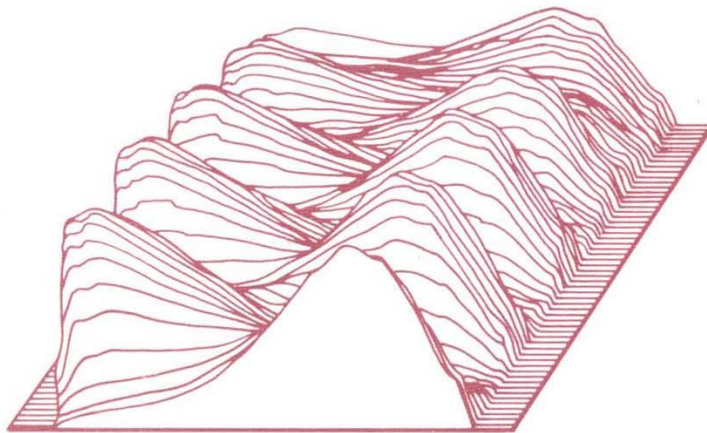


# NUCLEAR REACTOR

THEORY  
AND DESIGN

**Roger A. Rydin**



PBS SERIES IN REACTOR PHYSICS



# NUCLEAR REACTOR THEORY AND DESIGN

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# **NUCLEAR REACTOR THEORY AND DESIGN**

## **Third Edition**

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# PREFACE

There has not been a new or significantly revised textbook on Reactor Theory published for a number of years. In the meantime, computer codes have become more sophisticated and more universally available, and virtually every student has access to a computer. While a number of rather excellent older books exist, they usually contain at least one of two specific shortcomings. Either the books teach historic Reactor Theory, or they serve as compendia of knowledge for the advanced graduate student or researcher.

The purpose of the present work is very simply to teach the beginning graduate or undergraduate nuclear engineering student, who may have little or no previous knowledge of the field, the basic principles and ideas of present-day reactor physics design. The approach taken here is oriented towards the understanding and use of computer methods, but the material is carefully arranged so as to give a reasonable analytic foundation for the solutions.

The underlying physics and mathematics is continually emphasized.

Above all, the development of the ideas behind the methods is stressed. Where necessary, rigor has been sacrificed in order to present a detailed description of the essential underlying ideas. Advanced research areas are mentioned in many cases, but a conscious attempt has been made to keep the scope of the work confined to what material a first year graduate student should reasonably be expected to be exposed to in a single year. For many students, what is presented here is enough, because they will work in other areas of nuclear engineering. But for those who are interested in Reactor Theory as a career, this text should enable them to move to the advanced books and to tackle the literature.

The first three chapters are introductory in nature, and are

intended primarily as reference material for self-study. For a two-semester course, a reasonable division of the material would be coverage of chapters four through eight in the first semester and chapters nine through twelve in the second semester. A normal undergraduate program can reasonably be expected to have covered the equivalent of chapters one through eight, so that students with a bachelor's degree in nuclear engineering should be able to start the second semester directly.

As a departure from previous texts, a number of the problem sets given herein depend upon the use of commercial reactor design computer codes. These codes are available from the National Energy Software Center at Argonne National Laboratory or from the Oak Ridge Radiation Shielding Information Center. A number of these codes run on a PC. Problems are usually assigned to groups of two students, and each problem or problem set attempts to illustrate an idea, such as spatial reactor kinetics, which is difficult to demonstrate otherwise. On the other hand, there is great value in doing analytical derivations, which provide insight and understanding, and problems along these lines have not been neglected. The problems are considered to be an integral part of each chapter and not simply an appendage.

In the effort to produce this Third Edition of Reactor Theory and Design, I would like to gratefully acknowledge the help of Pamela Lockley and Vickie Thomas who did an excellent job of typing the manuscript in WORDPERFECT, from which the current form in Microsoft WORD, complete with figures, was extracted.

Roger A. Rydin  
Charlottesville, Virginia  
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## INTRODUCTION

### 1.1 Background

In 1932, Chadwick discovered that neutrons were emitted when alpha particles struck light materials such as beryllium. Soon afterwards, scientists bombarded many elements with neutrons in order to transmute these elements into new and heavier isotopes. In December of 1939, the German chemists, Otto Hahn and Fritz Strassmann discovered that some of the products from bombarding uranium with neutrons were lighter elements having about half the mass of uranium! Their colleagues, Lisa Meitner and Otto Frisch, soon worked out that the uranium was actually undergoing fission.

Fast neutrons were subsequently found to also be a byproduct of fission. Soon afterwards, the properties of natural uranium had been sufficiently well measured to be able to say something positive about the possibility of producing a sustained neutron chain reaction in a potentially controlled fashion. Natural uranium is composed of about 99.3% of the isotope  $^{238}_{92}\text{U}$ , and only 0.7% of the isotope  $^{235}_{92}\text{U}$ . The *abundant* isotope fissions, with a low probability, only for neutrons having energies above 1.3 MeV. This isotope is also a strong parasitic absorber of neutrons in the range of 6 to 1000 eV, where it has strong absorption resonances. On the other hand, the *rare* isotope fissions readily for neutrons having energies of less than an electron volt, which are called slow or thermal neutrons. Hence, the real question was whether or not the production of neutrons due to the fission of the  $^{235}_{92}\text{U}$  could overcome the capture of neutrons in the more abundant  $^{238}_{92}\text{U}$  isotope and other surrounding materials.

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Fission neutrons are born with energies in the range of 0.1 to about 10 MeV. Hence, in order to cause a significant amount of fission in  ${}^{235}_{92}\text{U}$ , these neutrons have to be slowed down by elastic collisions with other materials called moderators. Moderators are relatively light isotopes, because the most efficient energy transfer occurs when the masses of the colliding particles are equal or nearly so. However, a good moderator must also be a poor absorber, otherwise too many neutrons would be lost in the process of slowing down. Physical and chemical stability are also desirable properties of moderators.

The most commonly used moderator materials are water, heavy water, beryllium and graphite. Water is abundant, and also has useful properties as a coolant medium. Unfortunately, the absorption of neutrons by the hydrogen in water is sufficiently great that a chain reaction cannot be sustained using natural uranium. An enrichment of the isotope  ${}^{235}_{92}\text{U}$  to the range of 2 to 3% is needed to make the reaction feasible. Water moderated and cooled systems of this type are called Pressurized Water Reactors (PWRs) or Boiling Water Reactors (BWRs). Heavy water is a much better moderator than light water, because deuterium is a poor neutron absorber. Unfortunately, it is not easy to separate heavy water from light water, and high purity is needed to prevent too much absorption in the light water fraction. At present, most reactors use light water and slightly enriched uranium, rather than expensive heavy water and natural uranium. However, the Canadians manufacture a pressure tube reactor system using heavy water that is known by the acronym CANDU.

Beryllium has also been used in a variety of small reactors. Being a metal, it is readily machined into a variety of shapes. Unfortunately, beryllium is also toxic in a chemical sense, so that it must be handled with care. Furthermore, if any significant amount of power is produced in the reactor, a coolant such as water is also needed.



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Finally, graphite has been found to be a very fine moderator, at least after it has been chemically treated to remove natural impurities. Graphite is a strong readily machined solid, with a very high thermal heat capacity, that can operate at temperatures over 1000°C. Graphite moderated reactors usually use carbon dioxide or helium gas as a coolant, and such systems are called High-Temperature Gas-cooled Reactors (HTGRs).

### 1.2 Historical Approach

At the time when nuclear reactors were first being considered, there were no computers! Hence, it was necessary to develop analytical methods to solve the problem. A very wide range of energies had to be considered, with very strong neutron absorption and scattering resonance behavior occurring over parts of the spectrum. Strong local effects were expected for local heterogeneities, and global spatial effects were expected due to the relative arrangement of fuel and moderator materials. The approach that was taken was to *partition* the problem into a multiplicative set of terms, each representing a different *phenomenological* part of the problem. Thus was born the 4-factor formula for an infinitely large reactor, and the 6-factor or 7-factor formula for a finite-sized reactor.

The 4-factor formula is represented by the simple expression

$$k_{\infty} = \eta \phi f, \quad (1.1)$$

where the various terms are defined in words as follows:

- $k_{\infty}$     k-infinity is the multiplication factor of an infinite array of this material, where multiplication is defined as the number of slow neutrons produced per slow neutron absorbed;
- $\eta$        eta is the number of fast neutrons produced by fission

## NUCLEAR REACTOR THEORY AND DESIGN

per thermal neutron absorbed in the fuel material. It is composed of the fission-to-absorption fraction in the fuel times the number of neutrons produced per fission, which is called  $\nu$ ;

$\epsilon$  epsilon is the fast fission factor, representing the enhancement of thermal fissions by fast neutron fissions in the  ${}^{238}_{92}\text{U}$ ;

$p$  is the resonance escape or non-absorption probability, which represents the fraction of fast neutrons that escape capture during the moderation process to become thermal or slow neutrons; and

$f$  is the thermal utilization factor, or fraction of thermal neutrons captured in the fuel where they can cause fission, compared to capture in all materials present.

Each of these factors was calculated by an appropriate analytical approach. For a chain reaction to occur, the value of  $k_{\infty}$  has to be greater than unity. The factor  $\eta$  depends on the fuel, and is typically between 1.5 and 1.8. The factor  $\epsilon$  is usually only slightly greater than unity. Hence, the most important design factors are  $p$  and  $f$ . As the degree of fuel lumping in plates or pins increases,  $p$  rises because a greater fraction of neutrons slows down in the moderator that surrounds the lump. On the other hand, as the degree of fuel lumping increases, the center portion of the lump is shielded from thermal neutrons by absorption in the outer layers, and  $f$  decreases. Hence, there is an optimum lump size where  $k_{\infty}$  reaches a maximum.

The behavior of a finite-size reactor is obtained by adding in three new factors related to the physical size of the system and the mean distances a fast neutron and a thermal neutron can travel in the reactor material. This relationship is written as

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$$k_{eff} = \frac{k_{\infty}}{1 + (L^2 + \tau)B^2}, \quad (1.2)$$

where the new factors are defined in words as follows:

- $k_{eff}$   $k$ -effective is the multiplication factor of a finite reactor, given in terms of thermal neutrons produced per thermal neutron absorbed or lost across the boundaries of the reactor;
- $\tau$  tau is the age, which is actually related to the mean-square distance a fast neutron can move from its birthplace in the medium;
- $L^2$  is the diffusion length squared, which is related to the mean-square distance a thermal neutron can move in the medium, and
- $B^2$  is the buckling, related to the inverse square of the characteristic size of the reactor.

Although the 4-factor and 7-factor formulas were of great value in the early days of reactor theory, they are not relevant today. All of the pertinent quantities are *defined* or derived from those interactions that actually take place in the reactor, namely, neutrons reacting with the atoms of material comprising the reactor. Nonetheless, these factors do have value in summarizing what is happening in a phenomenological sense, and thus they aid in our understanding of reactor design trade-offs.

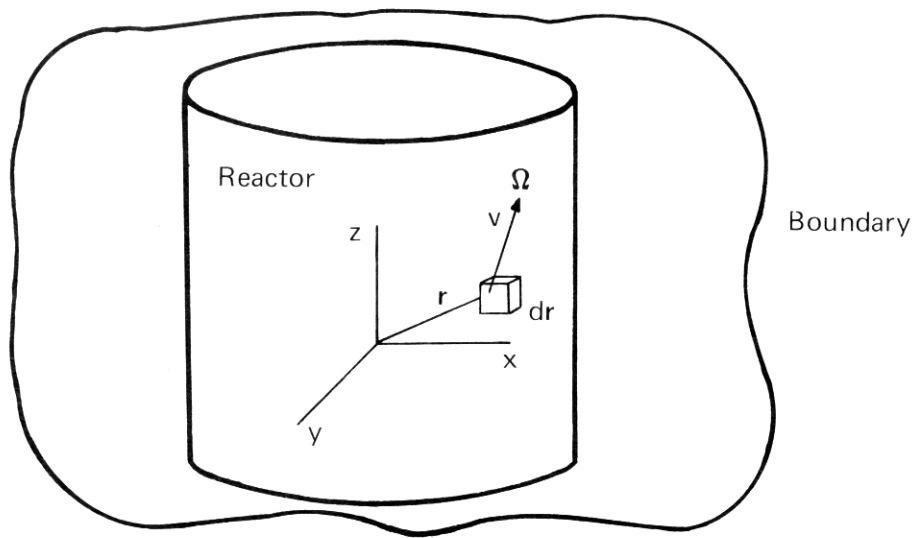
As a matter of fact, there are only two quantities that are of primary interest in reactor theory and design. These are:

1. the *neutron density* distribution function at any spatial position  $\vec{r}$ ; and,
2. the corresponding *reaction rates* for the various possible reactions occurring at this location.

Consider a schematic diagram of a reactor and its surroundings (Figure 1.1). The definition of the outer boundary is rather arbitrary. If one is interested mainly in the fuel-bearing

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region called the core, then the boundary is usually set near the edge of the core so that essentially all of the neutron reactions take place within the boundary. On the other hand, if one is interested in the problem of shielding personnel from the radiation emitted by the core, then the boundary must extend out to the point of interest, which may be several meters away from the core. The latter problem is sometimes decoupled from the former, by replacing the core region by an effective surface source.



**Fig. 1.1** Reactor and Surroundings

### 1.3 Neutron Density

When we consider the neutron density at position  $\vec{r}$ , we are interested not only in how many neutrons are located at  $\vec{r}$  per unit volume, but also in how fast they are traveling and in what directions they are traveling. In addition, we would like to know how this quantity varies with time. The neutron density distribution function is actually a 7-dimensional quantity that

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can be written as

$$n(x,y,z,v_x,v_y,v_z,t).$$

We have already denoted the position in space by the vector  $\vec{r}$ . The velocity components can then be given in terms of the scalar speed  $v$  and a unit direction vector  $\vec{\Omega}$  such that the velocity vector is  $\vec{v} = v\vec{\Omega}$ . In this case, the neutron density is often written as

$$n(\vec{r},\vec{\Omega},v,t).$$

Furthermore, since the energy of a neutron is related to its speed by  $E = \frac{mv^2}{2}$ , we can also write the neutron density as

$$n(\vec{r},\vec{\Omega},E,t).$$

Finally, in real reactors, the energy range of interest varies from 10 MeV down to a fraction of an eV, or over 9 to 10 decades, while the magnitude of the neutron density per unit energy also spans a number of decades. It then becomes convenient to introduce a dimensionless logarithmic variable called lethargy, defined as

$$u \equiv \ln \frac{E_0}{E}, \quad (1.3)$$

where  $E_0$  is typically taken to be 10 MeV and corresponds to  $u = 0$ . For a real reactor, the lethargy varies over a linear range of 0 to 20. Hence, the neutron density distribution function can also be written as

$$n(\vec{r},\vec{\Omega},u,t).$$

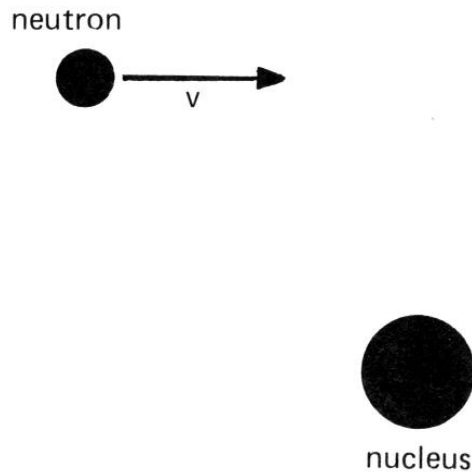
### 1.4 Reaction Rates

Reaction rates are governed by: the number of neutrons

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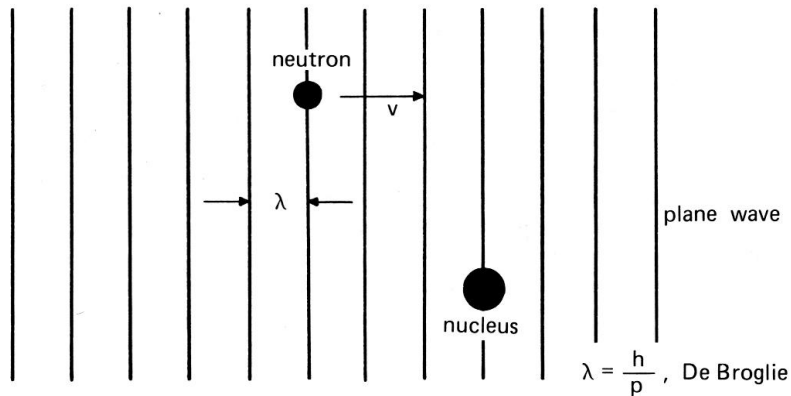
present, the speed at which they approach the target nuclei, the number of target nuclei present, and the probability that the nucleus will interact with the neutron. If we consider that the size of the nucleus is of the order of  $10^{-13}$  cm while the size of an atom is of the order of  $10^{-8}$  cm, we realize that matter is mostly empty space. The chance of a neutron actually hitting a nucleus in a pure billiard ball type of collision is extremely small, as indicated schematically in Figure 1.2. Recall that a neutron carries no charge and therefore does not interact with the electric fields of the nucleus or its surrounding electrons.

Using quantum mechanics, however, we can ascribe wave properties to the neutron. In this case, it can be seen that the neutron does not have to actually hit the nucleus in order to interact with it. For a collision, it is only necessary to have a portion of the neutron wave strike the nucleus, as shown in Figure 1.3.



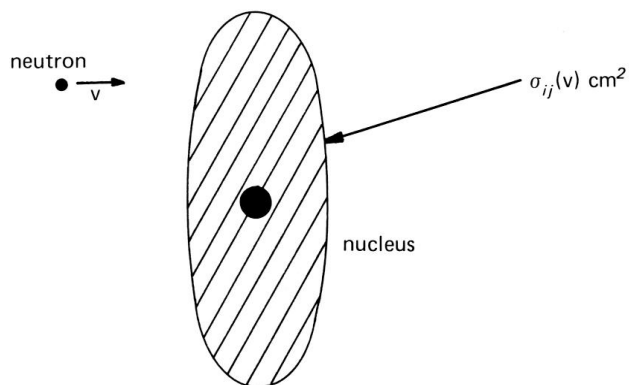
**Fig. 1.2** Neutron-nucleus Interaction on a Particle Basis

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**Fig. 1.3** Neutron-nucleus Interaction on a Wave Basis

We can graphically represent the probability of having a given interaction take place by drawing a shaded region about the nucleus whose cross-sectional area is proportional to the reaction probability, as shown in Figure 1.4. We call this the neutron "cross section", and denote it here by the symbol  $\sigma_{ij}(v)$  for reactions of the  $j$ th type with a nucleus of type  $i$ . This probability is a function of the relative velocity between the neutron and the nucleus.



**Fig. 1.4** Diagrammatic Representation of the Neutron Cross Section

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The number of interactions that take place per unit time in a given volume is proportional to the densities of both neutrons and nuclei, the reaction cross section, and the relative speed of approach. Therefore, the reaction rate is

$$R_{ij}(\vec{r}, \vec{\Omega}, E, t) = v n(\vec{r}, \vec{\Omega}, E, t) \sigma_{ij}(E) N_i(\vec{r}) \frac{\text{interactions}}{\text{cm}^3 \cdot \text{s} \cdot \text{ev} \cdot \text{sr}}, \quad (1.4)$$

where  $N_i(\vec{r})$  is the atom density of the  $i$ th atom type. The atom density can be calculated from the equation

$$N = \frac{\rho N_a}{M} \frac{\text{molecules}}{\text{cm}^3}, \quad (1.5)$$

where  $\rho$  is the density and  $M$  is the molecular weight of the compound. The remaining term,  $N_a = 6.025 \times 10^{23}$  molecules/mole, is Avagadro's number. For example, water has a density of  $\rho = 1 \text{ g/cm}^3$  and a molecular weight of  $M = 18$ . Hence,  $N = 0.0333 \times 10^{24}$  molecules/cm<sup>3</sup>. The individual atom densities are then obtained from the molecular formula. In this case, there are two hydrogen atoms and one oxygen atom per molecule. Hence  $N_H = 0.0666 \times 10^{24}$  atoms/cm<sup>3</sup> and  $N_O = 0.0333 \times 10^{24}$  atoms/cm<sup>3</sup>. If the water contained a small fraction of heavy water, then the appropriate hydrogen and deuterium atom densities could be obtained using the isotopic fractions.

The second two factors on the right-hand side of Eq. (1.4) give what is known as the macroscopic cross section, denoted by the symbol  $\Sigma$ , i.e.,

$$\sigma_{ij}(v) N_i(\vec{r}) \equiv \Sigma_{ij}(\vec{r}, v) \text{ cm}^{-1}. \quad (1.6)$$

Microscopic cross sections are usually quite small, so that a special unit called the "barn" has been coined, where  $1 \text{ barn} = 10^{-24} \text{ cm}^2$ . Most cross sections are of the order of magnitude of a barn, although there are notable exceptions. Since  $N$  contains a factor of  $10^{+24}$ , a usual practice in computer



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codes is to enter cross sections in barns and atom densities in atoms/barn-cm, so that these scale factors cancel.

The first two factors on the right-hand side of Eq. (1.4) are often grouped together into a quantity called the angular neutron flux, i.e.,

$$vn(\vec{r}, \vec{\Omega}, v, t) \equiv \Phi(\vec{r}, \vec{\Omega}, v, t) \frac{\text{neutrons}}{\text{cm}^2 \cdot \text{s} \cdot \text{ev} \cdot \text{sr}}. \quad (1.7)$$

Thus, the reaction rate is given as the product of the flux and the macroscopic cross section,

$$R_{ij}(\vec{r}, \vec{\Omega}, E, t) = \Sigma_{ij}(\vec{r}, E) \Phi(\vec{r}, \vec{\Omega}, E, t) \frac{\text{interactions}}{\text{cm}^3 \cdot \text{s} \cdot \text{ev} \cdot \text{sr}}. \quad (1.8)$$

Actually, the full definition of the angular flux contains more detail than we normally need. By integrating over the angular dependence, we obtain the energy-dependent flux,

$$\phi(\vec{r}, E, t) = \int \Phi(\vec{r}, \vec{\Omega}, E, t) d\Omega \frac{\text{neutrons}}{\text{cm}^2 \cdot \text{s} \cdot \text{eV}}. \quad (1.9)$$

By next integrating over energy, we obtain the total, or one-speed flux

$$\phi(\vec{r}, t) = \int \phi(\vec{r}, E, t) dE \frac{\text{neutrons}}{\text{cm}^2 \cdot \text{s}}. \quad (1.10)$$

Simple approximate relationships can be written for the energy-dependent flux over various ranges of the energy spectrum. The fission flux can be represented approximately over the range from 0.1 to 10 MeV as

$$\phi(E) = C_1 E e^{-E}, \quad (1.11)$$

where  $C_1$  is a normalization constant and  $E$  is given in dimensionless units corresponding to MeV. The slowing down region from 1 eV to 0.1 MeV can be represented approximately as a

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one-over-E flux,

$$\phi(E) = \frac{C_2}{E}, \quad (1.12)$$

where  $C_2$  is a constant. Finally, the thermal region, from 0 to 1 eV, can be represented by a Maxwellian distribution at the temperature of the moderator, namely

$$\phi(E) = C_3 E e^{-E/kT}, \quad (1.13)$$

where  $C_3$  is a constant,  $E$  is in units of eV,  $T$  is the temperature in degrees Kelvin, and  $k = 8.6173 \times 10^{-5}$  eV/°K is Boltzmann's constant.

It is typical to define some "room temperature" constants. At  $T_0 = 293^\circ\text{K}$ , the energy of the most probable neutron is  $E_0 = kT_0 = 0.025$  eV, which corresponds to a velocity of  $v_0 = 2200$  m/s. The absorption cross sections for most materials in the thermal energy range vary as one-over- $v$ , and can be represented by the equation

$$\sigma_a = \sigma_{a0} \frac{v_0}{v}, \quad (1.14)$$

where  $\sigma_{a0}$  is the 2200 m/s cross section.

The average absorption cross section over a Maxwellian distribution at a temperature  $T$  can then be obtained from the relationship

$$\sigma_a = \sqrt{\frac{\pi}{4}} \sigma_{a0} \sqrt{\frac{T_0}{T}}. \quad (1.15)$$

Hence, we look up the 2200 m/s cross section, multiply it by 0.886, and correct it for temperature to obtain the average value that is used with the one-speed flux to obtain the reaction rate in a Maxwellian spectrum. Scattering cross sections, on the other hand, tend to be relatively constant over the thermal

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range, so they are treated differently.

### 1.5 Design Approximations

For full information on the neutron density and the reaction rates, we need seven variables. This is generally beyond our computational abilities, even with the largest modern computers. Therefore, we usually make approximations in a sequential and iterative fashion to eventually obtain a valid synthesis of the actual problem solution. For example, detailed energy-dependent calculations are usually done as space- and time-independent computations for several different spatial regions of interest in a reactor. Average values over a gross energy representation (discretization into few-groups) are then used in detailed 1-, 2-, or 3-dimensional, time-independent, spatial flux calculations. The angular dependence is often averaged out leading to *Diffusion theory* as opposed to the full representation that is called *Transport theory*; this is a savings of two dimensions. Time-dependent problems using few-group diffusion theory rarely contain more than two spatial dimensions; and so on.

A desirable check of any approximation to the theory is an experiment that can be used to validate the calculations! Of course the experiments may be in error, so sometimes theory and experiment are used iteratively to validate each other. The nuclear industry has successfully validated its design methods to agree with experiment.

As a final comment, one saving grace in the study of reactor theory is the fact that the neutron density is rarely greater than  $10^{10}$  per  $\text{cm}^3$  while typical atom densities are of the order of  $10^{23}$ . Therefore, neutron-neutron collisions are extremely rare and the mathematical problem formulation is *linear*, which is an important simplification.

## NUCLEAR REACTOR THEORY AND DESIGN

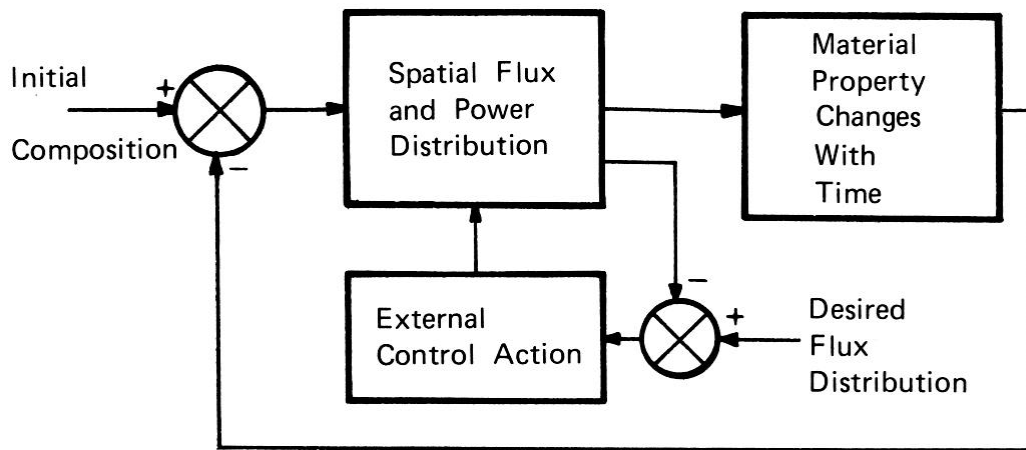
### 1.6 Reactor Design Implications

We have discussed the fact that the two most important quantities in reactor physics calculations are the *neutron density*,  $n(\vec{r}, \vec{\Omega}, E, t)$ , and the *reaction rate* with the  $i$ th type of nuclide, which can symbolically be written as  $R_i(\vec{r}, \vec{\Omega}, E, t)$ . We know the initial spatial distribution of all of the isotopes in the reactor. We must *calculate* the neutron density in the reactor at a given total operating power level that corresponds to the initial material distribution and any external sources that may be present.

Once we know the neutron density, the reaction rates are fully determined; these tell us, by virtue of simple rate equations, how the quantities of various isotopes that are present vary with time. Some isotopes burn up, such as  $^{235}\text{U}$  and  $^{10}\text{B}$ . Others are produced, such as the fission product  $^{135}\text{Xe}$  which has a very large ( $3 \times 10^{-18} \text{ cm}^2$ ) absorption cross section.

In turn, changes in the material properties affect the operating state of the reactor. In a sense we have a nontrivial feedback control problem (see Figure 1.5) where the object is to maintain the total power production at a desired value for a period of several months to years. We must compensate for all of the property changes that occur during the time period while preserving safety margins and material integrity constraints. In addition, as nuclear engineers, we want to make the entire process as economical as possible. This is, in essence, the process of reactor design.

## NUCLEAR REACTOR THEORY AND DESIGN



**Fig. 1.5** Schematic Reactor Operation Diagram

### Problems

- 1.1** This question concerns the relationship between energy, lethargy, velocity, and wavelength.
- If  $E_0$  is taken to be 10 MeV, find the values of energy  $E$  that correspond to each integer value of lethargy  $u$  from 0 to 20.
  - What are the corresponding neutron velocities,  $v$ , if the velocity of a "thermal" neutron at  $E_0 = 0.025$  eV is  $v_0 = 2200$  m/s?
  - What are the corresponding neutron wavelengths  $\lambda$ ? How do these compare to the size of a typical atom? Use  $\lambda = 2.86 \times 10^{-9} / \sqrt{E}$ , where  $E$  is in eV and  $\lambda$  is in cm.

## NUCLEAR REACTOR THEORY AND DESIGN

**1.2** The ceramic material  $\text{UO}_2$  has a sintered density of  $10.7 \text{ g/cm}^3$ .

- a) If the uranium is 3% enriched in  $^{235}\text{U}$ , find the number densities of all of the constituent atoms in the uranium dioxide fuel.
- b) If the average total microscopic cross sections of the constituent atoms are  $\sigma_{25} = 680$  barns,  $\sigma_{28} = 2.7$  barns, and  $\sigma_o = 0.18$  barns, find the macroscopic total cross section  $\Sigma_T$  for  $\text{UO}_2$ .

**1.3** A reactor shield is made up of a *mixture* of granulated lead in polyethylene. The resulting sheets contain 50%  $^{208}_{82}\text{Pb}$  by weight and the rest is polyethylene whose chemical formula can be assumed to be  $\text{CH}_2$ . If the measured density of the sheet is  $3.0 \text{ g/cm}^3$ , compute the atom densities of Pb, C and H.

**1.4** The material  $\text{B}_4\text{C}$  is often used in control rods.  $\text{B}_4\text{C}$  has a density of  $2.52 \text{ g/cm}^3$  and a molecular weight of 55.26. Natural boron contains 20% of the  $^{10}\text{B}$  isotope and 80% of the  $^{11}\text{B}$  isotope by weight. The 2200 m/s absorption cross sections for  $^{10}\text{B}$ ,  $^{11}\text{B}$ , and  $^{12}\text{C}$  are 3840, 0.0055 and 0.0034 barns, respectively.

- a) Find the total macroscopic thermal absorption cross section,  $\Sigma_a$ , for  $\text{B}_4\text{C}$  in a Maxwellian spectrum at a temperature of  $500^\circ\text{K}$ .
- b) The thermal neutron scattering cross sections are 2.2, 3.9 and 4.75 barns, respectively. Find the total macroscopic scattering cross section,  $\Sigma_s$ .

## NUCLEAR REACTOR THEORY AND DESIGN

**1.5** A region in a reactor contains the following atom densities,

$$H \text{ -- } 0.010 \times 10^{24} \text{ atoms/cm}^3$$

$$B \text{ -- } 0.001 \times 10^{24} \text{ atoms/cm}^3$$

$$C \text{ -- } 0.002 \times 10^{24} \text{ atoms/cm}^3.$$

Assuming that the material is in a Maxwellian thermal neutron distribution at  $T = 320^\circ\text{K}$  ( $47^\circ\text{C}$ ), compute the diffusion coefficient  $D$  for this material. As an approximation, take

$$D = \frac{l}{3(\Sigma_a + \Sigma_s)}.$$

**1.6** The total neutron flux, averaged over direction and energy, is typically  $10^{13} \text{ n/cm}^2\text{-s}$  at the center of a power reactor. Assume  $T = 600^\circ\text{K}$ .

- a) What is the neutron density at this position?
- b) If the macroscopic absorption cross section of the  $^{235}\text{U}$  at this location is  $\Sigma_{25} = 0.068 \text{ cm}^{-1}$ , and absorption in  $^{238}\text{U}$  can be ignored, find the local volumetric reaction rate in the uranium.
- c) If the reactor were operated at this flux level for an entire year, what fraction of the atoms in this location would be used up if the original atom density of the fuel was  $N_{25} = 10^{20} \text{ atoms/cm}^3$  and the cross sections were constant? Note that you must solve an ODE.
- d) Find what would happen if the power level were constant for the year instead of the flux being constant? Note that you must solve another ODE.

**1.7** In the slowing down region, the energy-dependent flux can be assumed to have the value  $\phi(E) = 10^{13}/E \text{ neutrons/cm}^2\text{-s-eV}$ . Find the total flux between 1 eV and 100 eV, and also the total flux between 1 keV and 100 keV. Compare the results.

## NUCLEAR REACTOR THEORY AND DESIGN

- 1.8** Prove that the maximum flux in a Maxwellian distribution occurs at

$$\hat{E} = kT.$$

- 1.9** Find the total flux in a Maxwellian distribution. Show that this corresponds to the average velocity times the neutron density.

- 1.10** Prove that, for a  $1/v$  absorber, the average cross section in a Maxwellian distribution is lower than the value at  $\hat{E} = kT$  by the factor  $\sqrt{\pi/4} = 0.887$ .

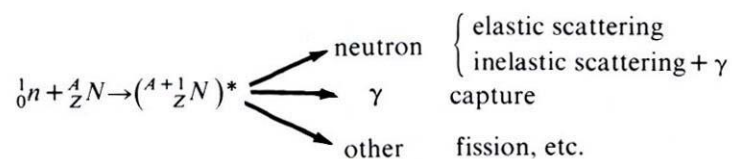


## INTERACTIONS OF NEUTRONS WITH MATTER

To begin with, we must point out that the *probability* of having a neutron reaction occur with a given nucleus is proportional to the associated reaction cross section, which is determined *only* by the nuclear properties of the nucleus with respect to the incident neutron. On the other hand, the *kinematics* of the reaction are completely decided by the conservation laws (i.e., conservation of energy, linear and angular momentum, charge, and nucleons). The actual collision can be considered to happen in a "black box", where we see only the "before" and "after" states. In fact, the Heisenberg Uncertainty Principle states that we *cannot* observe the exact details of the interaction because the region is too small and the particles move too fast to be observed fully.

### 2.1 Compound Nucleus-Cross Sections

We now turn to the physics of the interaction of the neutron with the target nucleus. One considers that the majority of events occur through the intermediary of formation of a compound nucleus that is in an excited state as a result of the addition of the binding energy of the extra neutron. This compound nucleus then decays by one of a number of processes as shown symbolically below:

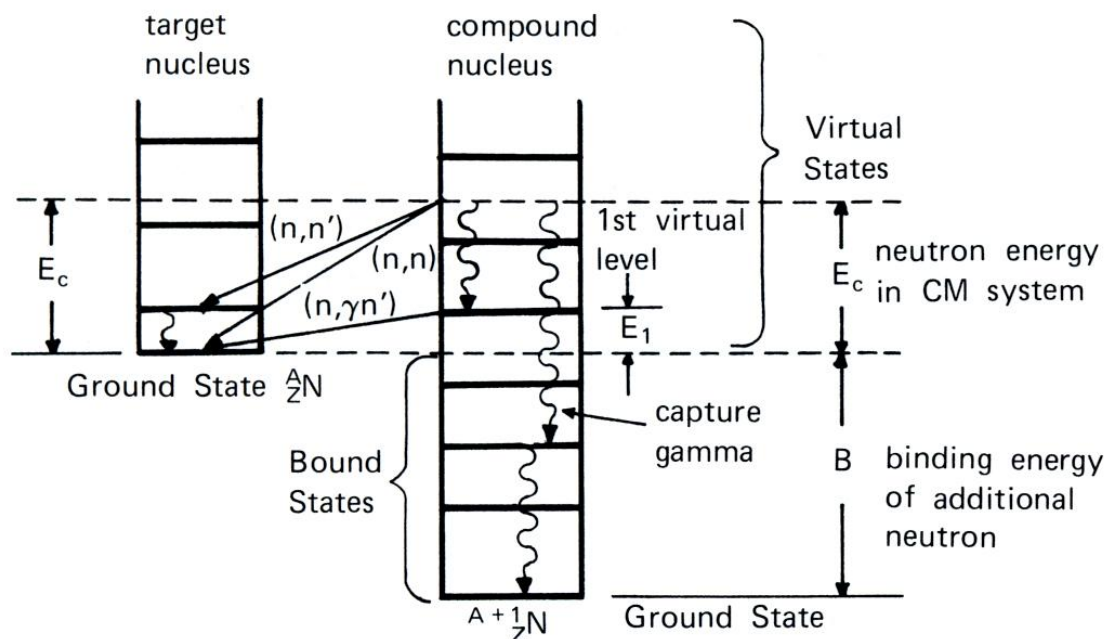


## NUCLEAR REACTOR THEORY AND DESIGN

Specifically, in order to examine the processes involved we must consider the energy level structure of the nucleus formed by the coalition of the neutron and the target nucleus. The kinetic energy of the neutron is transformed into internal energy of the compound nucleus and adds to the neutron binding energy to equal the total excitation energy. The level schemes of the target and compound nuclei are shown in Figure 2.1, where several things can happen to the excited compound nucleus:

1. A capture gamma ray (or cascade) can be emitted dropping the excitation level of the nucleus. If enough energy is lost to go below the virtual levels to the bound states, the neutron is captured and the ground state is reached by gamma emission.
2. The neutron (probably a different one) is re-emitted, with the same total kinetic energy shared between the particles, leaving the target nucleus in the ground state. A *transfer* of energy from one particle to the other usually takes place. This process is called elastic scattering.
3. The neutron can be re-emitted with somewhat less than the total kinetic energy shared between the particles, leaving the target nucleus in an excited state that decays by gamma emission. This is called  $n, n'$  inelastic scattering. The total inelastic cross section is the sum of the cross sections for exciting each level, as shown in Figure 2.2 for  $^{238}\text{U}(n, n')$ . The scattered neutron appears at an energy of  $E'_c = E_c - E_i$ , where  $E_i$  corresponds to the  $i$ th bound level of the target nucleus. Therefore, if one picks a single excitation energy, the resulting scattered neutrons will fall into rather well defined discrete ranges corresponding to each of the levels excited. Use of this fact allows one to prepare scattering transfer cross sections for inelastic scattering.

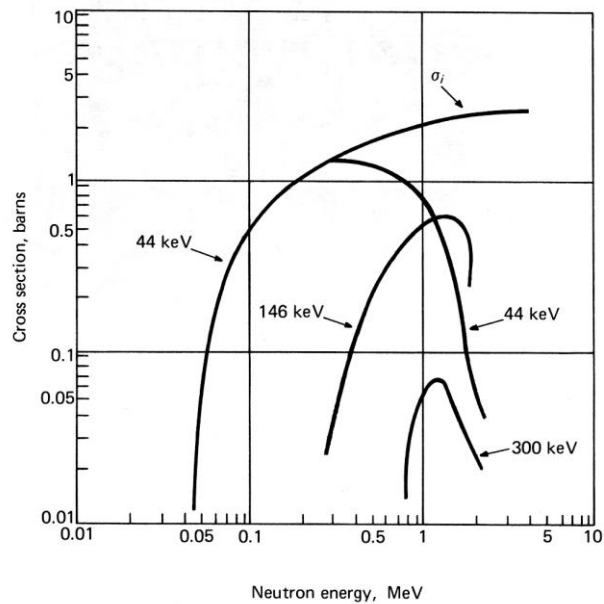
## NUCLEAR REACTOR THEORY AND DESIGN



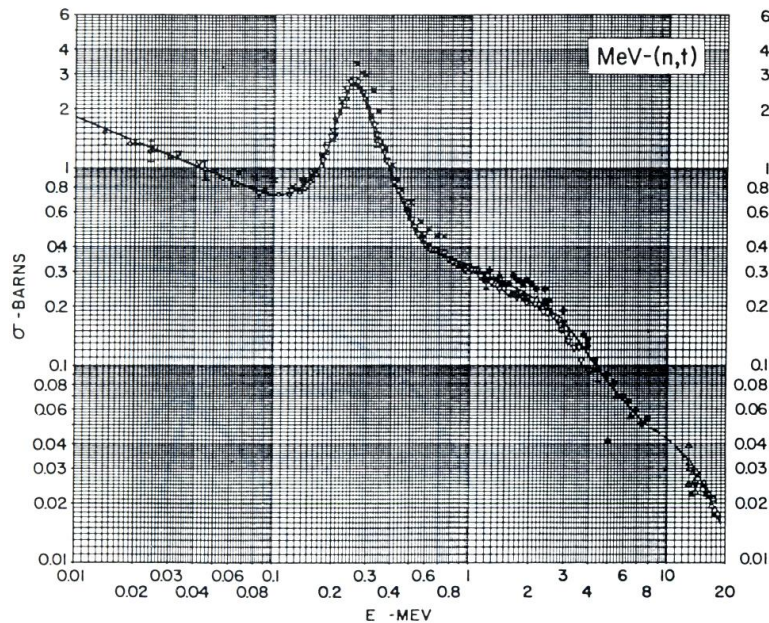
**Fig. 2.1** Energy Level Diagram for Compound Nucleus Formation

4. A gamma ray can be emitted by the compound nucleus followed by re-emission of a neutron. This is called  $n, \gamma n'$  inelastic scattering, and while it is much less important than  $n, n'$  scattering, its occurrence is not negligible. It is found that more energy is lost by the  $n, \gamma n'$  reaction than by the  $n, n'$  reaction and although the former is only a few percent of the total inelastic scattering, it cannot always be neglected.
5. A different particle, such as an  $\alpha$  particle, can be emitted, or fission can take place.

## NUCLEAR REACTOR THEORY AND DESIGN



**Fig. 2.2** Inelastic Scattering Cross Sections for  $^{238}\text{U}$   
 (From S. Yiftah, D. Okrent, P. A. Moldauer, *Fast Reactor Cross Sections*, 1960, Pergamon Press, Ltd.)



**Fig. 2.3** Lithium-6 Total Cross Section vs. Energy  
 (From BNL-325, Supl. 2, 1965)

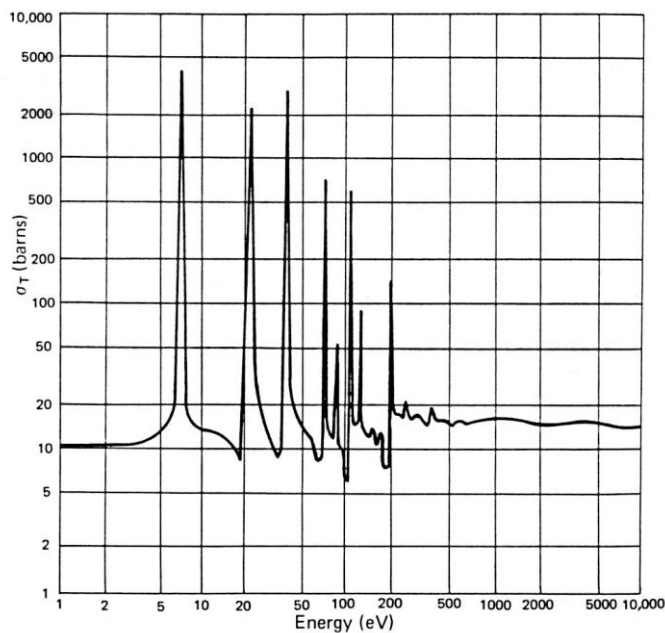
## NUCLEAR REACTOR THEORY AND DESIGN

We can compare the level structures of various nuclei to help us understand some of the features of the observed cross-section curves. Some general comments are in order:

- a. Light elements---the levels are widely separated in light elements. For example, the first excited level in  $^{12}\text{C}$  occurs at approximately 4.3 MeV. As a consequence, inelastic scattering is not observed at all except for high-energy neutrons, and we tend to have elastic slowing down in light moderators. Light elements also tend to have broad resonances at high energies, as illustrated in Figure 2.3.
- b. Heavy elements---the levels are narrowly spaced in heavy elements, often being only a few electron volts apart. Inelastic scattering is an important scattering mechanism. In fact, neutrons lose very little energy in elastic scattering by heavy elements, but can lose a considerable amount of energy by inelastic scattering. Resonances tend to be narrow and tightly spaced, as illustrated in Figure 2.4.
- c. Magic numbers---magic numbers correspond to closed shells of protons and neutrons, respectively, and are analogous to the closed electron shells in atomic physics that give rise to the noble gases. Nuclei having closed shells are especially tightly bound, and therefore a large amount of binding energy is available upon formation. Energy levels are widely spaced in such nuclei. The magic numbers are: 2, 8, 20, 28, 50, 82, and 126. Specific examples of such nuclei are:

## NUCLEAR REACTOR THEORY AND DESIGN

${}^4_2\text{He}$ —alpha particle	(2,2)
${}^{16}_8\text{O}$	(8,8)
${}^{208}_{82}\text{Pb}$	(82,126)

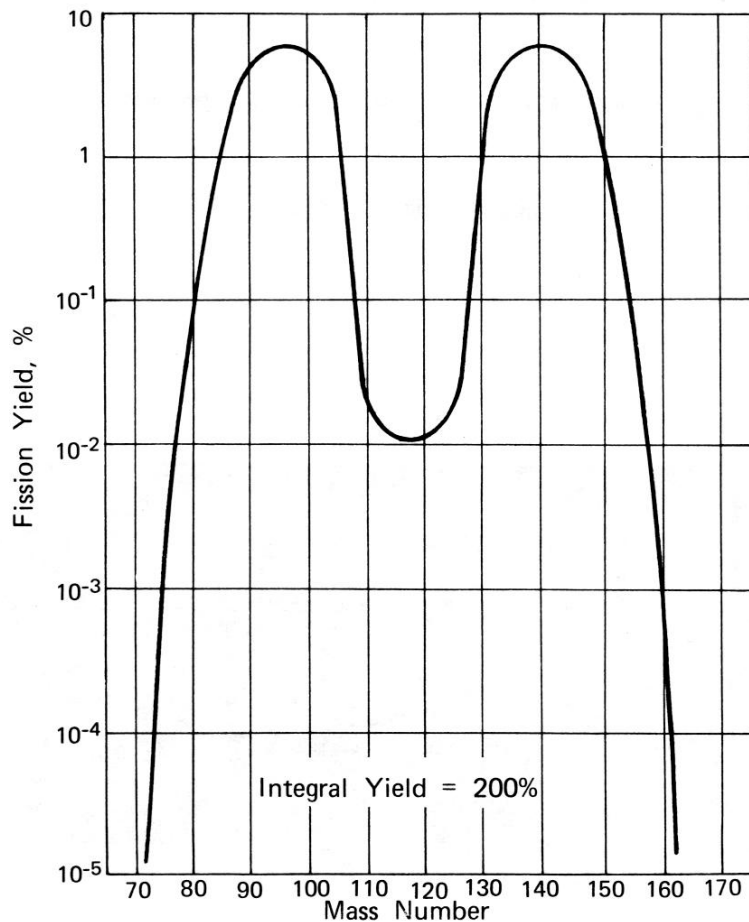


**Fig 2.4** Uranium-238 Total Cross Section vs. Energy  
(From BNL-325, Supl. 2, 1965)

The existence of these magic nuclei is very important in nuclear physics and accounts for such phenomena as:

1. alpha particle decay---deuteron, proton, etc., decay are not observed, but  $\alpha$  particles are so tightly bound that they can be emitted as an entity.
2. fission yield curves—the fission yield curves have a double hump shape as sketched in Figure 2.5 because the two fission fragments tend to form as combinations of magic numbers.

## NUCLEAR REACTOR THEORY AND DESIGN



**Fig. 2.5** Schematic Fission Yield Curve

3. delayed neutron emitters---some of the elements in the various fission product chains emit neutrons as they decay towards stability. The neutrons are invariably emitted as the precursor goes toward a magic number closed shell, using the additional binding energy to make neutron emission energetically possible. The delayed neutrons are part of the chain reaction balance in a nuclear reactor and modify the time scale for transient response from the microsecond range to the second range, thus making reactor control feasible.

## NUCLEAR REACTOR THEORY AND DESIGN

4. shielding materials---lead-208, being doubly magic, is the heaviest element which is stable to  $\alpha$  decay and is therefore not radioactive. High Z materials make good  $\gamma$ -ray shields.  $^{208}\text{Pb}$  also has a very small neutron absorption cross section.

### 2.2 Nuclear Systematics of Naturally Occurring Isotopes

If one examines the Periodic Chart of the Nuclides, several observations based on the relative occurrence of various nuclides in nature can be made. Because Coulomb repulsion varies as  $Z^2$ , heavy nuclides need more neutrons than light nuclides to "glue" them together. Therefore, the gross behavior of the Z versus N curve is as shown in Figure 2.6. Superimposed on the gross curve is a certain amount of fine structure. There are rather significant jumps that occur at the magic numbers because of the associated strong nuclear binding. In addition, there is a smaller systematic behavior that can be related to spin pairing of neutrons and protons, respectively, since each nucleon can have a quantum spin that is either up or down. The pairing gives additional binding, and is of three types:

proton-proton  
neutron-neutron  
neutron-proton (occurs only at the same energy level)

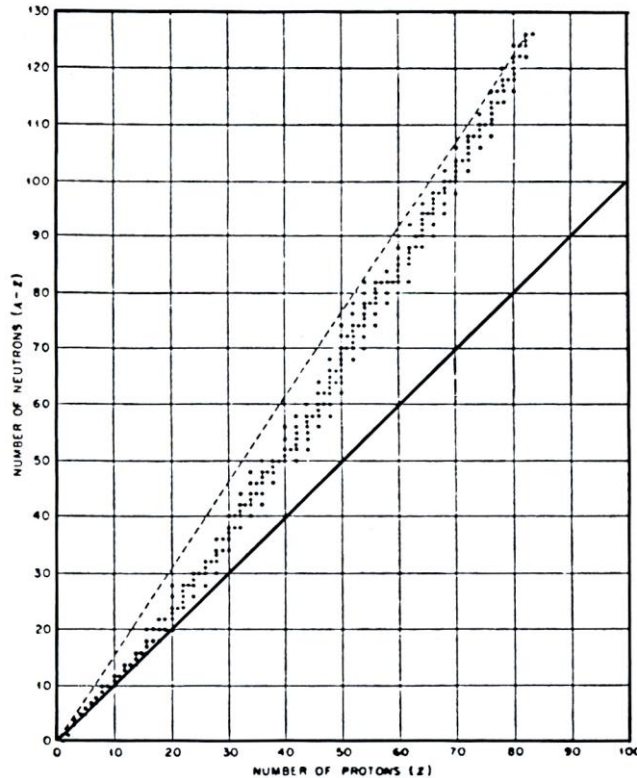
**Even-Even.** One finds that most naturally occurring nuclides are even-even. An example is  $^{238}_{92}\text{U}$ , which fissions only with neutrons of  $E > 1$  MeV because the addition of a neutron is a transition to the less stable even-odd state.

**Even-Odd or Odd-Even.** Almost all the rest of the naturally occurring nuclides fall into this category, which is far less



## NUCLEAR REACTOR THEORY AND DESIGN

numerous than above. An example is  ${}^{235}_{92}\text{U}$ , which fissions with thermal neutrons because neutron capture is a transition to the more stable even-even state, and the extra binding energy becomes available as excitation energy.

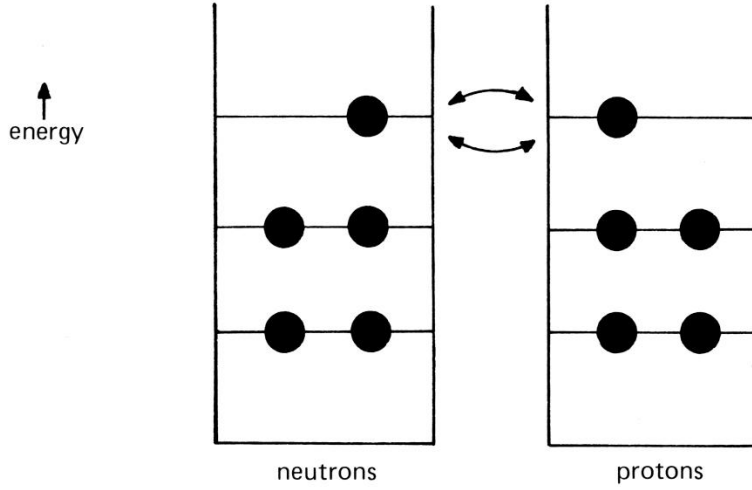


**Fig. 2.6** Diagram of Neutron Number vs. Proton Number for Naturally Occurring Isotopes

(From *The Elements of Nuclear Reactor Theory* by Glasstone and Edlund, 1952, Van Nostrand Reinhold Company)

**Odd-Odd.** There are only four odd-odd nuclides observed in nature. They exist because of neutron-proton spin pairing at the same energy level, as shown in Figure 2.7 for  ${}^{10}_5\text{B}$ . Since there are usually more neutrons than protons in nuclei, this case exists only for the light elements. The observed odd-odd nuclides are,  ${}^2_1\text{H}$ ,  ${}^6_3\text{Li}$ ,  ${}^{10}_5\text{B}$ , and  ${}^{14}_7\text{N}$ . The list stops here because  ${}^{16}_8\text{O}$  is doubly magic and upsets the progression.

## NUCLEAR REACTOR THEORY AND DESIGN



**Fig. 2.7** Neutron-Proton Spin-Pairing Diagram for  $^{10}_5\text{B}$

### 2.3 Level Widths and Partial Cross Sections

Up to this point, we have only considered the location of a given nuclear energy level. In fact, the level is a small band whose width can be related to the lifetime of the level. The mean lifetime of a level is the length of time that a nucleus in that state will exist before decaying to a more stable state. For example, the mean lifetime of the 6.67 eV level in  $^{238}\text{U}$  (which corresponds to the compound nucleus  $^{239}\text{U}^*$ ) is of the order of  $10^{-14}$  sec. Most of the time the neutron is captured and a gamma ray is given off. The decay constant for the level is the inverse of the mean lifetime,

$$\lambda = \frac{1}{\tau} \text{ s}^{-1}. \quad (2.1)$$

In turn, the total level width  $\Gamma$  is related to  $\lambda$  by Planck's constant

$$\Gamma = \hbar \lambda \text{ eV}, \quad (2.2)$$

## NUCLEAR REACTOR THEORY AND DESIGN

where  $\hbar = h/2\pi$ . We usually measure  $\Gamma$  and calculate  $\tau$ .

Since the total level width is proportional to the total probability of decay of the compound nucleus, it is also equal to the sum of the probabilities of decay into all channels, which is given as

$$\begin{array}{cccc} \text{total} & \text{neutron} & \text{radiation} & \text{fission} \\ & \text{width} & \text{width} & \text{width} \\ & (\text{scattering}) & (\text{capture}) & \end{array} \quad (2.3)$$

$$\Gamma = \Gamma_n + \Gamma_\gamma + \Gamma_f + \dots \text{etc.}$$

As far as the compound nucleus is concerned, the total level width corresponds to the cross section for formation of the compound nucleus, and the partial level widths correspond to the scattering, capture, fission, etc., cross sections. In the general case,

$$\begin{array}{ccccccc} & \text{total} & & \text{scattering} & & \text{capture} & \text{fission} \\ \sigma_T & = & \sigma_s & + & \sigma_c & + & \sigma_f + \dots \end{array} \quad (2.4)$$

The cross sections given above are furthermore often given in the form

$$\sigma_T = \sigma_s + \sigma_a, \quad (2.5)$$

where the scattering is further subdivided into elastic and inelastic contributions,

$$\sigma_s = \sigma_{elas} + \sigma_{inelas}, \quad (2.6)$$

and the absorption is subdivided into capture, fission, etc.

$$\sigma_a = \sigma_c + \sigma_f + \dots \quad (2.7)$$

One often sees in the literature the term non-elastic cross section, which is related to the above by the expression

$$\sigma_{ne} = \sigma_T - \sigma_{elas}. \quad (2.8)$$

## NUCLEAR REACTOR THEORY AND DESIGN

The relationship between the total cross section and the cross section for formation of the compound nucleus is obtained by adding what is known as potential scattering (billiard ball effect) and interference scattering that is a cross term between potential scattering and compound nucleus scattering. Hence,

$$\sigma_T = \sigma_{CN} + \sigma_p + \sigma_{interference} . \quad (2.9)$$

### 2.4 Cross Section for Formation of the Compound Nucleus

We have examined the process of neutron scattering with regard to energy diagrams of the unexcited and compound nuclei, noting the presence and role of various allowed energy levels. Experimentally, at energies in the eV to KeV range, heavy nuclides exhibit rapidly varying cross sections whose peak magnitudes are often thousands of times greater than the values found in between peaks. The cross-section curve resonances correspond directly to the *virtual levels* in the compound nucleus, as shown in Figure 2.8. For a single isolated resonance at energy  $E_r$ , the wave-mechanical solution can be put into a form called the Breit-Wigner single level formula:

$$\sigma_{CN}(E_c) = \frac{A}{(E_c - E_r)^2 + \Gamma^2/4}, \quad (2.10)$$

where A is essentially constant.

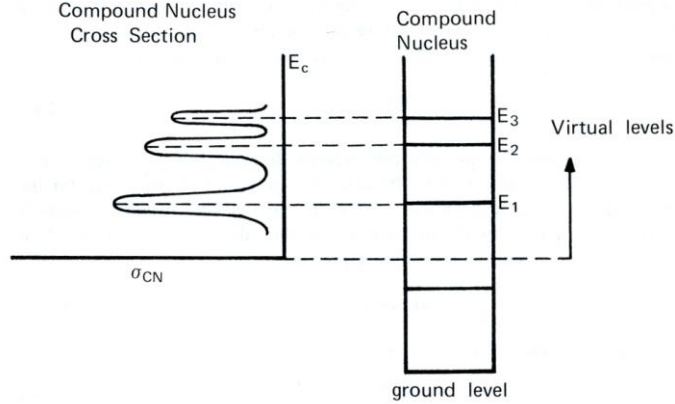
This is the cross section for formation of the compound nucleus. The probability of obtaining any given mode of de-excitation is proportional to the ratio of the partial level width to the total level width. Thus, for scattering from the compound nucleus,

$$\sigma_{sCN}(E_c) = \sigma_{CN}(E_c) \frac{\Gamma_n}{\Gamma}, \quad (2.11)$$

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while for radiative capture,

$$\sigma_c(E_c) = \sigma_{CN}(E_c) \frac{\Gamma_\lambda}{\Gamma}, \text{ etc.} \quad (2.12)$$



**Fig. 2.8** Cross Section vs. Energy Relative to the Levels of the Compound Nucleus

### 2.5 Reaction Probabilities

We have examined the nature of the microscopic cross sections of various materials as a function of energy. We now turn to the probability that an interaction will occur as a neutron passes through matter. Specifically, we observe that the macroscopic total cross section at any energy, denoted as  $\Sigma_T(E)$ , is really the *probability* of having any kind of interaction take place per centimeter of the material through which the neutron passes. Hence, the average number of interactions that a single neutron will have in passing through a distance  $dx$  is

$$\text{Probability of interaction in } dx = \Sigma_T dx = [\Sigma_c + \Sigma_f + \Sigma_s + \dots] dx. \quad (2.13)$$

## NUCLEAR REACTOR THEORY AND DESIGN

If it were possible to consider each neutron to be an *intensity* rather than a single particle, then we could lose a fractional part of that intensity rather than the whole neutron in an interaction (this is the equivalent of considering a beam of neutrons where there are so many that we can talk about statistical averages). The fractional attenuation of neutrons in a given distance  $dx$  is therefore

$$\frac{dn}{n} = -\Sigma_T dx, \quad (2.14)$$

where the minus sign indicates that the intensity decreases with each interaction. This is a first-order homogeneous differential equation that can be solved for the probability that a single neutron will survive the traversal of a distance  $x$  without interaction. If  $n_o$  represents the initial intensity, then the equation can be solved using an integrating factor to obtain the expression

$$n(x) = n_o e^{-\Sigma_T x}. \quad (2.15)$$

The corresponding survival probability is

$$p_x = \frac{n}{n_o} = e^{-\Sigma_T x}. \quad (2.16)$$

Again, this probability applies to a single neutron. Note that it is *not* the sum of the partial probabilities for absorption, fission, scattering, etc. Also note that this equation says nothing about what happens to a neutron that is scattered; we are only counting first-collision events.

As an example, consider the probability that a thermal (0.025 eV) neutron will traverse a thickness of 1 cm of water without interaction. Since  $\Sigma_T = 3.3 \text{ cm}^{-1}$ , we have  $p_{(1\text{cm})} = e^{-3.3} = 0.037$ . Only about 4% of the neutrons will pass through a distance of 1 cm without interaction. On the other hand, since scattering

## NUCLEAR REACTOR THEORY AND DESIGN

is the predominant mode of interaction, most of the neutrons will survive to have multiple-scattering collisions and therefore will penetrate a considerably greater distance before being lost.

However, since each scattering event involves an energy transfer, the neutrons that survive will be at a different energy than when they started. This is the process of neutron moderation, and the above considerations imply that moderation is a function of both space and energy.

Let  $p(x) dx$  be the probability that the neutron will penetrate a distance  $x$  and then have an interaction in the interval  $dx$ , i.e., between  $x$  and  $x + dx$ . This factor is given as the product of the individual probabilities that a neutron will survive in passing through  $x$  and then have its next interaction in  $dx$ , namely,

$$p(x)dx = e^{-\Sigma_T x} \Sigma_T dx. \quad (2.17)$$

If the medium were of infinite extent, the total probability of interaction would be unity, since

$$\int_0^\infty p(x)dx = -e^{-\Sigma_T x} \Big|_0^\infty = 1.0. \quad (2.18)$$

This is to say that the neutron would interact somewhere with absolute certainty. The probability  $p(x)$  is useful as a weighting function. For example, the average distance that a neutron would move before it has an interaction, which is called the mean free path  $\lambda_T$ , is given by the expression

$$\lambda_T = \bar{x} = \frac{\int_0^\infty xp(x)dx}{\int_0^\infty p(x)dx} = \frac{1}{\Sigma_T}. \quad (2.19)$$

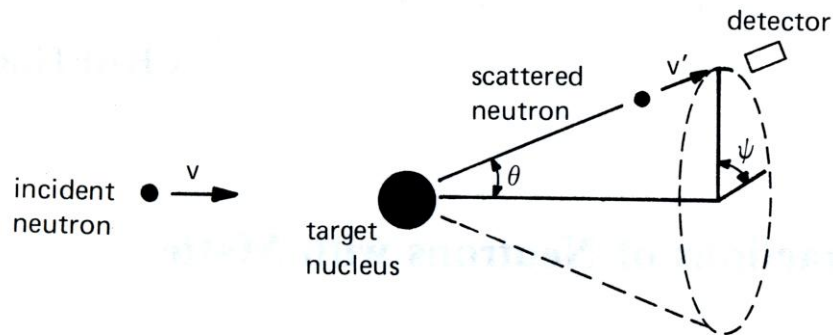
This result can be obtained by integrating Eq. (2.19) by parts.

### 2.6 Kinematics in the Center-of-Mass System

It is possible to treat the neutron scattering or absorption

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event directly in the Laboratory System (LAB) such that the process corresponds directly with an experiment. This configuration is shown in Figure 2.9. Unfortunately, the target nucleus considers itself to be at the "center of the universe" at the moment that the incident neutron has coalesced with it, and the resulting probabilities or cross sections for re-emission of the neutron (or other product) are generally symmetric (even isotropic) about this center point. Hence, it is most convenient to view the collision in the Center-of-Mass System (CM), which gives the simplest form for the reaction probability. We then translate back to the LAB system to observe the results.



**Fig. 2.9** Neutron Scattering in the LAB System

The center of mass of a system lies along the straight line that joins the two particles and moves with respect to a fixed observer in the laboratory as the particles move. In general, the velocity diagrams are vectors, but in the special (and important) case where the target nucleus is initially at rest, all velocities are collinear. Consider that the neutron has mass  $m$  and velocity  $v$  before the collision, and the nucleus has mass  $M$  and is at rest. With the origin of the coordinate system placed at the site of target nucleus, we have the diagram shown in Figure 2.10. The neutron instantaneously lies at a distance  $x$



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from the nucleus while the center of mass lies at  $x_o$ .

Since the center of mass is located at the balance point of the system, we write

$$(m+M)x_o = mx,$$

or

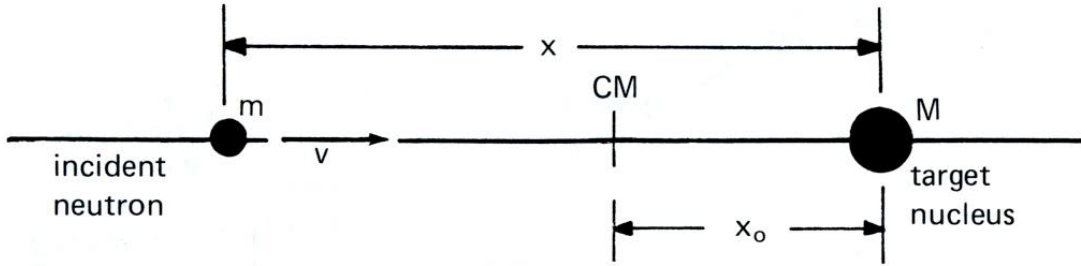
$$x_o = \frac{mx}{m+M} = \frac{x}{1+A}, \quad (2.20)$$

where  $A = M/m$  is the atomic weight of the target nucleus. The velocity of the center of mass is obtained by differentiating the position variable with respect to time, i.e.,

$$V_{CM} = \frac{dx_o}{dt} = \frac{1}{1+A} \frac{dx}{dt}. \quad (2.21)$$

Hence,

$$V_{CM} = \frac{1}{1+A} v. \quad (2.22)$$



**Fig. 2.10** Neutron-nucleus Location With Respect to the Center of Mass

If we imagine ourselves at the center of mass, we see both particles approach from opposite directions. The neutron has a relative velocity  $v_c$  given by

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$$v_c = v - V_{CM} = \frac{A}{A+I}v, \quad (2.23)$$

while the nucleus approaches from the opposite direction with a relative velocity  $V_c$  given by

$$V_c = 0 - V_{CM} = -\frac{I}{I+A}v. \quad (2.24)$$

The total momentum in the CM system is found by direct substitution of the above values, giving

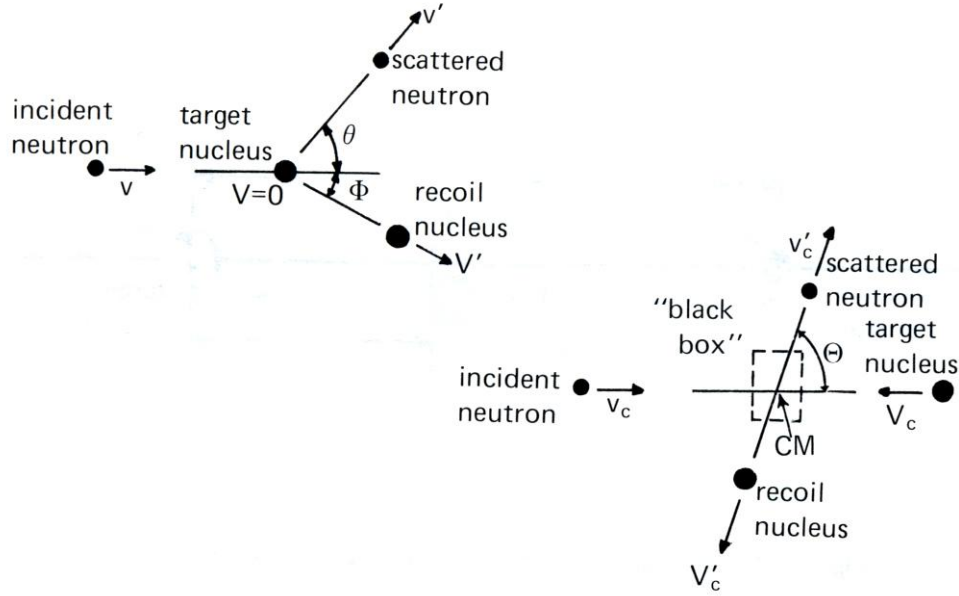
$$mv_c + MV_c = 0. \quad (2.25)$$

Hence, the CM System is a *zero momentum system*. The net momentum before the interaction is zero and it must remain so afterwards. An important consequence of this result is, that in an *elastic* collision in the CM system, the particles leave back-to-back with the *same* velocities that they had before the collision. The two versions of the same collision are shown in Figure 2.11. Conceptually, the collision is much simpler in the CM system because there is only one angle involved and the velocities are unchanged by the collision.

Now, consider the total energy in the two systems. For elastic scattering, the energy of the incident neutron in the LAB system is exactly equal to the total energy and is given as

$$E = \frac{1}{2}mv^2. \quad (2.26)$$

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**Fig. 2.11** Comparison of a Scattering Collision in the LAB and CM Systems

In the CM system the total energy is the sum of the energies of the two particles as seen by an observer located at the center of mass. This value is

$$\begin{aligned}
 E_c &= \frac{1}{2}(mv_c^2 + MV_c^2) \\
 &= \frac{1}{2}m\left(\frac{A}{A+1}\right)v^2 = \frac{1}{2}\left[\frac{mM}{m+M}\right]v^2.
 \end{aligned}
 \tag{2.27}$$

The quantity in brackets is called the "reduced mass," denoted by the symbol  $\mu_m$ , and is given in general by the equation

$$\mu_m = \frac{mM}{m+M} = \frac{mA}{A+1}.
 \tag{2.28}$$

Note that, comparing  $E$  with  $E_c$ ,  $E_c$  is smaller, i.e.,

$$E_c = \frac{A}{A+1}E.
 \tag{2.29}$$

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The difference in energy is not lost, it is simply the energy of motion of the center of mass itself. On the other hand, as far as a nuclear reaction is concerned, the energy of motion of the center of mass, given by the expression

$$E_{CM} = \frac{1}{2} \left( \frac{m}{1+A} \right) v^2 = \frac{1}{A+1} E, \quad (2.30)$$

is *unavailable* to excite the nucleus. This means that for endothermic reactions (negative  $Q$  value) the reaction threshold is greater than  $Q$  by the factor  $(A+1)/A$ . Note that the sum of  $E_c$  and  $E_{CM}$  is equal to  $Q$  as it should be for conservation of energy to hold. The proof that the velocities in the CM system remain unchanged after an elastic collision is straightforward and is left as an exercise.

We now relate the scattering collision in the two systems by using a vector diagram that combines the two previous scattering diagrams. After the collision we have the situation where the final velocity in the LAB system is obtained by adding the velocity of the center of mass to the final velocity in the CM system (Figure 2.12). We note that in the perpendicular direction,

$$v' \sin \theta = v_c' \sin \Theta, \quad (2.31)$$

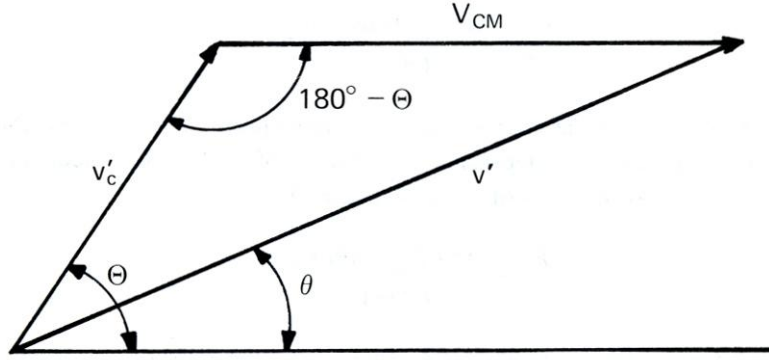
while in the parallel direction

$$v' \cos \theta = v_{CM} + v' \cos \Theta. \quad (2.32)$$

The ratio of these quantities is

$$\tan \theta = \frac{\sin \Theta}{V_{CM} / v_c' + \cos \Theta}. \quad (2.33)$$

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**Fig. 2.12** Scattered Neutron Velocities in the CM and LAB Systems

Thus, we have one useful relationship between  $\theta$  and  $\Theta$ . By applying the law of cosines,

$$v'^2 = v_c'^2 + V_{CM}^2 - 2v_c'V_{CM}\cos(180^\circ - \Theta).$$

But,

$$\cos(180^\circ - \Theta) = -\cos\Theta.$$

Hence, the laboratory velocity is related to the CM velocity by the expression

$$v'^2 = v_c'^2 + V_{CM}^2 + 2v_c'V_{CM}\cos\Theta. \quad (2.34)$$

Recall that for elastic scattering

$$v_c' = v_c = \frac{A}{A + I}v. \quad (2.35)$$

Introducing this value into Eq. (2.34), and simplifying, we obtain the useful result

$$\frac{v'^2}{v^2} = \frac{A^2 + 2A\cos\Theta + I}{(A + I)^2}. \quad (2.36)$$

Since the energy of a particle is proportional to the square of

## NUCLEAR REACTOR THEORY AND DESIGN

its velocity, the ratio of the energy of the scattered neutron to the energy of the incident neutron in the LAB system, expressed in terms of the CM angle  $\Theta$ , is

$$\frac{E'}{E} = \frac{A^2 + 2A\cos\Theta + I}{(A + I)^2}. \quad (2.37)$$

Note that for  $\Theta = 0^\circ$ , i.e., a glancing collision,  $E'_{\max} = E$  and there is no energy exchange. On the other hand, for a head-on collision where  $\Theta = 180^\circ$ ,

$$\frac{E'_{\min}}{E} = \frac{A^2 - 2A + I}{(A + I)^2} = \left( \frac{A - I}{A + I} \right)^2 \equiv \alpha. \quad (2.38)$$

Hence, for a collision which gives the maximum energy exchange in an elastic collision,

$$E'_{\min} = \alpha E. \quad (2.39)$$

### 2.7 Relationships Between the Scattering Angles in the LAB and CM Systems

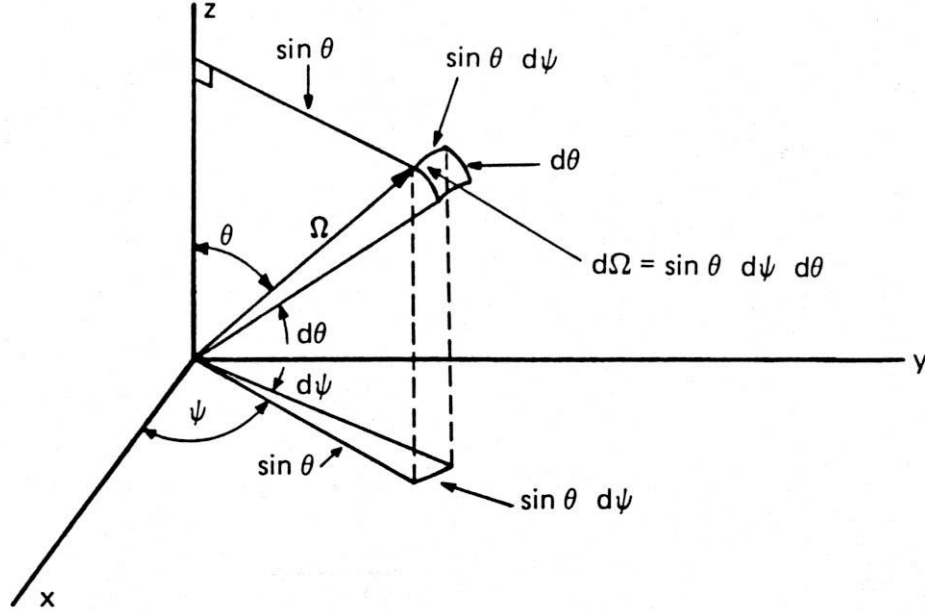
We can also find a relationship between the angle  $\theta$  in the LAB system and the angle  $\Theta$  in the CM system. We start with the vector diagram result given by Eq. (2.32),

$$\cos\theta = \frac{V_{CM} + v_c' \cos\Theta}{v'},$$

and substitute the values for  $V_{CM}$  and  $v_c'$  in terms of  $v$  (for elastic scattering) to obtain

$$\cos\theta = \frac{I + A\cos\Theta}{\sqrt{A^2 + 2A\cos\Theta + I}}. \quad (2.40)$$

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**Fig. 2.13** Differential Solid Angle Diagram

This expression, relating the LAB angle of scattering to the CM angle of scattering, can be used to relate the cross sections in the two systems. Recall that the unit vector  $\vec{\Omega}$  gives the direction of travel of the neutrons. Associated with  $\vec{\Omega}$  is a differential surface element  $d\Omega$  through which these neutrons pass. This is shown in detail in Figure 2.13. The quantity  $d\Omega$  is an element of surface area on the unit sphere given by the expression

$$d\Omega = \sin \theta d\psi d\theta. \quad (2.41)$$

Referring back to Figure 2.9, one must remark that for most materials there is no polarization and the scattering is only dependent upon the polar angle  $\theta$  and not on the azimuthal angle  $\psi$  (that is, we have rotational symmetry about the azimuth). The same holds true in the CM system. We relate the cross sections as a function of angle by writing that the probability that a neutron crosses the corresponding surface area in the two cases

## NUCLEAR REACTOR THEORY AND DESIGN

is equal, i.e.,

$$\sigma_s(\theta, \psi) d\Omega = \sigma_s(\Theta, \Psi) d\Omega_{CM}. \quad (2.42)$$

But because of azimuthal symmetry, the cross sections are only functions of the polar angle, giving

$$\sigma_s(\theta, \psi) = \sigma_s(\theta)/2\pi, \text{ and } \sigma_s(\Theta, \Psi) = \sigma_s(\Theta)/2\pi.$$

The differential solid angles in the two systems are

$$d\Omega = \sin\theta \, d\theta \, d\psi$$

*and*

$$d\Omega_{CM} = \sin\Theta \, d\Theta \, d\Psi.$$

Moreover, the rotational angles  $\psi$  and  $\Psi$  must be equivalent to conserve momentum. Hence, by substitution,

$$\sigma_s(\theta) \sin\theta \, d\theta = \sigma_s(\Theta) \sin\Theta \, d\Theta. \quad (2.43)$$

We note that

$$\sin\Theta \, d\Theta = -d(\cos\Theta) \text{ and}$$

$$\sin\theta \, d\theta = -d(\cos\theta)$$

Therefore, the desired relationship is

$$\sigma_s(\theta) = \sigma_s(\Theta) \frac{d(\cos\Theta)}{d(\cos\theta)}. \quad (2.44)$$

The factor  $d(\cos\Theta)/d(\cos\theta)$  is called the Jacobian of the transformation of the cross section from the CM system to the LAB system.

Using the previously obtained expression relating the cosines in the two systems, plus Eq. (2.40), and performing the derivatives, we obtain the useful equation



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$$\sigma_s(\theta) = \sigma_s(\Theta) \left[ \frac{A^2 + 2A \cos \Theta + 1}{A^2(A + \cos \Theta)} \right]^{3/2}. \quad (2.45)$$

Thus, if we know  $\sigma_s(\Theta)$ , which is a constant for isotropic scattering in the CM system, we can easily compute  $\sigma_s(\theta)$ . For isotropic scattering in the CM system,

$$\sigma_s(\Theta, \psi) = \sigma_s(\Theta)/2\pi = \sigma_s/4\pi,$$

where  $\sigma_s$  is the total scattering across section given by the relationship

$$\sigma_s = \int \sigma_s(\theta, \psi) d\Omega = \int \sigma_s(\Theta, \Psi) d\Omega_{CM}. \quad (2.46)$$

We must pick an angle  $\theta$  in the laboratory system, compute the corresponding  $\Theta$  using the cosine relation given by Eq. (2.40), compute the Jacobian for this  $\Theta$ , and then multiply it by  $\sigma_s(\Theta)$  to obtain the value of  $\sigma_s(\theta)$ . The process must be repeated for each value of  $\theta$ .

Next, let us consider in somewhat more detail what happens to the neutrons that scatter. Scattering is usually isotropic in the CM system but anisotropic in the LAB system. Anisotropic scattering implies a net migration of the neutron in the original direction of travel after multiple collisions.

A measure of the amount of anisotropy is the average cosine of the scattering angle, defined as  $\bar{\mu} = \cos \theta$ . The average cosine of the scattering angle is computed by weighting the quantity  $\cos \theta$  by the probability of scattering through angle  $\Theta$ , which is given by the angular cross section  $\sigma_s(\Theta)$ . Hence,

$$\bar{\mu} \equiv \frac{\int_{all\Omega} \sigma_s(\theta, \psi) \cos \theta d\Omega}{\int_{all\Omega} \sigma_s(\theta, \psi) d\Omega} = \frac{\int_{all\Omega_{CM}} \sigma_s(\Theta, \Psi) \cos \theta d\Omega_{CM}}{\int_{all\Omega_{CM}} \sigma_s(\Theta, \Psi) d\Omega_{CM}}. \quad (2.47)$$

For azimuthal symmetry, the differential solid angle of a ring is

## NUCLEAR REACTOR THEORY AND DESIGN

$$\int_0^{2\pi} d\Omega = 2\pi \sin\theta d\theta.$$

Also, the integral of  $\sigma_s(\Theta)$  over all  $\Theta$  is simply  $\sigma_s$ . Thus the expression reduces to

$$\begin{aligned} \bar{\mu} &= \frac{1}{\sigma_s} \int_0^\pi \sigma_s(\theta) \cos\theta \sin\theta d\theta = \frac{1}{\sigma_s} \int_0^\pi \sigma_s(\Theta) \cos\theta \sin\Theta d\Theta \\ &= \frac{1}{\sigma_s} \int_{-1}^{+1} \sigma_s(\mu) \mu d\mu. \end{aligned} \quad (2.48)$$

We already have relationships between the angles  $\theta$  and  $\Theta$ , which for elastic scattering are simply

$$\tan\theta = \frac{A \sin\Theta}{1 + A \cos\Theta}, \text{ and } \cos\theta = \frac{1 + A \cos\Theta}{\sqrt{A^2 + 2A \cos\Theta + 1}}.$$

We also have a relationship between the cross sections  $\sigma_s(\theta)$  and  $\sigma_s(\Theta)$ . Furthermore, for isotropic scattering in the CM system,  $\sigma_s(\Theta) = \sigma_s/2$ . We can therefore insert the above information into the expression for  $\bar{\mu}$  and perform the integrals to obtain a result that is good for elastic scattering that is isotropic in the CM system, namely,

$$\bar{\mu} = \frac{2}{3A}. \quad (2.49)$$

For heavy nuclei,  $A$  is large and  $\bar{\mu}$  is small. The average scattering angle is near  $90^\circ$ , which states that scattering is approximately isotropic in the LAB system as well as in the CM system.

For hydrogen,  $\bar{\mu} = 2/3$ , which corresponds to an average scattering angle of  $48^\circ$ . This means that the scattering is primarily forward directed in the LAB system. In fact, letting  $A = 1$ , the tangent relationship gives

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$$\tan\theta = \frac{\sin\Theta}{1+\cos\Theta} = \frac{2\sin(\Theta/2)\cos(\Theta/2)}{2\cos^2(\Theta/2)} = \tan\frac{\Theta}{2}.$$

Hence,  $\theta = \Theta/2$ . Since  $\Theta_{\max} = 180^\circ$ ,  $\theta_{\max} = 90^\circ$  and there is no backscattering at all in the LAB system!

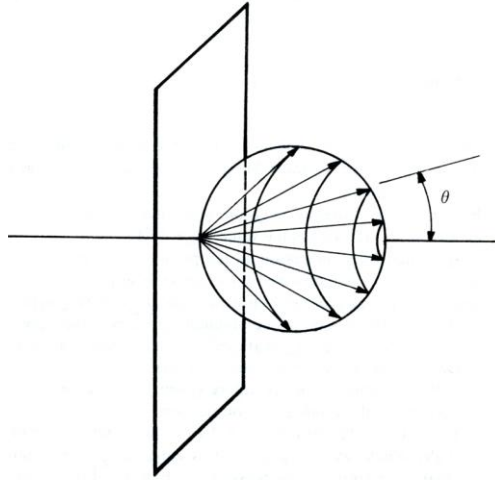
Using the cross-section relationship, the corresponding angular cross section in the LAB system is

$$\sigma_s(\theta) = \frac{\sigma_s}{2} \frac{(2 + 2\cos\Theta)^{3/2}}{1 + \cos\Theta} = \frac{\sigma_s}{2} 2^{3/2} (1 + \cos\Theta)^{1/2}.$$

Using the half-angle relationship, we obtain

$$\sigma_s(\theta) = 2\sigma_s \cos\frac{\Theta}{2} = 2\sigma_s \cos\theta; \quad 0 < \theta < \frac{\pi}{2}.$$

This cross section is strongly peaked forward. In fact, the distribution is a uniform sphere tangent to the point of interaction, as shown in Figure 2.14.



**Fig. 2.14** Angular Differential Scattering Cross Section of Hydrogen in the LAB System

Recall that  $\lambda_T = 1/\Sigma_T$ . We can also define a mean free path for scattering as  $\lambda_s = 1/\Sigma_s$ , where  $\lambda_s$  is the average distance

## NUCLEAR REACTOR THEORY AND DESIGN

between elastic scattering collisions. But since we do not lose the neutron, we should really increase or reduce the average path length to account for the fact that there may be predominant forward or backward scattering in the LAB system. We call this corrected quantity the transport mean free path and define it as

$$\lambda_{tr} = \frac{\lambda_s}{1 - \bar{\mu}}. \quad (2.50)$$

Note that  $\bar{\mu}$  lies between 0 and 1 for isotropic scattering in the CM system so that  $\lambda_{tr} > \lambda_s$ . On the other hand, if the scattering cross section in the CM system is anisotropic, so that it peaks in the backward direction, then  $\bar{\mu}$  is negative and  $\lambda_{tr} < \lambda_s$ .

We can now define a transport cross section that includes both absorption and corrected scattering. It is given by the expression

$$\Sigma_{tr} \equiv \Sigma_a + \Sigma_s(1 - \bar{\mu}) = \Sigma_T - \Sigma_s \bar{\mu}. \quad (2.51)$$

This expression will be encountered again in Chapter 4 when we deal with neutron transport.

### Problems

- 2.1 Prove that the initial velocities of both the neutron and the target particle remain unchanged in the CM system after an elastic scattering collision through an angle  $\Theta$ .
- 2.2 For an elastic scattering collision, show that the ratio  $\gamma = V_{CM}/v_c$  which appears in Eq. (2.33), has the value  $\gamma_{elas} = 1/A$ .
- 2.3 Suppose that for some reason all red protons had a mass of 1/2 instead of the normal value of 1 observed for ordinary

## NUCLEAR REACTOR THEORY AND DESIGN

blue protons. We know that the neutron scattering cross section is isotropic in the CM system.

- a) What are the maximum and minimum energies in the laboratory system of neutrons of energy  $E_0$  scattered by an initially stationary red proton? Derive your answer from basic principles.
- b) Is the scattering in the laboratory system isotropic, forward, or backward? Give physical reasoning for your answer.
- c) The text gives the formula  $\bar{\mu} = 2/(3A)$  for the average cosine of the scattering angle, which says  $\bar{\mu} = 4/3$  when  $A$  is equal to  $1/2$ ; this is obviously wrong because the cosine varies between  $\pm 1$ . Explain what is going on, and make a reasonable estimate of the proper value of  $\bar{\mu}$ .

**2.4** The differential elastic neutron cross section in the CM system for a material of mass number  $A = 2$  is given by the expression

$$\sigma_s(\Theta) = \frac{0.5}{2}(1 + 0.8 \cos \Theta) \frac{\text{barns}}{\text{sr}}.$$

- a) What is the value of the total elastic scattering cross section  $\sigma_s$ ?
- b) Plot the differential elastic scattering cross section in both the CM system and the LAB system versus the corresponding scattering angles  $\Theta$  and  $\theta$  on both linear graph paper and polar graph paper.
- c) What fraction of the neutrons are backscattered in the CM system and in the LAB system?
- d) Compute the average cosine of the scattering angle  $\bar{\mu}$ .

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- 2.5\*** For elastic scattering, the relationship between the laboratory neutron energies before and after collision is given by the expression

$$\frac{E'}{E} = \frac{A^2 + 2A\cos\theta + 1}{(A+1)^2}.$$

Derive the corresponding relationship for inelastic scattering to the first excited level at energy  $E_1$  above the ground state of a target nucleus of mass  $M$ .

- 2.6\*** Using the nuclear data sheets or the chart of the nuclides to obtain mass values, compute the binding energy of the last neutron for the following light isotopes using the formula

$$B = \left[ {}^A_Z M + {}^1_0 n - {}^A_Z M \right] c^2,$$

where  $1 \text{ AMU} \approx 931 \text{ MeV}$ .

- |                        |                        |                        |                        |
|------------------------|------------------------|------------------------|------------------------|
| a. ${}^2_1\text{H}$    | b. ${}^3_1\text{H}$    | c. ${}^4_2\text{He}$   | d. ${}^7_3\text{Li}$   |
| e. ${}^8_3\text{Li}$   | f. ${}^8_4\text{Be}$   | g. ${}^9_4\text{Be}$   | h. ${}^{10}_5\text{B}$ |
| i. ${}^{11}_5\text{B}$ | j. ${}^{12}_6\text{C}$ | k. ${}^{13}_6\text{C}$ | l. ${}^{14}_6\text{C}$ |

Comment on any systematic behavior or unusually large or small values that you observe.

- 2.7\*** You are given the general nuclear reaction  $a(b,c)d$ , where the corresponding masses are  $M_a$ ,  $M_b$ ,  $M_c$ , and  $M_d$ , and  $M_a + M_b \approx M_c + M_d$ .

- a) Show that the quantity  $\gamma$  is given by the expression

$$\gamma \equiv \frac{V_{CM}}{v_c^-} \approx \left[ \frac{M_a M_c}{M_b M_d} \left\{ \frac{E_c}{E_c + Q(1 + M_a/M_b)} \right\} \right]^{1/2},$$

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where  $E_c$  represents the kinetic energy brought into the CM system by the particle b and Q is the Q-value of the reaction.

- b) Find an expression for the laboratory energy of particle c in terms of the laboratory energy of particle b and the scattering angle relationship

$$\delta = [\cos\theta + \cos(\Theta - \theta)/\gamma]^2.$$

- 2.8 For elastic scattering that is isotropic in the CM system, prove that

$$\bar{\mu} = \frac{2}{3A}.$$

## References

**R.D. Evans**, *The Atomic Nucleus*, (McGraw Hill Book Company, New York, NY, 1955), Chapters 2 and 12, Appendices B and C.

**J.R. Lamarsh**, *Nuclear Reactor Theory*, (Addison Wesley Publishing Company, Reading, M.A., 1966), Chapters 1 and 2.

## NUCLEAR REACTOR THEORY AND DESIGN



## NUCLEAR FISSION

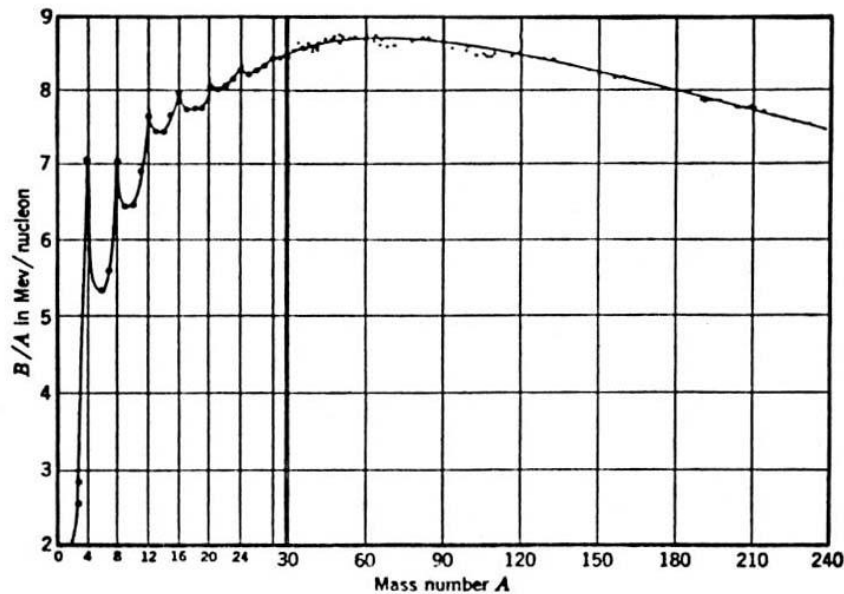
In this chapter we examine the energetics of the fission process in terms of the binding energy of a nucleus. We will see that the reason that some nuclides fission with thermal neutrons while others fission only with fast neutrons is related to the spin-pairing effect between similar nucleons. For heavy nuclides, such as uranium, the nucleus is held together against the disruptive Coulomb forces between protons by short-range strong nuclear forces provided by both protons and neutrons. When fission takes place, the lower  $Z$  products find themselves with a surplus of neutrons, which leads to prompt neutron emission during fission and a subsequent series of  $\beta^-$  decays of the fission fragments. These excess fast neutrons form the basis for a chain reaction, while the instability of the fission fragments to  $\beta^-$  decay leads to a large inventory of radioactive species in a power reactor and forms the basis for problems of decay heat removal, reactor safety and waste handling and disposal.

We shall also see that the magic numbers, which pertain to closed shells of neutrons or protons, play the major role in determining the shapes of the fission product yield curves for various fissionable isotopes. Magic numbers are involved in delayed neutron emission, which, in turn, is the basis for allowing a nuclear reactor to be controlled on a time scale of seconds with mechanically driven control rods. They are also responsible for the high yield and large cross section of  $^{135}\text{Xe}$ , which leads to the xenon poisoning and xenon-induced power oscillation problems in thermal power reactors.

## NUCLEAR REACTOR THEORY AND DESIGN

### 3.1 Binding Energy

If one sketches the curve of binding energy per nucleon versus mass number, one obtains a curve that increases initially from zero, peaks at about 8 MeV/nucleon near mass number 60, and then slowly decreases as the mass number increases further. Superimposed upon the general curve is a certain amount of fine structure, as shown in Figure 3.1. Note that the binding energy per nucleon is higher for elements with mass numbers near 60 than for elements of high mass number such as  $^{235}\text{U}$  or  $^{238}\text{U}$ . Therefore, there exists a configuration at medium mass numbers that is more stable than the one that occurs at high mass numbers: and one might expect that heavy nuclei would undergo spontaneous fission into smaller pieces in an attempt to reach the more stable state. In most cases this does not happen; energy must usually be supplied to start the reaction.



**Fig. 3.1** Binding Energy per Nucleon versus Mass Number

(From R. D. Evans, *The Atomic Nucleus*, 1955, McGraw Hill)

## NUCLEAR REACTOR THEORY AND DESIGN

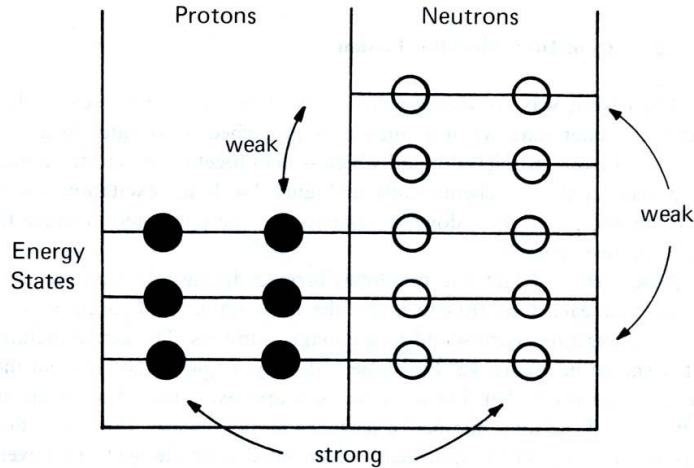
The semi-empirical binding energy equation explains Figure 3.1 in the following manner. The primary force that holds the nucleus together is due to short-range nucleon-nucleon attraction that is essentially proportional to the total number of nucleons present; this is, in turn, proportional to the nuclear volume. We must subtract something from the nuclear forces to account for the fact that some nucleons are near the nuclear surface and do not have neighbors on all sides. Hence, the binding energy curve increases with mass number at small mass numbers. The primary force trying to disrupt the nucleus is Coulomb repulsion, which is proportional to  $Z^2$ , the square of the number of protons present in the nucleus. This term tends to be largest at high mass numbers. Furthermore, we must subtract something for asymmetry, i.e., having either too many protons or neutrons in the nucleus. These extra particles must lie at higher quantum states and are therefore less tightly bound, as shown in Figure 3.2. Because of spin pairing, we must add or subtract a term; we subtract when the nucleus is odd-odd (i.e., an odd number of both protons and neutrons) and add when it is even-even. This contribution is represented by the saw-tooth structure superimposed on the binding energy curve. Finally, we have the effects of closed shells of nucleons, which we shall call magic. To summarize, the contributions symbolically are the following:

$$\begin{aligned} \text{Binding energy} = & \left( \begin{array}{c} \text{Volume} \\ \text{term} \end{array} \right) - \left( \begin{array}{c} \text{Coulomb} \\ \text{term} \end{array} \right) - \left( \begin{array}{c} \text{Surface} \\ \text{term} \end{array} \right) \\ & - \left( \begin{array}{c} \text{Asymmetry} \\ \text{term} \end{array} \right) \pm \left( \begin{array}{c} \text{Pairing} \\ \text{term} \end{array} \right) + (\text{Magic}). \end{aligned}$$

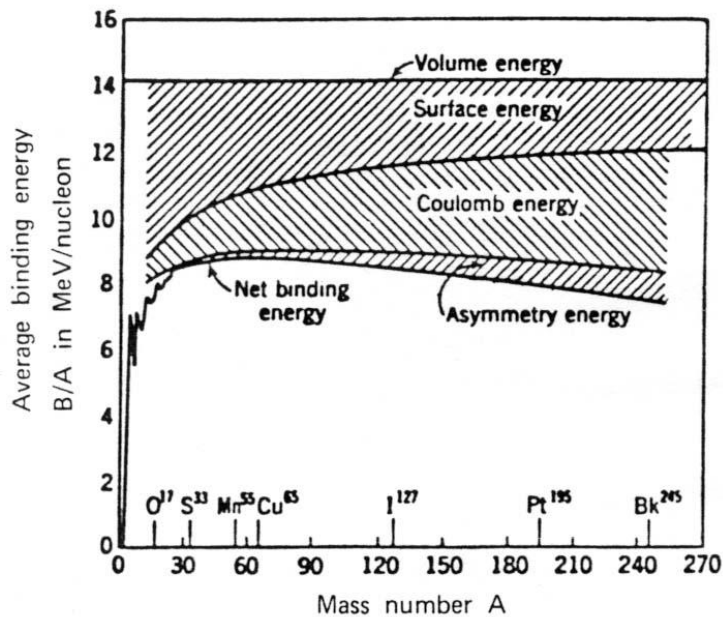
We can easily see from this expression why the binding energy per nucleon decreases above  $A = 60$ . As  $Z$  increases, the Coulomb repulsion term increases rapidly, requiring considerably more

## NUCLEAR REACTOR THEORY AND DESIGN

neutrons to hold the nucleus together. On the other hand, these extra neutrons lend a certain asymmetry to the binding that prevents one from adding neutrons ad infinitum. The contributions of the various terms are shown in Figure 3.3.



**Fig. 3.2** Binding in Asymmetric Nuclei



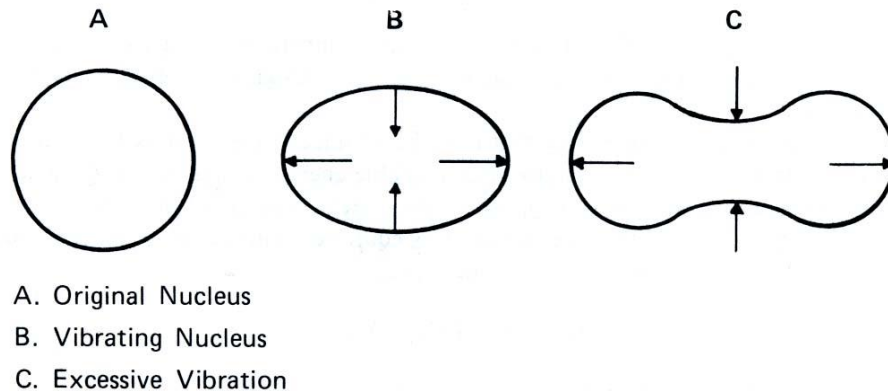
**Fig. 3.3** Binding Energy Contributions

(From R. D. Evans, *The Atomic Nucleus*, 1955, McGraw Hill)

## NUCLEAR REACTOR THEORY AND DESIGN

### 3.2 Liquid Drop Model of Fission

The easiest way to visualize fission is in terms of the so-called liquid drop model. Consider that, when a nucleus is perturbed, it vibrates in a longitudinal fashion just like a droplet of liquid that is held together by surface tension forces. The process is shown schematically in Figure 3.4. If the excitation is sufficient to cause the nucleus to neck down at some point, there is a good chance that it will break into two pieces.



**Fig. 3.4** Vibration of a Perturbed Nucleus

As a matter of fact, the two lobes formed during vibration are not of equal size, because each lobe tries to attain the most stable configuration possible, and these configurations correspond to the magic numbers. The actual picture is closer to that shown in Figure 3.5. One lobe is doubly magic at (50;82) and the other is doubly magic at (28;50). The neck contains approximately 25 nucleons making up the balance of the total number of particles in the nucleus. The actual point of the break is not fixed, but is statistically distributed over the neck. However, there is reason to believe that it is more likely that the neck will break in the middle than at the ends where it

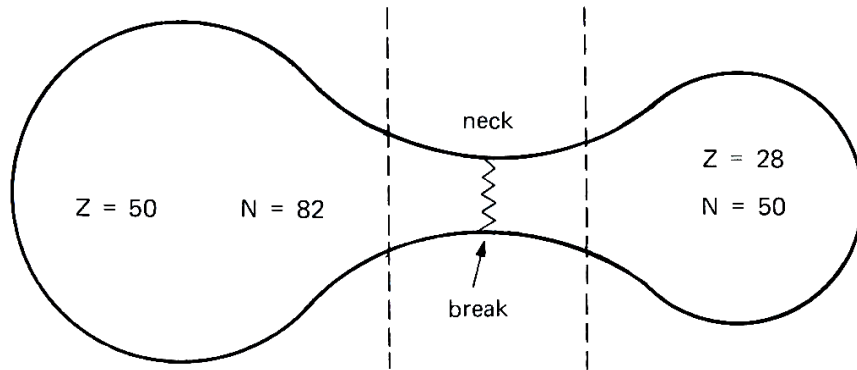
## NUCLEAR REACTOR THEORY AND DESIGN

is somewhat wider.

What causes the break to occur at all? Basically, the break is due to the Coulomb repulsion. When the nucleus is spherical, the short-range nuclear forces can hold it together, but when it is distorted, the short-range forces are diluted by the additional surface area, and Coulomb repulsion predominates. The Coulomb repulsion can be calculated classically; for example, for the two just-touching spheres shown in Figure 3.6, it is given by the expression

$$E_q = \frac{Z_1 Z_2 e^2}{(R_1 + R_2)}, \quad (3.1)$$

where  $(Z_1; A_1)$  and  $(Z_2; A_2)$  are the atomic numbers and weights of the two fragments and  $(Z = Z_1 + Z_2; A = A_1 + A_2)$  is the designation of the compound nucleus.



**Fig. 3.5** Nucleus at the Moment of Fission

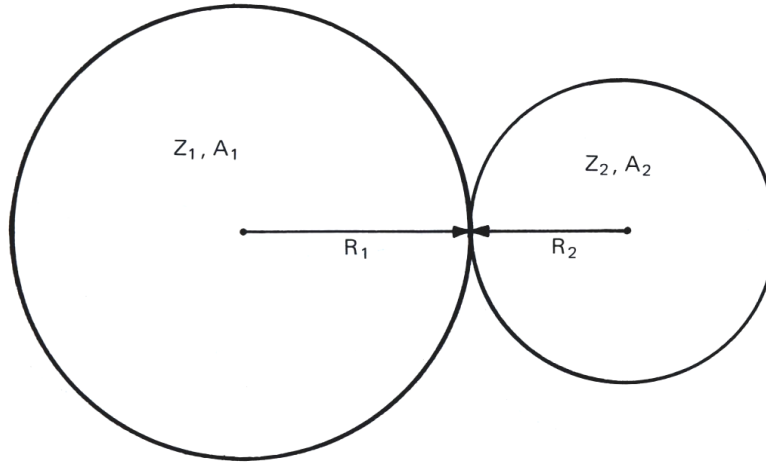
$E_q$  is the minimum energy that must be attained if the break is to occur and the two fragments are to separate. The available energy is equal to the  $Q$  value of the reaction plus the energy supplied to the system externally. The  $Q$  value is, of course, equal to the difference in rest mass equivalent energies between the initial and final ground states of the constituents, i.e.,

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$$Q = [M_A - (M_{A1} + M_{A2})]c^2. \quad (3.2)$$

Fission will occur whenever

$$E_{available} = E_{supplied} + Q > E_q. \quad (3.3)$$



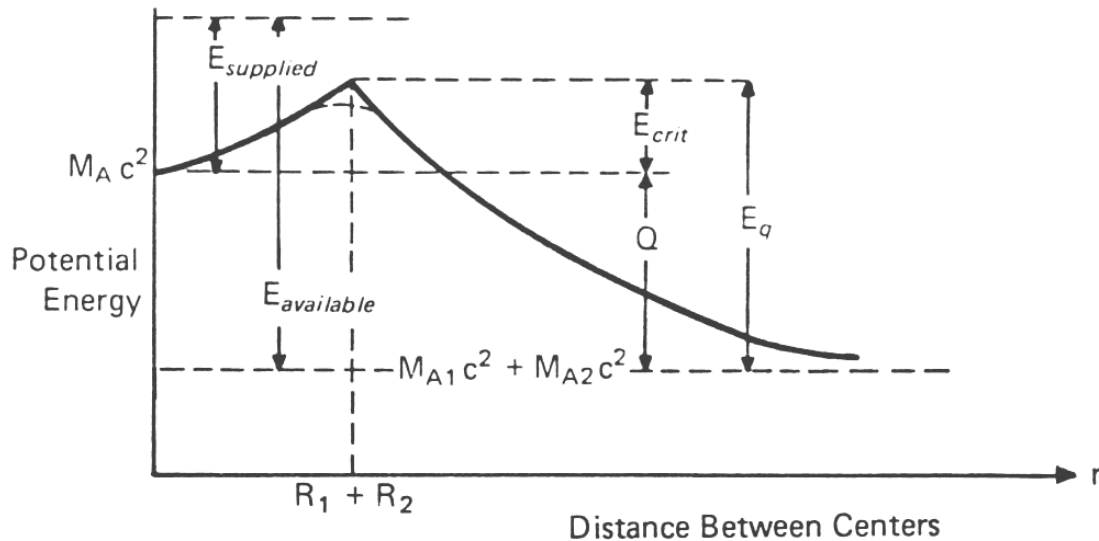
**Fig. 3.6** Two Touching Fission Fragments

The point of interest is that the binding energy of the last neutron, the one captured to form the compound nucleus, is a significant contributor to the needed value. In some cases, the binding energy of the last neutron can supply enough energy so that fission will occur with thermal neutrons having essentially zero kinetic energies.

We have already written an expression for the Coulomb energy,  $E_q$ , which corresponds to the amount of energy required to bring the two spheres from infinity to the point where they just touch. If the spheres were pushed together a bit more, they would in fact begin to merge and the forces of nuclear attraction would then pull them together into a single nucleus. This process, when plotted on a potential energy diagram, is as shown in Figure 3.7. Fission is the exact opposite process. We must

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now supply some energy to stretch the nucleus out of its spherical shape, and if we do not supply enough energy, it will spring back. But if we manage to supply  $E_{crit}$  or more, fission will occur. Upon fission, we will get back the energy  $Q$  plus the energy supplied,  $E_{supplied}$ .



**Fig. 3.7** Potential Energy Diagram for Two Fission Fragments

Where can this excess excitation energy be obtained? There are at least four processes that are commonly observed:

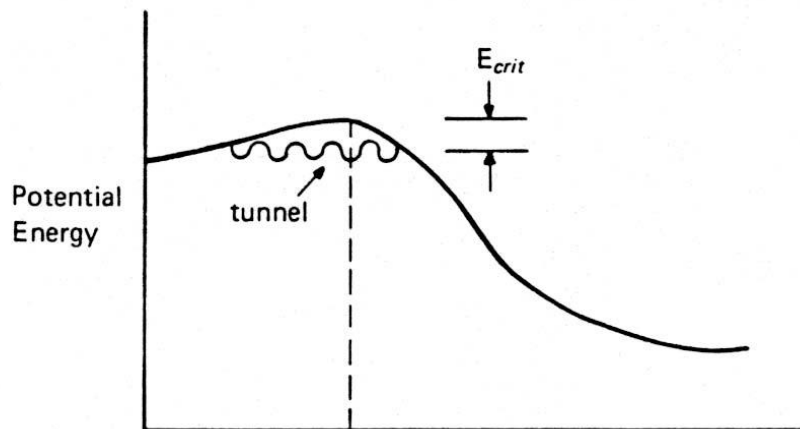
1. The nucleus captures an energetic  $\gamma$  ray. Capture  $\gamma$  rays have energies of 4-8 MeV. If this is greater than  $E_{crit}$ , the result is called photofission.
2. Capture of a slow neutron. The binding energy  $B$  of the last neutron is available as excitation of the compound nucleus. This is sometimes sufficient to cause fission, which is the case when  $^{235}\text{U}$  captures a neutron and the compound nucleus  $^{236}\text{U}^*$  fissions. If the nucleus de-excites by gamma emission, fission does not occur.
3. Capture of an energetic neutron. The kinetic energy  $E_c$ ,



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when added to B, can be sufficient to cause fission. This is a threshold reaction and is exemplified by  $^{238}\text{U}$  and  $^{232}\text{Th}$  which fission upon capture of a neutron having an energy greater than about 1.3 MeV. Of course, the nuclide that fissions is  $^{239}\text{U}^*$  or  $^{233}\text{Th}^*$ .

4. Spontaneous fission. If the value of  $E_{\text{crit}}$  is relatively small, there is a fairly good chance that a random fragment can "tunnel" through the potential barrier as shown in Figure 3.8. This is a quantum-mechanical effect, which is well known in  $\alpha$ -particle emission. The higher the barrier, the longer the half life for fission. An example is  $^{252}\text{Cf}$ , which has a half life of 2.64 years.  $^{238}\text{U}$  also fissions spontaneously but with an effective half life of  $10^{16}$  years!



**Fig. 3.8** Potential Energy Diagram for Spontaneous Fission

The critical energies for fission of various nuclides are given in Table 3.1; for those nuclei that are usually formed by neutron capture, the binding energy of the last neutron is also given. One notes that the critical energies are only small for the very heavy nuclides, which may be traced to the increasing Coulomb repulsion effect. One also notes that the spin-pairing effect is very important, since those nuclei that start out odd-

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even and become even-even by neutron capture gain a pairing energy of 1-2 MeV, which is usually enough to make fission with thermal neutrons possible. The fissile nuclei such as  $^{235}\text{U}$ ,  $^{233}\text{U}$ , and  $^{239}\text{Pu}$  fall into this class.

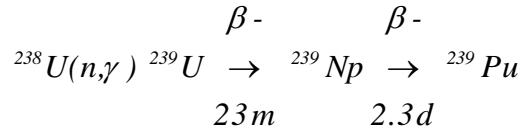
**Table 3.1**  
Critical Energies of Fissionable Nuclides

Parent Nuclide	Fissioning Nuclide	Critical Energy (Mev)	Binding Energy B of Last Neutron (Mev)	$E_{\text{crit}} - B$ (MeV)
-	$^{208}\text{Pb}$	20.	-	-
-	$^{232}\text{Th}$	5.9	-	-
$^{232}\text{Th}$	$^{233}\text{Th}^*$	6.5	5.1	1.4
-	$^{233}\text{U}$	5.5	-	-
$^{233}\text{U}$	$^{234}\text{U}^*$	4.6	6.6	negative
-	$^{235}\text{U}$	5.75	-	-
$^{235}\text{U}$	$^{236}\text{U}^*$	5.3	6.4	negative
-	$^{238}\text{U}$	5.85	-	-
$^{238}\text{U}$	$^{239}\text{U}^*$	5.5	4.9	0.6
-	$^{239}\text{Pu}$	5.5	-	-
$^{239}\text{Pu}$	$^{240}\text{Pu}^*$	4.0	6.4	negative

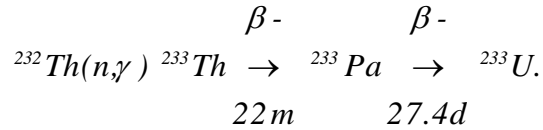
(Adapted from J. R. Lamarsh, *Nuclear Reactor Theory*, 1966, Addison-Wesley)

On the other hand, those nuclei that are even-even to start with and become even-odd by neutron capture lose the pairing energy. One must therefore supply kinetic energy to make these nuclides fission. Examples are  $^{232}\text{Th}$  and  $^{238}\text{U}$ , which have thresholds at about 1 MeV. These nuclides are considered to be fertile, however, because the decay chain eventually leads to a fissile element, e.g.,

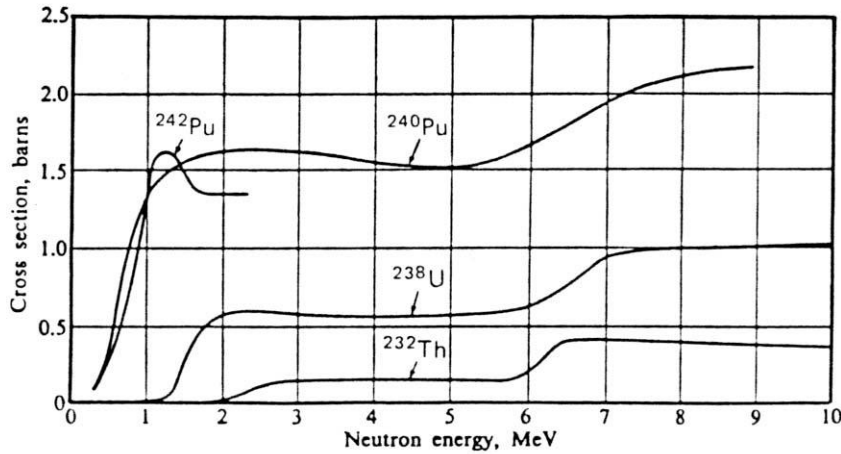
## NUCLEAR REACTOR THEORY AND DESIGN



and



The fission cross sections for several even-even nuclides are given in Figure 3.9 where the threshold nature is obvious.



**Fig. 3.9** Threshold Cross Sections

(From S. Yiftah, J. Okrent, and P. Moldauer, *Fast Reactor Cross Sections*, 1960, Pergamon)

For the even-odd fissile nuclides, the fission cross sections for thermal neutrons are rather high, as is illustrated in Table 3.2. A measure of the efficiency of a fissile element is its spectrum-averaged capture-to-fission cross-section ratio, given as

$$\bar{\alpha} \equiv \frac{\bar{\sigma}_c}{\sigma_f}. \quad (3.4)$$

This quantity represents the relative number of neutrons that

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are captured, and hence lead to the nonproductive loss of a fuel atom, compared to those that lead to fission. When a nucleus fissions, the products are neutron rich and some of the excess neutrons are released immediately. We state that  $\bar{\nu}$  neutrons are "boiled off" in the fission process. Hence, the net number of neutrons produced in the fuel per neutron captured, which is a figure of merit for the fuel, is given by

$$\bar{\eta} \equiv \bar{\nu} \frac{\bar{\sigma}_f}{\bar{\sigma}_a} = \frac{\bar{\nu}}{1 + \bar{\alpha}}. \quad (3.5)$$

**Table 3.2**

Microscopic Thermal Neutron Fission Cross Sections in Barns

Nuclide	Absorption	Fission	Capture	$\bar{\nu}$
$^{233}\text{U}$	579	531	48	2.49
$^{235}\text{U}$	681	582	99	2.42
$^{239}\text{Pu}$	1011	743	268	2.87

There is a corresponding definition for natural or enriched uranium that involves macroscopic cross sections. We would like  $\bar{\eta}$  to be as large as possible. In fact,  $\bar{\eta}$  can be classified as follows:

- $\bar{\eta} > 1$       for a chain reaction to be feasible;
- $2 > \bar{\eta} > 1$       for the possibility of *converting* fertile atoms to fissile, which is the case for thermal reactors fueled with  $^{235}\text{U}$ ;
- $\bar{\eta} > 2$       for the possibility of *breeding* as much fuel as is consumed, which is the case for fast reactors fueled with  $^{239}\text{Pu}$ .

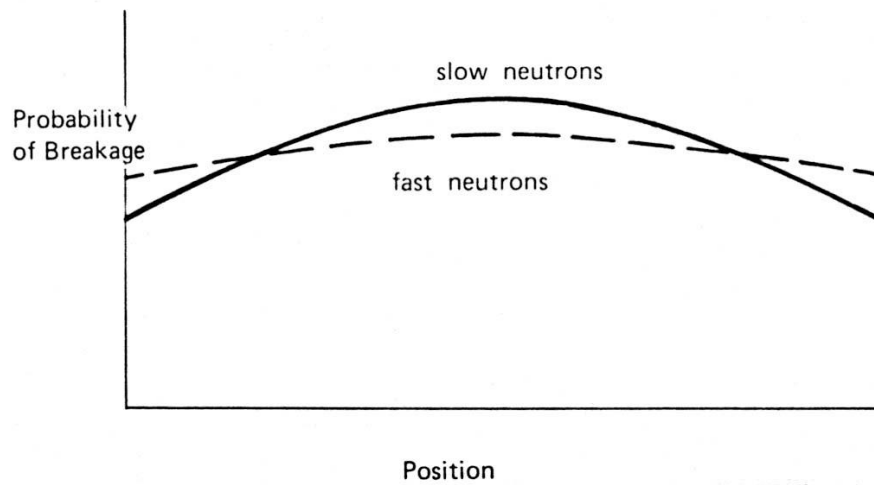
## NUCLEAR REACTOR THEORY AND DESIGN

### 3.3 Fission Product Yields

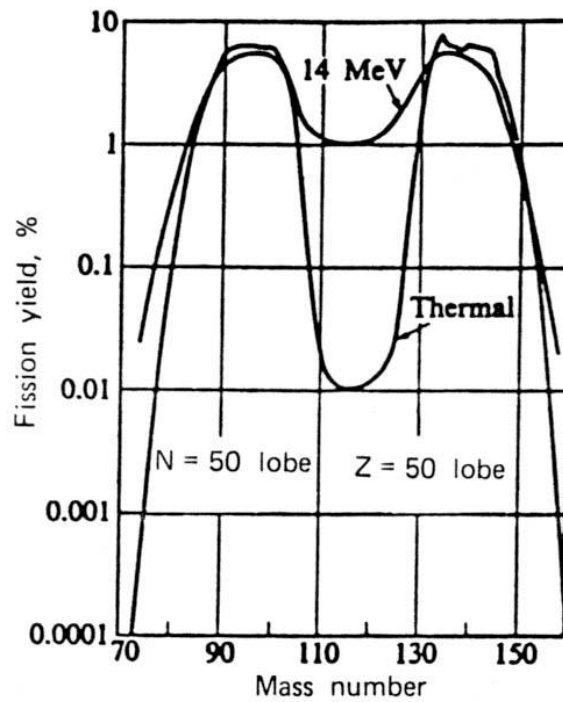
We have shown that the process of fission is asymmetric because each lobe tends to be doubly magic in the perturbed nucleus. Actually, many different modes of fission are possible, because the products formed are dependent upon where the "neck" between the two lobes breaks. The total energy released is therefore an average over all possible modes. The average yield of each product depends upon the probability distribution for breakage along the neck; breakage is most probable in the center of the neck and varies as a function of neutron energy, as shown schematically in Figure 3.10.

With these generalities in mind, we can examine the experimentally obtained fission product yield curves. The yield curves have been obtained by using very quick and efficient radiochemical procedures to separate and identify a number of specific isotopes in the various mass chains. Sample yield curves are shown in Figure 3.11. The maximum yields are about 7%, with considerable variation in magnitude as the mass number varies. The yield curves for heavier fissionable elements are somewhat different, being slightly shifted to the right because there are more particles in the "neck". The fact that the delayed neutron emitters are fission products means that the yields of delayed neutrons will be different for different fissionable nuclides simply because the fission product yield curves are different. The mass chain  $A = 135$ , which leads to the fission product  $^{135}\text{Xe}$  ( $\sigma_{\text{Xe}} \approx 3 \times 10^6$  barns!), has a yield of the order of 6%. Hence xenon poisoning in thermal reactors operating at moderate power levels is a definite reactor operation problem that would not exist if the yields were lower.

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**Fig. 3.10** Schematic Breakage Probability vs. Position in the "Neck"



**Fig. 3.11** Fission Product Yield Curves for  $^{235}\text{U}$

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### 3.4 Fission Neutron Spectrum

The prompt fission spectrum for a number of fissionable isotopes has been measured by proton-recoil techniques using both hydrogen-filled proportional counters and photographic emulsions. In the former, a voltage pulse is measured for each neutron detected, while in the latter the track length of the scattered proton is measured in the developed film. In either case, what is measured is the proton energy spectrum from which the incident neutron spectrum must be derived by some sort of unfolding procedure. Fortunately, the response function for a mono-energetic neutron source at energy  $E_n$  is essentially a rectangular distribution of proton energies from the neutron energy  $E_n$  down to zero, as shown in Figure 3.12. If the protons are only observed at a fixed angle to the neutron source, there is a direct proportionality between the proton and the neutron spectra. However, if all angles are measured, as in emulsions, then the neutron spectrum is essentially proportional to the derivative of the proton spectrum.

The experimental results, when plotted versus neutron energy, can be fit by a variety of functions. The basic nature of the curve is shown in Figure 3.13. We shall use the symbol  $\chi(E)$  to denote the normalized fission neutron spectrum such that

$$\int_{all E} \chi(E) dE = 1. \quad (3.6)$$

For  $^{235}\text{U}$  fission, the following formulae are often used

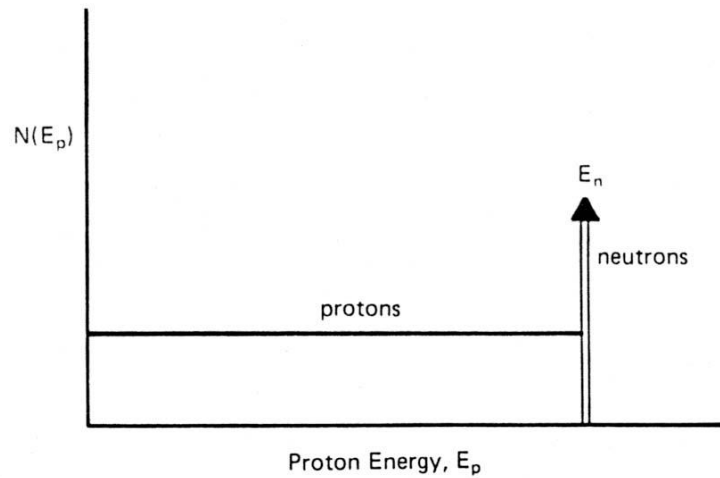
$$\text{Maxwellian } \chi(E) = 0.770 e^{-0.776E} \sqrt{E}; \quad (3.7)$$

$$\text{Cranberg-Frye } \chi(E) = 0.453 e^{-1.036E} \sinh \sqrt{2.29E}; \quad (3.8)$$

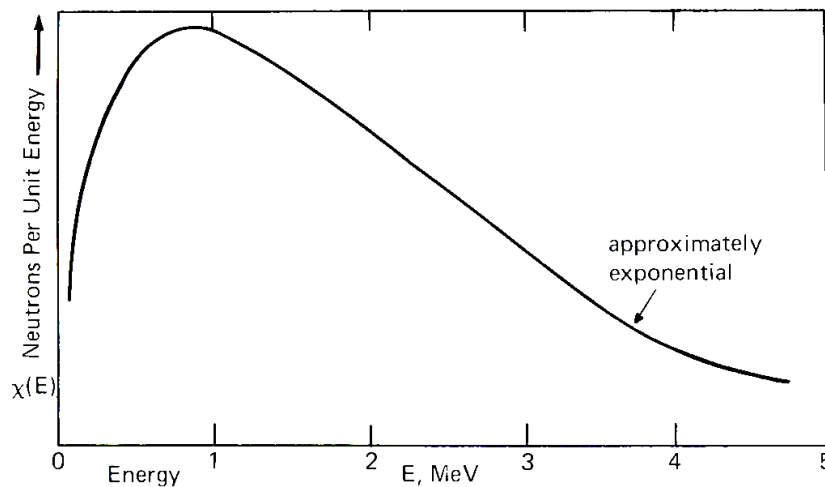
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$$\text{Harris } \chi(E) = \text{numerical tabulation of best data available.} \quad (3.9)$$

From the reactor designer's standpoint, the numerical tabulation is probably the most appropriate choice, although the analytical forms have some advantages when doing theoretical computations.



**Fig. 3.12** Energy Distribution of Scattered Protons for a Monoenergetic Neutron Source



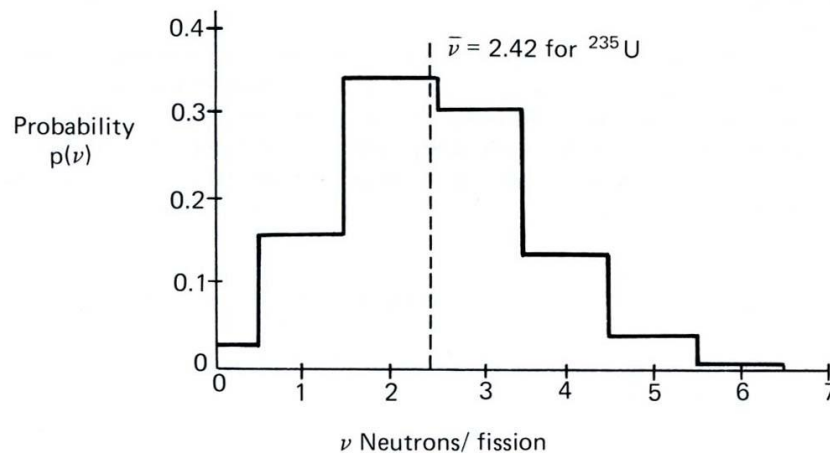
**Fig. 3.13** Fission Neutron Spectrum



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### 3.5 Prompt Neutrons

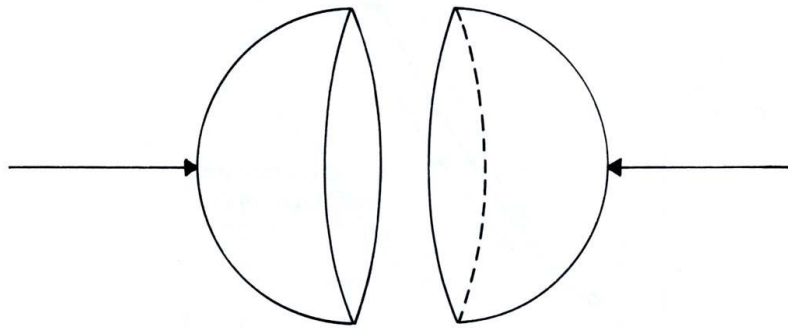
The neutrons that are emitted in the fission process all contribute to the maintenance of the steady-state chain reaction, whether they are emitted immediately (i.e., within  $10^{-17}$  s of the fission event) or are emitted in the decay of some of the fission fragments or their daughters (which delays the emission to the time range of seconds after the fission event). The number of prompt neutrons that are "boiled off" of the nucleus that is undergoing fission is a purely statistical quantity that can vary from a minimum of zero up to as many as 6 or 7. The distribution has been measured and has the general shape plotted in Figure 3.14. When we have a large number of neutrons in a reactor we can use the mean value of  $\bar{\nu} = 2.42$  to characterize the behavior of the system. On the other hand, when we consider the source-less startup of a "new" reactor, the statistical nature of the neutron yield comes into play, as has been observed in the Godiva bare core assembly experiments. There we encounter the spread or variance of the distribution as well as the mean or average behavior.



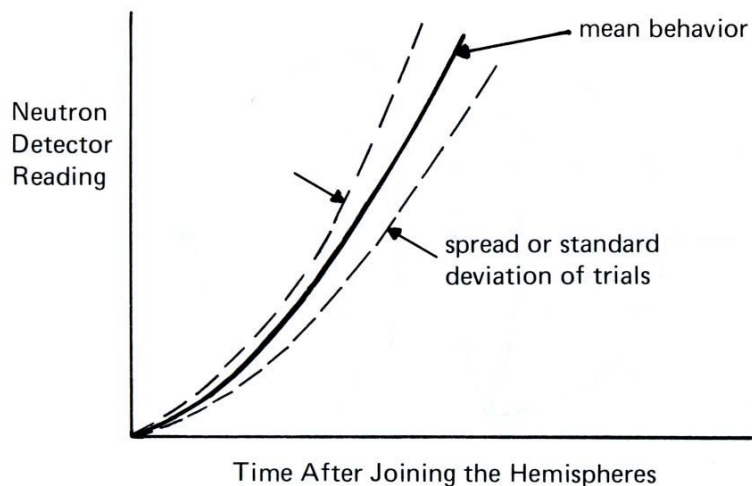
**Fig. 3.14** Probability Distribution of Fission Neutron Yields

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A Godiva experiment consisted of the assembly of two small  $^{235}\text{U}$  hemispheres (see Figure 3.15) such that the assembly became supercritical. After a very short period of time, the hemispheres were separated to terminate the excursion. The experiment was repeated 89 times. In each case, the same excess reactivity effect was introduced but the flux level vs. time history was different depending upon how many neutrons were emitted in the initial few fission events. The results are sketched in Figure 3.16.



**Fig. 3.15** Godiva Hemispheres



**Fig. 3.16** Results of the Godiva Excursion Experiments

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These experiments have been successfully analyzed using a probability generating function technique in the balance equations. The mean or first moment of the distribution corresponds to the average behavior when the neutron population is very large (deterministic), while the second moment predicts the spread or variance of the distribution. Ordinarily there are so many neutrons present in a reactor that we need worry only about the average behavior and need not consider statistical fluctuations.

Because the amount of excitation of a fissioning nucleus is a function of the binding energy plus the kinetic energy of the last neutron, one would expect to see some variation in the neutron yield with neutron energy. As a matter of fact, this effect is observed. An approximate formula for  $\nu$  (dropping the average bar) as a function of energy is

$$\nu(E) = \nu_0 + aE, \quad (3.10)$$

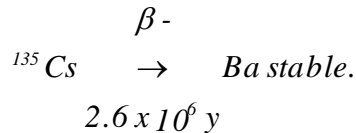
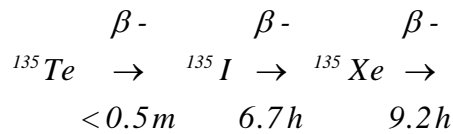
where  $\nu_0$  is the value at thermal energy or at the threshold energy and  $a$  is a small positive constant value which is different for different nuclides.

### 3.6 Delayed Neutrons

The delayed neutrons are neutrons that are emitted by certain members of various fission product chains when the available binding energy makes neutron emission a competitive process with  $\beta^-$  decay. To examine this process more fully, we first examine the nature of the driving force in the fission product decay chains. Specifically, the fission products that are emitted are neutron rich, and the asymmetry effect in the semi-empirical binding energy equation drives the decay to a point of stability for the given mass number by effectively

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converting neutrons to protons ( $\beta^-$  decay). The 135-mass chain is shown below as an example:

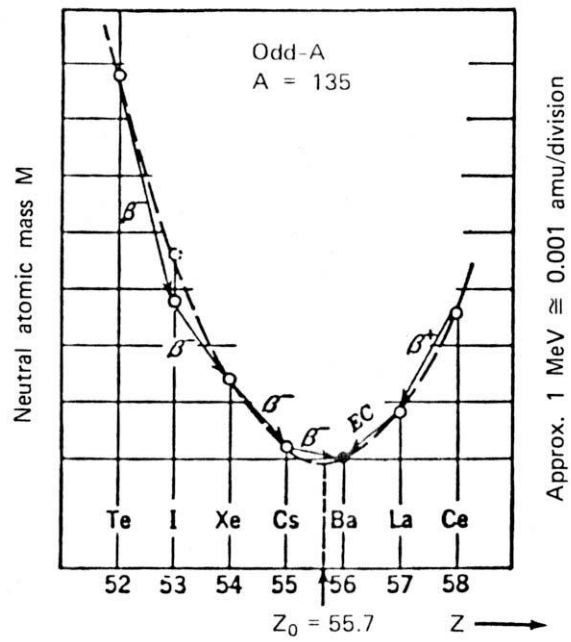


Four successive  $\beta^-$  decays are needed to attain stability, and in general the half-life increases as stability is approached, which implies that the driving energy is a decreasing function as  $Z$  increases. As a matter of fact, by taking the derivative of the semi-empirical binding energy equation with respect to  $Z$  for constant  $A$ , one obtains a parabola for mass numbers that are odd (see Figure 3.17). One sees that isotopes on the left-hand side of the figure will undergo  $\beta^-$  decay to reach stability, while those on the right-hand side will undergo  $\beta^+$  decay or electron capture. Fission products are always on the left-hand side. The situation is similar for even  $A$ , but there is a double parabola, as shown in Figure 3.18.

The emission of delayed neutrons is invariably related to the magic numbers, as illustrated by the  $A=87$  decay scheme shown in Figure 3.19. The isotope  ${}^{87}\text{Kr}$  has 51 neutrons, one more than needed for a closed shell. If the isotope is formed at an excited level above the ground state of  ${}^{86}\text{Kr}$ , this excess neutron will be emitted in competition with the emission of a  $\gamma$  ray to the ground state of  ${}^{87}\text{Kr}$ . The isotope  ${}^{86}\text{Kr}$  is even-even and also has a magic neutron number. This extra binding energy is the source of the energy favoring neutron emission. Note that the emitted neutron has a discrete energy that is generally less than 500 KeV; each type of delayed neutron emitter has its

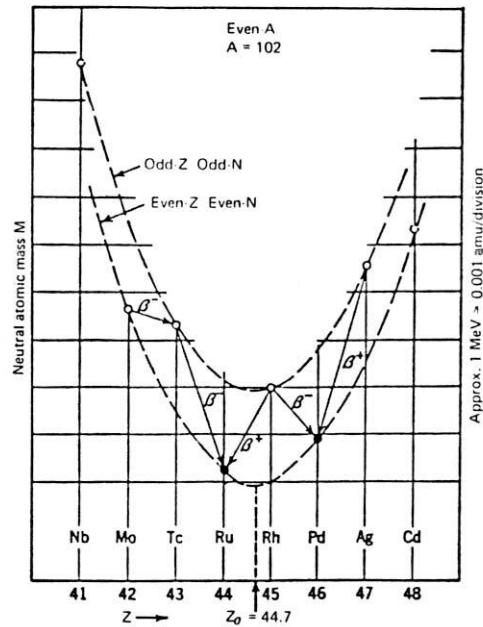
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own discrete neutron energy.



**Fig. 3.17** Mass Parabola for Odd A Nuclides

(From R. D. Evans, *The Atomic Nucleus*, 1955, McGraw Hill)

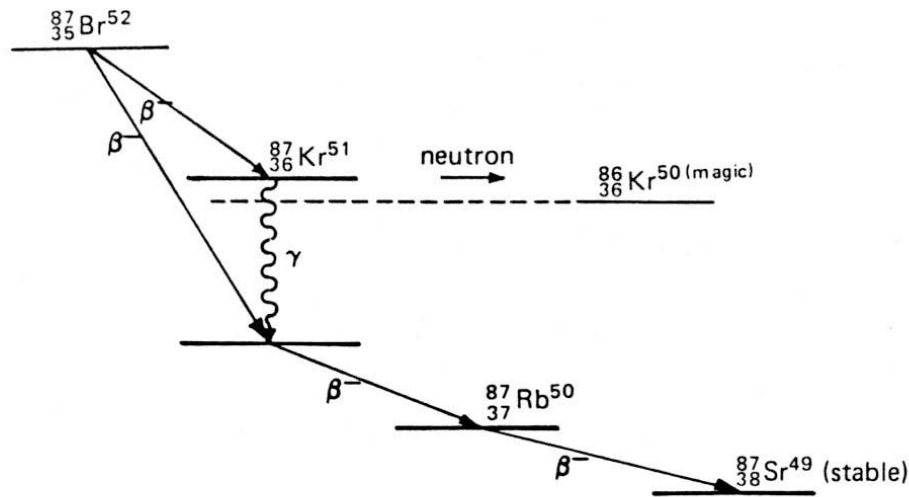


**Fig. 3.18** Mass Parabola for Even A Nuclides

(From R. D. Evans, *The Atomic Nucleus*, 1955, McGraw Hill)

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There are numerous isotopes that can emit delayed neutrons. These are experimentally classified into six groups by half-life. The total delayed neutron fraction is  $\beta = .0064$  for  $^{235}\text{U}$  and  $\beta = .0021$  for  $^{239}\text{Pu}$ . The effective half-lives range from approximately 0.2 s to 54 s. The delayed neutron spectrum for each group is a composite of its constituents. The presence of the delayed neutrons, even in such a small fraction, slows down the response time of a reactor system from the range of microseconds to the range of seconds, and therefore makes the problem of reactor control feasible.



**Fig. 3.19** Delayed Neutron Precursor Chain

### 3.7 Energy Production in Fission

The average  $Q$  value for fission is about 180 MeV. This energy appears as kinetic energy of the fission fragments, kinetic energy of fission neutrons, and as prompt  $\gamma$  rays. The balance of the energy obtained in fission is released by the fission products as they decay towards a stable state. A

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summary of the energy released in the fission of  $^{235}\text{U}$  is given in Table 3.3. The amount of energy released by the fission products is a function of the length of time that the reactor has operated. This is because many of the fission product chains require time to build up to saturation levels. After shutdown, all of the chains decay. If  $t$  is the time after shutdown and  $T$  is the time of operation, both in seconds, then an empirical formula for estimating the energy release as a fraction of the original operating power level is the Borst-Wheeler formula

$$f(t) = 0.065 [t^{-0.2} - (t+T)^{-0.2}] \quad (3.11)$$

**Table 3.3**  
Energy Released in Fission

Form	Emitted Energy (MeV)	Recoverable Energy
Fission fragments	168	168
Fission product decay		
$\beta$	8	8
$\gamma$	7	7
neutrinos	12	escape
Prompt $\gamma$	7	7
Fission neutrons	5	5
Capture $\gamma$ rays	-	3-12
Total	207 MeV	198-207 MeV

Note that when a power reactor is shut down after long-term operation, several percent of its operating power is still released initially, requiring some provision for continued cooling.

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### Problems

**3.1** Tables of fission product decay chains and yields for  $^{235}\text{U}$  fission are available in the literature.

- a) Pick the first member of several representative chains with mass numbers between  $A = 72$  and  $A = 161$ , postulate reasonable corresponding fission fragments, and calculate the Coulomb energy  $E_q$  needed to bring the particles together so that they just touch. Use the following approximate equation to calculate the radii of the particles:

$$R = 1.2 \times 10^{-13} A^{1/3} \quad (\text{cm}).$$

- b) Look at the trend of  $E_q$  as fission becomes more asymmetric. Is the observed fission yield versus mass number curve for  $^{235}\text{U}$  consistent with this trend? Explain.

**3.2** Define, describe, and discuss the important consequences to reactor physics of the following two topics, giving as many examples as you can:

- a) Spin-pairing;
- b) Magic numbers;

**3.3** Show that the fission spectrum  $\chi(E)$  is normalized to unity, and calculate the average energy and most probable energy of the fission neutrons in the following spectra:

- a) Maxwellian spectrum;
- b) Cranberg-Frye spectrum.



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**3.4** Using the data given in Figure 3.14 for  $p(\nu)$  of  $^{235}\text{U}$ , compute the following quantities:

- a)  $\bar{\nu}$ ;
- b)  $\overline{\nu^2}$ ;
- c)  $D(\nu) = \overline{\nu(\nu-1)}/\bar{\nu}^2$ , which is called the Diven parameter, and which appears in formulations of neutron fluctuation "noise" analysis.

**3.5** A power reactor has operated steadily at a thermal power of 3000 MW for one year. Plot the subsequent power release as a function of time over the period of one minute to one month following shutdown for refueling. Comment on the need for cooling the fuel elements.

## References

- R.D. Evans**, *op. cit.*, Chapters 9 and 11.  
**J.R. Lamarsh**, *op. cit.*, Chapter 3.

## NUCLEAR REACTOR THEORY AND DESIGN

## DERIVATION OF THE NEUTRON DIFFUSION EQUATION

There are two different ways to derive the neutron diffusion equation. The most straightforward, but approximate, approach is to simply assume that neutrons in a medium diffuse from regions of high concentration to low concentration in a manner similar to the way that heat flows from regions of high temperature to low temperature. A simple model is used to calculate the diffusion coefficient. Then, the equation governing neutron flow is applied to calculate the net leakage from a differential volume element for use in the overall balance equation that we call the diffusion equation.

In order to accomplish the above derivation, several approximations must be made. The basic defect is that neutrons do not simply flow continuously, but rather they travel in straight lines until they collide with an atom, and then they are either captured, or they abruptly change energy and direction. Therefore, we shall next derive the correct integro-differential equation that governs the neutron behavior at any position and in any material composition region in a reactor, and reduce it to the diffusion equation. For simplicity, we shall consider only the case where all of the neutrons have the same speed and do not change energy but only change direction in a scattering collision (the one-group model). In Chapter 6 we will expand our derivation to cover the energy-dependent case that leads to the multigroup diffusion theory model. Our equation will be a neutron balance over a small volume element  $d\mathbf{r}$ , and will have associated with it a term that accounts for each physically

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significant process which takes place, such as neutron transport, absorption, fission, or scattering.

### 4.1 Fick's Law Derivation of the Diffusion Equation

Under certain conditions, the net current of neutrons that flows per second through a unit area normal to the direction of flow is given by Fick's law of diffusion as

$$\vec{J} = -D\nabla\phi, \quad (4.1)$$

where the gradient  $\nabla$  is expressed in Cartesian coordinates as

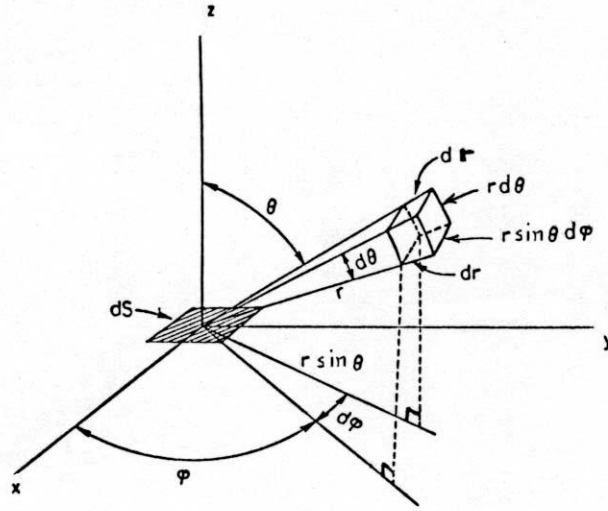
$$\nabla = \vec{i} \frac{\partial}{\partial x} + \vec{j} \frac{\partial}{\partial y} + \vec{k} \frac{\partial}{\partial z}. \quad (4.2)$$

By net current, we mean the difference between the normal projections of all neutron paths that cross the surface going in any direction. The factor of proportionality, called the diffusion coefficient  $D$ , is a function of the material properties of the medium.

We can derive Fick's law for mono-energetic neutrons using a set of fairly restrictive assumptions:

- 1) the medium is infinite in extent;
- 2) the material properties are spatially constant;
- 3) there are no sources present;
- 4) neutron absorption is negligible relative to scattering;
- 5) scattering is isotropic in the LAB system;
- 6) the neutron flux varies slowly with position;
- 7) there is no time variation of the flux.

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**Fig. 4.1** Calculation of Neutron Current Density

We shall first calculate the  $z$ -component of the current,  $J_z$ , and then generalize to the net current  $\vec{J}$ . Consider a small area  $dS$  lying in the  $x$ - $y$  plane of the coordinate system shown in Figure 4.1. Neutrons scatter in the volume element  $d\mathbf{r}$  at the rate of  $\Sigma_s \phi(\vec{r}) d\mathbf{r}$  per second. These neutrons are assumed to be scattered isotropically into a sphere centered about  $d\mathbf{r}$  such that the un-collided number that would cross the surface of the sphere at a radius  $r$ , corresponding to the distance to  $dS$ , is inversely proportional to the surface area  $4\pi r^2$ . Unfortunately,  $dS$  is not perpendicular to the radius of this sphere, so that the potential fraction actually crossing  $dS$  is based on the projection of  $dS$  along  $r$ , namely,

$$[\text{fraction}] = \frac{dS \cos \theta}{4\pi r^2}.$$

But not all of these neutrons reach  $dS$ . Because of scattering, the fraction  $e^{-\Sigma_s r}$  scatters to another direction. We ignore multiple scattering.

As seen in Figure 4.1, the differential volume element in

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spherical coordinates is

$$dr = r^2 \sin \theta dr d\theta d\psi. \quad (4.3)$$

The total number of neutrons that pass through the area  $dS$  in the negative direction is the integral of all possible downward contributions from the entire upper half plane, or

$$J \cdot dS = \frac{dS}{4\pi} \sum_s \int_0^\infty \int_0^{2\pi} \int_0^{\pi/2} \phi e^{-\Sigma_s r} \cos \theta \sin \theta d\theta d\psi dr. \quad (4.4)$$

In order to evaluate this integral, the flux must be known as a function of position. We make the approximation that the flux varies slowly with position, even though the distance is not differentially small, such that the flux at any point  $\vec{r}$  can be expressed in terms of flux at the position of  $dS$  by the truncated Taylor series expansion

$$\phi(x,y,z) = \phi_o + x \left( \frac{\partial \phi}{\partial x} \right)_o + y \left( \frac{\partial \phi}{\partial y} \right)_o + z \left( \frac{\partial \phi}{\partial z} \right)_o + \dots, \quad (4.5)$$

The independent variables may be expressed in spherical coordinates by the expressions

$$x = r \sin \theta \cos \psi$$

$$y = r \sin \theta \sin \psi \quad (4.6)$$

$$z = r \cos \theta.$$

When Eq. (4.5) is inserted into Eq. (4.4), and the integral over  $d\psi$  is performed over the range of 0 to  $2\pi$ , one finds that the  $x$  and  $y$  contributions are zero due to symmetry. The remaining two terms can be evaluated to obtain the expression

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$$\begin{aligned}
 J_- &= \frac{\Sigma_s}{4\pi} \left[ \phi_o \int_0^\infty \int_0^{2\pi} \int_0^{\pi/2} e^{-\Sigma_s r} \cos\theta \sin\theta \, d\theta \, d\psi \, dr \right. \\
 &\quad \left. + \left( \frac{\partial\phi}{\partial z_o} \right) \int_0^\infty \int_0^{2\pi} \int_0^{\pi/2} r e^{-\Sigma_s r} \cos^2\theta \sin\theta \, d\theta \, d\psi \, dr \right] \\
 &= \frac{\phi_o}{4} + \frac{1}{6\Sigma_s} \left( \frac{\partial\phi}{\partial z} \right)_o.
 \end{aligned} \tag{4.7}$$

A similar integration can be performed over the lower half plane to give the number of neutrons that pass upward through  $dS$  in the positive direction. The integration over  $\theta$  proceeds from  $\pi/2$  to  $\pi$ , giving the expression

$$J_+ = \frac{\phi_o}{4} - \frac{1}{6\Sigma_s} \left( \frac{\partial\phi}{\partial z} \right)_o. \tag{4.8}$$

The net current  $J_z$  in the positive  $z$ -direction is the difference between  $J_+$  and  $J_-$ , or

$$J_z = J_+ - J_- = -\frac{1}{3\Sigma_s} \left( \frac{\partial\phi}{\partial z} \right)_o. \tag{4.9}$$

Similar expressions are obtained for  $J_x$  and  $J_y$ . These may be added together vectorially to give Fick's law in the form

$$\begin{aligned}
 \vec{J} &= \vec{i} J_x + \vec{j} J_y + \vec{k} J_z \\
 &= \frac{1}{3\Sigma_s} \left[ \vec{i} \frac{\partial\phi}{\partial x} + \vec{j} \frac{\partial\phi}{\partial y} + \vec{k} \frac{\partial\phi}{\partial z} \right] = -D\nabla\phi,
 \end{aligned} \tag{4.10}$$

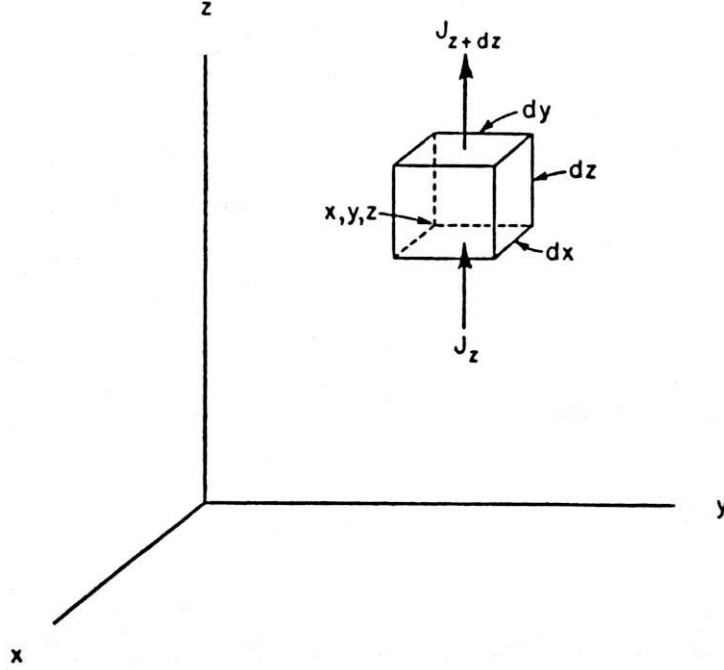
where the diffusion coefficient in this approximation is defined as

$$D \equiv \frac{1}{3\Sigma_s}.$$

In Section 4.5 a similar expression, with a somewhat modified

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form of the diffusion coefficient, is obtained from the transport derivation.



**Fig 4.2** Calculation of Neutron Leakage

We now consider the neutron balance in the volume element shown in Figure 4.2. The net leakage of neutrons out of the region in the positive z-direction is the difference between the net currents entering and leaving in that direction, or

$$(J_{z+dz} - J_z) dx dy = -D \left[ \left( \frac{\partial \phi}{\partial z} \right)_{z+dz} - \left( \frac{\partial \phi}{\partial z} \right)_z \right] dx dy. \quad (4.11)$$

A truncated Taylor's series expansion of the derivative of the flux at  $z + dz$  can be made in terms of the derivative of the flux at  $z$ . This expansion, which is consistent with that made for the flux itself, is

$$\left( \frac{\partial \phi}{\partial z} \right)_{z+dz} = \left( \frac{\partial \phi}{\partial z} \right)_z + \left( \frac{\partial^2 \phi}{\partial z^2} \right)_z dz + \dots \quad (4.12)$$



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When Eq. (4.12) is inserted into Eq. (4.11), the result is,

$$\left[ \begin{array}{c} \text{Net leakage in the} \\ z\text{-direction} \end{array} \right] = -D \frac{\partial^2 \phi}{\partial z^2} dx dy dz. \quad (4.13)$$

Similar expressions are obtained in the x and y directions, leading to an expression for the total leakage of the form

$$\left[ \begin{array}{c} \text{Neutron leakage per unit} \\ \text{volume per second} \end{array} \right] = -D \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right) = -D \nabla^2 \phi, \quad (4.14)$$

where  $\nabla^2$  is the Laplacian operator.

The diffusion equation is the equation that describes the total neutron balance in the volume element  $d\mathbf{r} = dx dy dz$ . When all of the possible contributions in the one-speed case are included, we obtain the equation

$$\text{rate of change} = \text{source} - \text{fission} - \text{absorption} - \text{leakage} \quad (4.15)$$

$$\frac{1}{v} \frac{\partial \phi}{\partial t} = S + \nu \sum_f \phi - \sum_a \phi + D \nabla^2 \phi.$$

Note that there is a theoretical *contradiction* here, since the leakage was derived in the *absence* of sources, absorption and time-dependence of the spatial flux.

In order to solve the diffusion equation, two boundary conditions are needed. Heuristically, we will assume that the flux must be continuous everywhere, since otherwise it would not be slowly varying, which was a condition used in deriving Fick's Law. For the second boundary condition, we will assume that the current  $\vec{J}$  is also continuous, since in the absence of sources those neutrons that enter a surface area must leave on the other side.

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### 4.2\* The One-Speed Transport Equation

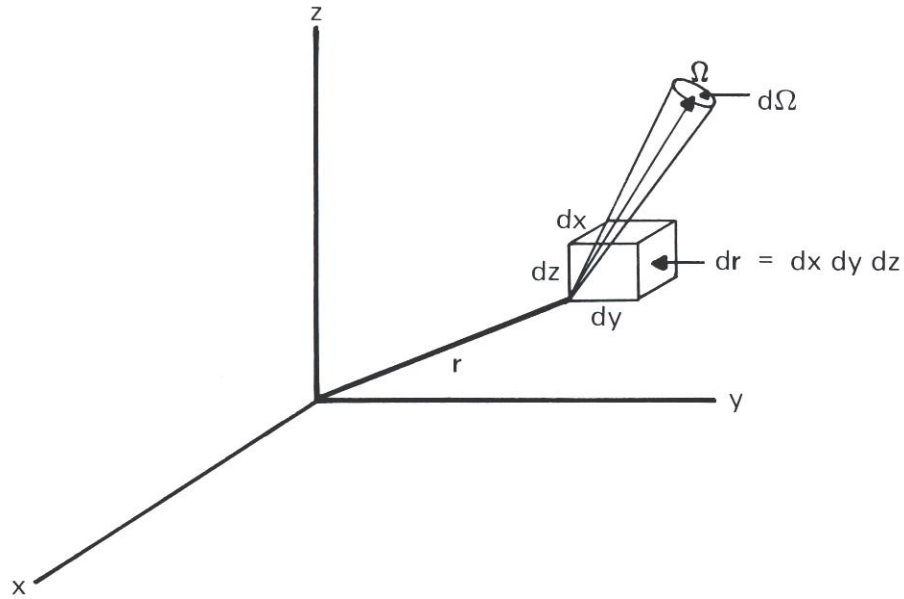
In the context of the one-speed model, the quantity  $n(\vec{r}, \vec{\Omega}, t) d\vec{r} d\vec{\Omega}$  is the total number of neutrons in a volume element  $d\vec{r}$  about  $\vec{r}$ , traveling in direction  $d\vec{\Omega}$  about  $\vec{\Omega}$ , at time  $t$ . In Cartesian coordinates, the situation is as depicted in Figure 4.3.

Associated with the neutron density is the angular neutron flux, which is given by the expression

$$\Phi(\vec{r}, \vec{\Omega}, t) = v n(\vec{r}, \vec{\Omega}, t). \quad (4.16)$$

A related quantity is the directed neutron flux, which is obtained by multiplying the angular neutron flux by the direction vector  $\vec{\Omega}$ , i.e.,

$$\vec{\Phi}(\vec{r}, \vec{\Omega}, t) = \vec{\Omega} \Phi(\vec{r}, \vec{\Omega}, t). \quad (4.17)$$



**Fig. 4.3** Neutron Density in Cartesian Coordinates

The macroscopic cross sections at position  $\vec{r}$  are related by the

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expression

$$\Sigma_T(\vec{r}) = \Sigma_s(\vec{r}) + \Sigma_a(\vec{r}),$$

where  $\Sigma_T$  is the total cross section,  $\Sigma_s$  contains both elastic and inelastic scattering, and  $\Sigma_a$  contains both capture and fission. Recall that the total scattering cross section is the integral over the differential angular scattering cross section, i.e.,

$$\Sigma_s = \int_{all \Omega} \Sigma_s(\vec{\Omega}) d\Omega.$$

Beginning with an element of phase space defined as

$$d\tau = dr d\Omega,$$

we define our balance equation in words as

$$\left[ \begin{array}{l} \text{rate of change} \\ \text{of neutrons in } d\tau \end{array} \right] = \left[ \begin{array}{l} \text{production} \\ \text{rate in } d\tau \end{array} \right] - \left[ \begin{array}{l} \text{loss rate} \\ \text{in } d\tau \end{array} \right]. \quad (4.18)$$

The production rate term includes neutrons produced by independent sources (e.g., a plutonium-beryllium source), neutrons scattered elastically or inelastically into the direction  $d\Omega$  about  $\vec{\Omega}$  from any other direction  $\vec{\Omega}'$ , and neutrons produced by fission, which are assumed to appear at the site of the fission event. The loss rate is due to the absorption processes of capture and fission, and is also due to streaming across the faces of the volume element without collision (i.e., leakage). We also include all scattering processes that take a neutron out of the direction  $d\Omega$  about  $\vec{\Omega}$  and send it into any other direction  $\vec{\Omega}'$ .

Probably the most complicated term is the leakage term, which will be treated first. We will work with only one Cartesian direction at a time and then sum the results into a

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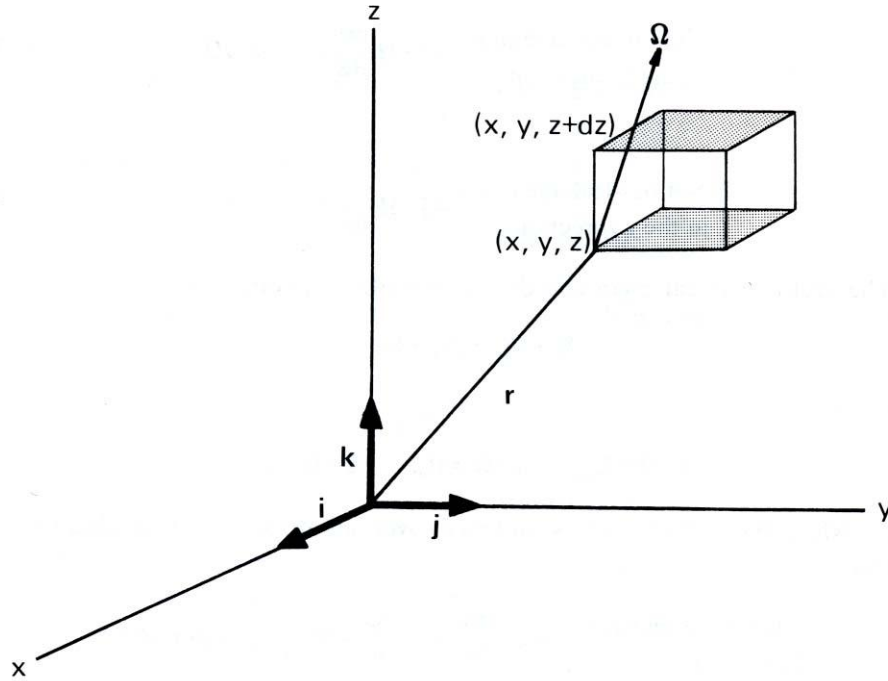
vector form. The result will, in fact, be valid for any coordinate system. It is convenient at this point to redraw the volume element so as to emphasize the faces of the cube in the  $z$  direction, as shown in Figure 4.4.

The number of neutrons going in the direction  $d\Omega$  about  $\vec{\Omega}$  that cross into the volume element  $d\mathbf{r}$  per second through the lower surface  $dS = dx dy$  is given by the projection of the vector flux in the  $z$  direction, namely,

$$\vec{k} \cdot \vec{\Omega} \Phi(x, y, z, \vec{\Omega}, t) dx dy d\Omega$$

The number leaving the top surface is similarly given by the expression

$$\vec{k} \cdot \vec{\Omega} \Phi(x, y, z + dz, \vec{\Omega}, t) dx dy d\Omega$$



**Fig. 4.4** Leakage Component in the  $z$ -direction

The net out-leakage, which we want to include in the neutron

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balance as a loss term, is the net of the number leaving minus the number entering, i.e.,

$$\left[ \begin{array}{c} \text{Out-leakage rate in} \\ \text{the } z \text{ direction} \end{array} \right] = \vec{k} \bullet \vec{\Omega} [\Phi((x,y,z+dz,\vec{\Omega},t) - \Phi(x,y,z,\vec{\Omega},t))] dx dy d\Omega. \quad (4.19)$$

We expand the first term in a Taylor series and truncate it to the order of  $dz$ , giving the approximation

$$\Phi(x,y,z+dz,\vec{\Omega},t) = \Phi(x,y,z,\vec{\Omega},t) + \frac{\partial \Phi(x,y,z,\vec{\Omega},t)}{\partial z} dz + O(dz)^2. \quad (4.20)$$

We then insert this expression into the equation for out-leakage to obtain

$$\left[ \begin{array}{c} \text{Net out-leakage rate} \\ \text{in the } z \text{ direction} \end{array} \right] = \vec{k} \bullet \vec{\Omega} \frac{\partial \Phi(x,y,z,\vec{\Omega},t)}{\partial z} dx dy dz d\Omega. \quad (4.21)$$

Likewise, for the  $x$  and  $y$  directions we obtain the contributions

$$\left[ \begin{array}{c} \text{Net out-leakage rate} \\ \text{in the } x \text{ direction} \end{array} \right] = \vec{i} \bullet \vec{\Omega} \frac{\partial \Phi}{\partial x} dx dy dz d\Omega, \quad (4.22)$$

and

$$\left[ \begin{array}{c} \text{Net out-leakage rate} \\ \text{in the } y \text{ direction} \end{array} \right] = \vec{j} \bullet \vec{\Omega} \frac{\partial \Phi}{\partial y} dx dy dz d\Omega. \quad (4.23)$$

The vector  $\vec{\Omega}$  in Cartesian coordinates is written in components as

$$\vec{\Omega} = \vec{i} \Omega_x + \vec{j} \Omega_y + \vec{k} \Omega_z.$$

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Note that:

$$\vec{i} \cdot \vec{\Omega} = \Omega_x, \quad \vec{j} \cdot \vec{\Omega} = \Omega_y, \quad \vec{k} \cdot \vec{\Omega} = \Omega_z.$$

Hence, when the out-leakage is summed over all directions, one obtains the quantity

$$\begin{aligned} \left[ \begin{array}{c} \text{Total out-leakage} \\ \text{rate in } d\tau \end{array} \right] &= (\Omega_x \frac{\partial \Phi}{\partial x} + \Omega_y \frac{\partial \Phi}{\partial y} + \Omega_z \frac{\partial \Phi}{\partial z}) dx dy dz d\Omega \\ &= \vec{\Omega} \cdot \nabla \Phi(x, y, z, \vec{\Omega}, t) dx dy dz d\Omega \\ &= \vec{\Omega} \cdot \nabla \Phi(\vec{r}, \vec{\Omega}, t) d\vec{r} d\Omega, \end{aligned} \quad (4.24)$$

which is a vector form that is valid for any coordinate system.

The loss rate term due to collisions of all types is simply:

$$\left[ \begin{array}{c} \text{Loss rate in } d\tau \text{ due to} \\ \text{absorption and outscatter} \end{array} \right] = (\Sigma_s + \Sigma_a) \Phi(x, y, z, \vec{\Omega}, t) dx dy dz d\Omega \quad (4.25)$$

$$= \Sigma_T(\vec{r}) \Phi(\vec{r}, \vec{\Omega}, t) d\vec{r} d\Omega.$$

We include the total scattering cross section because we are interested in all scattering out of  $\vec{\Omega}$  into any other direction.

The production rate due to in-scattering is somewhat more complicated. Here we must include scattering of neutrons going in any direction  $\vec{\Omega}'$  where the scattered neutron ends up in the interval  $d\Omega$  about direction  $\vec{\Omega}$ . This process is governed by the differential angular scattering cross section between the two angles, which we call the transference function. We must sum over all such starting angles  $\vec{\Omega}'$ , i.e., we write the integral

$$\left[ \begin{array}{c} \text{Production rate in } d\tau \text{ due} \\ \text{to inscatter from } \vec{\Omega}' \end{array} \right] = \int_{\text{all } \vec{\Omega}'} \Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(\vec{r}, \vec{\Omega}', t) d\Omega' d\vec{r} d\Omega. \quad (4.26)$$

Fission assumes a similar form in the one-speed approximation, where we neglect the fact that the fission neutrons have an energy spectrum and only account for the average

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number of neutrons produced per fission,  $\nu$ . Hence, the fission term is

$$\left[ \begin{array}{c} \text{Production rate in } d\tau \\ \text{due to fission} \end{array} \right] = \int_{\text{all } \vec{\Omega}} \sum_f (\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(\vec{r}, \vec{\Omega}', t) d\Omega' d\vec{r} d\Omega. \quad (4.27)$$

The source rate is given very simply by the term

$$\left[ \begin{array}{c} \text{Source rate} \\ \text{in } d\tau \end{array} \right] = S(\vec{r}, \vec{\Omega}, t) d\vec{r} d\Omega. \quad (4.28)$$

Finally, the rate of change of the neutron density in  $d\tau$  is given by the expression

$$\begin{aligned} \left[ \begin{array}{c} \text{Rate of change of} \\ \text{neutron density in } d\tau \end{array} \right] &= \frac{\partial n(\vec{r}, \vec{\Omega}, t)}{\partial t} d\vec{r} d\Omega \\ &= \frac{1}{\nu} \frac{\partial \phi(\vec{r}, \vec{\Omega}, t)}{\partial t} d\vec{r} d\Omega. \end{aligned} \quad (4.29)$$

Combining all of the above contributions to the balance equation, we obtain the following equation after cancellation of the differential elements  $d\vec{r} d\Omega$  that appear in each term:

$$\begin{aligned} \frac{1}{\nu} \frac{\partial \Phi(\vec{r}, \vec{\Omega}, t)}{\partial t} &= S(\vec{r}, \vec{\Omega}, t) + \int_{\text{all } \vec{\Omega}'} \sum_s (\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(\vec{r}, \vec{\Omega}', t) d\Omega' \\ &+ \int_{\text{all } \vec{\Omega}'} \sum_f (\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(\vec{r}, \vec{\Omega}', t) d\Omega' \\ &- \sum_T (\vec{r}) \Phi(\vec{r}, \vec{\Omega}, t) - \vec{\Omega} \cdot \nabla \Phi(\vec{r}, \vec{\Omega}, t). \end{aligned} \quad (4.30)$$

This is known as the one-speed neutron transport equation, or the Boltzmann equation. As a point of interest, this equation corresponds to the Eulerian interpretation as found in fluid mechanics. If one takes the Lagrangian interpretation of moving along with the vector field, one can combine the rate of change and leakage terms into what is known as the total derivative,

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defined as

$$\frac{Dn}{Dt} \equiv \frac{\partial n}{\partial t} + v\vec{\Omega} \cdot \nabla n,$$

and rewrite the balance equation accordingly.

### 4.3\* One-Dimensional, One-speed Transport Equation

It is possible to proceed directly towards the reduction of the Boltzmann equation to the diffusion equation using vector operators and expansions. At this point we will avoid most of the detailed mathematics by treating a fairly straightforward special case that illustrates the steps that need to be taken and the proper form of the general result. We will use only the first two terms of a series expansion for the flux, and these will be written out explicitly.

We look at the case where the system is infinite in both the x and y directions so that the only variation of interest occurs in the z direction. We redraw our Cartesian coordinate system so as to explicitly show the components of the vector  $\vec{\Omega}$ , as illustrated in Figure 4.5. In terms of our previous notation, the angular components are

$$\Omega_x = \sin\theta \cos\psi, \quad \Omega_y = \sin\theta \sin\psi, \quad \Omega_z = \cos\theta.$$

Looking at the leakage term, we rewrite this expression as

$$\vec{\Omega} \cdot \nabla \Phi = \Omega_x \frac{\partial \Phi}{\partial x} + \Omega_y \frac{\partial \Phi}{\partial y} + \Omega_z \frac{\partial \Phi}{\partial z}.$$

But  $\frac{\partial \Phi}{\partial x} = \frac{\partial \Phi}{\partial y} = 0$  for this special case, and  $\cos\theta = \mu$ . Hence, the vector operation in the leakage term is reduced to the scalar form



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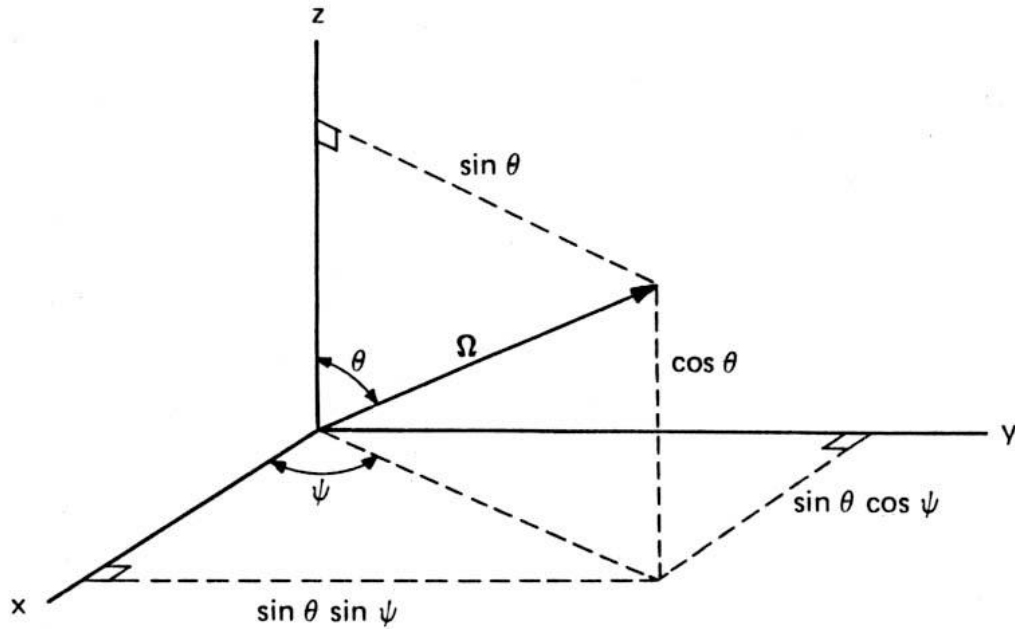
$$\vec{\Omega} \cdot \nabla \Phi(\vec{r}, \vec{\Omega}) = \mu \frac{\partial \Phi(z, \vec{\Omega})}{\partial z}. \quad (4.31)$$

Next, notice that the flux in the one-dimensional model is not dependent upon the azimuthal angle  $\psi$  but only on the polar angle  $\theta$  (i.e.,  $\mu$ ) as shown in Figure 4.6. We take advantage of this rotational symmetry. We therefore integrate the transport equation over the azimuthal angle  $\psi$  by applying the operator  $\int_0^{2\pi} d\psi$  separately to each term of the equation. We make the following definitions:

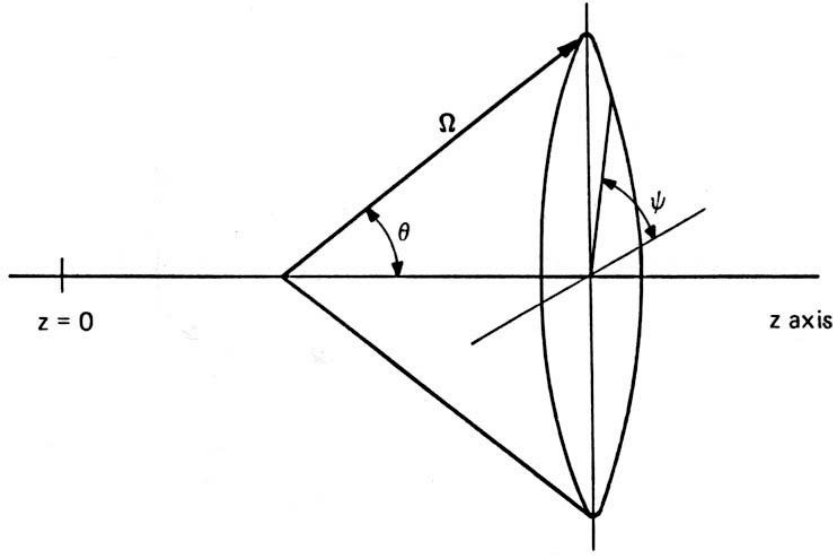
$$\int_0^{2\pi} \Phi(z, \vec{\Omega}) d\psi \equiv \Phi(z, \mu) \quad (4.32)$$

and

$$\int_0^{2\pi} S(z, \vec{\Omega}) d\psi \equiv S(z, \mu). \quad (4.33)$$



**Fig. 4.5** Cartesian components of  $\vec{\Omega}$



**Fig. 4.6** Directional Dependence of  $\vec{\Omega}$  in the One-Dimensional Case

Upon integration over the rotational angle, the Boltzmann equation is reduced to the following form:

$$\begin{aligned} & \frac{1}{v} \frac{\partial \Phi(z, \mu)}{\partial t} + \mu \frac{\partial \Phi(z, \mu)}{\partial z} + \Sigma_T(z) \Phi(z, \mu) \\ &= S(z, \mu) + \int_0^{2\pi} d\psi \int_{all \vec{\Omega}'} \Sigma_s(\vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(z, \vec{\Omega}') d\Omega' \\ &+ \int_0^{2\pi} d\psi \int_{all \vec{\Omega}'} \Sigma_f(\vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(z, \vec{\Omega}') d\Omega'. \end{aligned} \quad (4.34)$$

Note that the  $\vec{\Omega}$  dependence still remains in the integral terms so that further reduction is necessary.

The transference cross sections are normally not dependent upon the values of the vectors  $\vec{\Omega}$  and  $\vec{\Omega}'$ , but only upon the polar angle  $\theta_0$  between them. Making use of rotational symmetry, we can write these terms as

$$\Sigma_s(z, \vec{\Omega}' \rightarrow \vec{\Omega}) = \Sigma_s(z, \vec{\Omega}' \cdot \vec{\Omega}) = \Sigma_s(z, \mu_0)/2\pi$$

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and

$$\Sigma_f(z, \vec{\Omega}' \rightarrow \vec{\Omega}) = \Sigma_f(z, \vec{\Omega}' \bullet \vec{\Omega}) = \Sigma_f(z, \mu_o)/2\pi,$$

where  $\mu_o$  is defined as  $(\vec{\Omega}' \bullet \vec{\Omega}) \equiv \mu_o = \cos \theta_o$ . Furthermore, the fission cross section is usually isotropic in the laboratory system and has the form  $\Sigma_f(z, \vec{\Omega}' \bullet \vec{\Omega}) = \nu \Sigma_f(z)/4\pi$ . Noting that  $d\Omega' = -d\mu' d\psi'$ , we see that the fission integral becomes

$$\int_0^{2\pi} d\psi \int_0^{2\pi} \int_{-1}^1 \frac{\nu \Sigma_f(z)}{4\pi} \Phi(z, \vec{\Omega}') d\mu' d\psi' = \frac{\nu \Sigma_f(z)}{2} \int_{-1}^1 \Phi(z, \mu') d\mu', \quad (4.35)$$

where use has been made of the definition of  $\Phi(z, \mu)$  given by Eq. (4.32).

In order to proceed further with the scattering transference function we need to do two things:

1. expand the actual cross-section data in a convenient angular series; and
2. find a relationship between  $\mu_o$  and  $\mu$ ,  $\mu'$ ,  $\psi$  and  $\psi'$ .

As a first approximation for the elastic and inelastic scattering terms we try an expansion in terms of Legendre polynomials. These are natural functions for the system under consideration because the Legendre polynomials are functions of  $\mu$  and are orthogonal over the range of  $-1 < \mu < +1$ . We truncate after the first two terms (this is an arbitrary choice) and therefore write

$$\Sigma_s(z, \vec{\Omega}' \rightarrow \vec{\Omega}) = \frac{\Sigma_s(z, \mu_o)}{2\pi} \approx \frac{1}{2\pi} \left[ \frac{\Sigma_{s0}(z)}{2} + \frac{3\mu_o \Sigma_{s1}(z)}{2} \right], \quad (4.36)$$

which comes from the first two terms of the general expansion

$$\Sigma_s(z, \mu_o) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_{\ell}(\mu_o) \Sigma_{s\ell}(z), \quad (4.37)$$

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where

$$\begin{aligned} P_0(\mu_o) &= 1, \\ P_1(\mu_o) &= \mu_o, \\ P_2(\mu_o) &= \frac{1}{2}(3\mu_o^2 - 1), \\ P_3(\mu_o) &= \frac{1}{2}(5\mu_o^3 - 3\mu_o), \end{aligned}$$

*etc.*

The Legendre polynomials also obey the recursion relationship

$$\mu_o P_n(\mu_o) = \frac{1}{2n+1} [(n+1)P_{n+1}(\mu_o) + nP_{n-1}(\mu_o)].$$

The factor  $1/2\pi$  is included because the cross sections are assumed to possess rotational symmetry.

The orthogonality property of Legendre polynomials states that

$$\int_{-1}^1 P_m(\mu_o) P_\ell(\mu_o) d\mu_o = \frac{2}{2\ell+1} \delta_{\ell m}, \quad (4.38)$$

where  $\delta_{\ell m}$  is the Kroniker delta. We have experimental data for  $\Sigma_s(\mu_o)$ . We can actually fit this data by choosing the coefficients  $\Sigma_{s1}$  properly. Hence, the  $\Sigma_{s1}$  values can be considered to be known data. An interpretation of the terms follows by multiplying Eq. (4.37) by  $P_1(\mu_o)$  and integrating over  $\mu_o$  for  $l = 0, \dots, n$ . For  $l = 0$ ,

$$\Sigma_{s0} = \int_{-1}^1 \Sigma_s(\mu_o) d\mu_o = \Sigma_s, \quad (4.39)$$

which is the total scattering cross section.

For  $l = 1$ ,

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$$\Sigma_{sl} = \int_{-1}^{+1} \mu_o \Sigma_s(\mu_o) d\mu_o = \bar{\mu}_o \Sigma_s, \quad (4.40)$$

which is proportional to the total scattering cross section since the average cosine of the scattering angle for a single atom species is defined as

$$\bar{\mu}_o \equiv \frac{\int_{all \Omega} \sigma_s(\theta_o) \cos \theta_o d\Omega}{\int_{all \Omega} \sigma_s(\theta_o) d\Omega} = \frac{\int_{-1}^{+1} \mu_o \sigma_s(\mu_o) d\mu_o}{\sigma_s}. \quad (4.41)$$

This is the place where  $\bar{\mu}_o$  enters naturally into the transport equation. Of course, for a mixture of atom species, an appropriate average  $\bar{\mu}_o$  must be used.

Now we need a transformation between  $\mu_o$  and the actual angle cosines  $\mu'$  and  $\mu$ . Recall the definition of  $\mu_o$ :

$$\begin{aligned} \mu_o &= \vec{\Omega}' \bullet \vec{\Omega} = (\vec{i} \sin \theta' \cos \psi' + \vec{j} \sin \theta' \sin \psi' + \vec{k} \cos \theta') \\ &\quad \bullet (\vec{i} \sin \theta \cos \psi + \vec{j} \sin \theta \sin \psi + \vec{k} \cos \theta) \\ &= (\sin \theta \sin \theta' \cos(\psi - \psi') + \mu \mu'). \end{aligned} \quad (4.42)$$

This result is a simplified form of a more general expression known as the addition theorem for Legendre functions. (See Appendix D.)

We use the foregoing terms in the scattering integral to obtain

$$\int_0^{2\pi} \int_0^{2\pi} \int_{-1}^{+1} \left[ \frac{\Sigma_{so}(z)}{4\pi} + \frac{3\Sigma_{sl}(z)}{4\pi} \{ \mu \mu' + \sin \theta \sin \theta' \cos(\psi - \psi') \} \right] \Phi(z, \vec{\Omega}') d\mu' d\psi' d\psi. \quad (4.43)$$

The first term in the square brackets is treated easily and gives

$$\int_0^{2\pi} \int_0^{2\pi} \int_{-1}^{+1} \frac{\Sigma_{so}(z)}{4\pi} \Phi(z, \vec{\Omega}') d\mu' d\psi' d\psi = \frac{\Sigma_{so}}{2} \int_{-1}^{+1} \Phi(z, \mu') d\mu'. \quad (4.44)$$

The second term in the square brackets simplifies considerably by

noting that

$$\int_0^{2\pi} \cos(\psi - \psi') d\psi' = 0.$$

The balance of the expression is therefore

$$\begin{aligned} & \int_0^\pi \int_0^\pi \int_{-1}^1 \frac{3 \Sigma_{sl}(z)}{4\pi} \mu \mu' \Phi(z, \bar{\Omega}') d\mu' d\psi' d\psi \\ &= \frac{3\mu \Sigma_{sl}(z)}{2} \int_{-1}^1 \mu' \Phi(z, \mu') d\mu'. \end{aligned} \quad (4.45)$$

Putting all of the terms together, the final form of the one-dimensional, one-speed Boltzmann transport equation is

$$\frac{I}{v} \frac{\partial \Phi(z, \mu)}{\partial t} + \mu \frac{\partial \Phi(z, \mu)}{\partial z} + \Sigma_T(z) \Phi(z, \mu) = \frac{\nu \Sigma_f(z)}{2} \int_{-1}^1 \Phi(z, \mu') d\mu' \quad (4.46)$$

$$+ \frac{\sum_{so}(z)}{2} \int_{-1}^{+1} \Phi(z, \mu') d\mu' + \frac{3 \sum_{sl}(z) \mu}{2} \int_{-1}^{+1} \mu' \Phi(z, \mu') d\mu' + S(z, \mu).$$

Note that the entire equation has been reduced considerably. There are no vector terms, and the angular dependence is no worse than the product of  $\mu$  and  $\Phi(z, \mu)$ . But there are still flux integrals. To proceed further, we must simplify the flux and source terms by yet another expansion.

#### 4.4\* Derivation of the $P_1$ Equations

We now have a form of the one-speed, one-dimensional Boltzmann transport equation that is considerably simpler than

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our previous equation but is still difficult to solve. There are three possible approaches.

1. Separation of variables - This is a use of Case's method of singular eigenfunctions, which will give exact solutions to certain simple problems when one does a great deal of difficult mathematical manipulation. This is not the most practical solution method.
2. Discretization of the angular variable into several discrete directions, followed by numerical solution - This is the discrete ordinates or  $S_n$  method that is widely used in industry.
3. Reduction of the equations by further expansion in Legendre polynomials - These are the  $P_n$  methods that lead to diffusion theory and higher-order solutions. The resulting equations are often discretized in space and solved numerically.

We proceed with the third approach to the problem. Note that the source terms are known functions while the flux terms are the unknowns to be determined.

We make an expansion of the source and the flux in the same Legendre form that enabled simplification of the transport equation. Let the known source be written as

$$S(z, \mu) = \frac{1}{2} S_0(z) + \frac{3}{2} \mu S_1(z). \quad (4.47)$$

Again, we fit the coefficients  $S_0$  and  $S_1$  to the actual data. The physical interpretation of the terms is obtained by successively

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multiplying Eq. (4.47) by  $P_1(\mu)$  and integrating over  $\mu$ . For  $l = 0$ ,

$$\int_{-1}^{+1} S(z, \mu) d\mu = S_o(z), \quad (4.48)$$

which is the total source at  $z$ .

For  $l = 1$ ,

$$\int_{-1}^{+1} \mu S(z, \mu) d\mu = S_1(z), \quad (4.49)$$

which is the total source current in the  $z$  direction at  $z$ .

The unknown flux is expanded similarly as

$$\Phi(z, \mu) \approx \frac{l}{2} \phi_o(z) + \frac{3}{2} \mu \phi_1(z). \quad (4.50)$$

The physical interpretation for  $l = 0$  is

$$\int_{-1}^{+1} \Phi(z, \mu) d\mu = \phi_o(z), \quad (4.51)$$

which is the total flux at  $z$ .

For  $l = 1$ ,

$$\int_{-1}^{+1} \mu \Phi(z, \mu) d\mu = \phi_1(z) \equiv J(z), \quad (4.52)$$

which is the net neutron current in the  $z$  direction at  $z$ . Note that the current is directed along the axis, which implies that it is a *vector* quantity. The balance equation with the two-term source and flux expansion is the following:



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*rate of change*

*leakage*

*removal*

$$\frac{1}{v} \left( \frac{1}{2} \frac{\partial \phi_o}{\partial t} + \frac{3\mu}{2} \frac{\partial \phi_l}{\partial t} \right) + \left( \frac{\mu}{2} \frac{\partial \phi_o}{\partial z} + \frac{3\mu^2}{2} \frac{\partial \phi_l}{\partial z} \right) + \left( \frac{1}{2} \Sigma_T \phi_o + \frac{3}{2} \mu \Sigma_T \phi_l \right)$$

*source*

*fission*

$$= \left( \frac{1}{2} S_o + \frac{3}{2} \mu S_l \right) + \frac{1}{2} v \Sigma_f \int_{-1}^{+1} \left( \frac{1}{2} \phi_o + \frac{3}{2} \mu' \phi_l \right) d\mu' \quad (4.53)$$

*isotropic*

*anisotropic*

*inscatter*

*inscatter*

$$+ \frac{1}{2} \Sigma_{so} \int_{-1}^{+1} \left( \frac{1}{2} \phi_o + \frac{3}{2} \mu' \phi_l \right) d\mu' + \frac{3}{2} \Sigma_{sl} \mu \int_{-1}^{+1} \left( \frac{1}{2} \mu' \phi_o + \frac{3}{2} \mu'^2 \phi_l \right) d\mu'.$$

Since we have two unknowns,  $\phi_o(z)$  and  $\phi_l(z)$ , we need two equations. These are obtained by successively multiplying Eq. (4.53) by  $P_0(\mu)$  and  $P_1(\mu)$  and integrating over  $\mu$ . For  $l = 0$ , using the orthogonality of the Legendre polynomials, we obtain

$$\frac{1}{v} \frac{\partial \phi_o}{\partial t} + \frac{\partial \phi_l(z)}{\partial z} + \Sigma_T \phi_o(z) = S_o(z) + v \Sigma_f \phi_o(z) + \Sigma_{so} \phi_o(z). \quad (4.54)$$

For  $l = 1$ , we obtain

$$\frac{1}{v} \frac{\partial \phi_l}{\partial t} + \frac{1}{3} \frac{\partial \phi_o(z)}{\partial z} + \Sigma_T \phi_l(z) = S_l(z) + \Sigma_{sl} \phi_l(z). \quad (4.55)$$

If the flux expansion had been carried out to more terms, say  $l = 3$ , we would have repeated the above process by weighting by  $P_2(\mu)$  and  $P_3(\mu)$  to obtain a total of four equations in four unknowns. Note that the source and cross sections need not be expanded to the same order as the flux.

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Once we solve the coupled set of equations for the terms  $\phi_o(z)$ ,  $\phi_1(z)$ , etc., we can reconstruct the angular flux  $\Phi(z, \mu)$  from the defining expansion given by Eq. (4.50). In order to solve the equations, we need boundary conditions at the outer surfaces. The spatial boundary condition on the original Boltzmann equation is that the angular flux  $\Phi(z, \mu)$  is continuous across the boundary (i.e., any neutron that leaves the surface going in direction  $\mu$  arrives in the other region). The corresponding  $P_n(\mu)$  boundary conditions are:

$$\begin{aligned}\phi_o(z) & \text{ is continuous;} \\ \phi_1(z) & \text{ is continuous;} \\ & \text{etc.}\end{aligned}$$

### 4.5 The $P_1$ Diffusion Theory Approximation

If we now write the time-dependent  $P_n$  equations and truncate to order  $n = 1$ , we have the following set:

$$\frac{1}{v} \frac{\partial \phi_o}{\partial t} = S_o + (\Sigma_{so} - \Sigma_T) \phi_o + \nu \Sigma_f \phi_o - \frac{\partial \phi_1}{\partial z} \quad (4.56)$$

and

$$\frac{1}{v} \frac{\partial \phi_1}{\partial t} = S_1 + (\Sigma_{s1} - \Sigma_T) \phi_1 - \frac{1}{3} \frac{\partial \phi_o}{\partial z} - \frac{2}{3} \frac{\partial \phi_2}{\partial z}. \quad (4.57)$$

Note that an extra derivative term appears in the second equation. In order to obtain the diffusion equation, we must make the following additional approximations to the second equation:

1. Neglect the source current,  $S_1(z)$ :
2. Neglect the next higher spatial derivative,  $\partial \phi_2(z) / \partial z$ ;

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3. Neglect the time derivative of the current,  $\partial\phi_1(z)/\partial t$ .

Also recall that

$$\Sigma_{so} = \Sigma_s,$$

$$\Sigma_{sl} = \bar{\mu}_o \Sigma_s,$$

and

$$\Sigma_T = \Sigma_a + \Sigma_s.$$

Inserting these quantities into our two equations, we obtain the expressions

$$\frac{1}{\nu} \frac{\partial \phi_o}{\partial t} = S_o + \nu \Sigma_f \phi_o - \Sigma_a \phi_o - \frac{\partial \phi_l}{\partial z} \quad (4.58)$$

and

$$0 = (\bar{\mu}_o \Sigma_s - \Sigma_T) \phi_l - \frac{1}{3} \frac{\partial \phi_o}{\partial z}. \quad (4.59)$$

We solve Eq. (4.59) for  $\phi_l(z)$ , obtaining

$$\phi_l(z) = - \frac{1}{3(\Sigma_T - \bar{\mu}_o \Sigma_s)} \frac{\partial \phi_o(z)}{\partial z}. \quad (4.60)$$

If we define the  $P_1$  diffusion coefficient as

$$D \equiv \frac{1}{3(\Sigma_T - \bar{\mu}_o \Sigma_s)} = \frac{1}{3\Sigma_{tr}}, \quad (4.61)$$

which is different from that used in Eq. (4.10), we obtain Fick's Law for the total current in the  $z$  direction, namely,

$$\phi_l(z) \equiv J(z) = -D \frac{\partial \phi_o(z)}{\partial z}. \quad (4.62)$$

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Note that we had to ignore three separate quantities, listed above, to obtain this result. The transport cross section  $\Sigma_{tr}$  enters here also.

At this point, we take the spatial derivative of Eq.(4.62) and use it to eliminate the  $\partial\phi_1/\partial z$  term in Eq. (4.58). If D is a function of position, then

$$\frac{\partial\phi_1}{\partial z} = -\frac{\partial}{\partial z}\left(D\frac{\partial\phi_o}{\partial z}\right). \quad (4.63)$$

The insertion of this expression into Eq. (4.58) gives

$$\frac{1}{v}\frac{\partial\phi_o(z)}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial\phi_o}{\partial z}\right) - \Sigma_a\phi_o + \nu\Sigma_f\phi_o + S_o. \quad (4.64)$$

Generalization to three dimensions now leads to the usual form of the Diffusion equation, namely

$$\begin{array}{ccccccc} \text{rate of change} & \text{out-leakage} & \text{absorption} & \text{fission} & \text{source} & & \\ \frac{1}{v}\frac{\partial\phi_o(\vec{r})}{\partial t} & = \nabla \bullet D(\vec{r})\nabla\phi_o(\vec{r}) & - \Sigma_a(\vec{r})\phi_o(\vec{r}) & + \nu\Sigma_f(\vec{r})\phi_o(\vec{r}) & + S_o(\vec{r}), & & \end{array} \quad (4.65)$$

with the associated boundary conditions,

$$\phi_o(\vec{r}) \text{ is continuous across a boundary}$$

and

$$\vec{J}(\vec{r}) = -D(\vec{r})\nabla\phi_o(\vec{r}) \text{ is continuous across a boundary.}$$

When D is independent of position, the leakage term is replaced by

$$[\text{out-leakage}] = -D\nabla^2\phi_o(\vec{r}).$$

Note that scattering enters the one-speed balance equation only in the leakage term because scattering does not otherwise lead to the loss of a neutron.

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### 4.6 Comments on the $P_1$ Equations of Diffusion Theory

The Boltzmann equation is valid everywhere. The  $P_n$  approximation for odd  $n$  truncates some of the more asymmetric components of the flux and therefore an error is made in regions where these components are important. Specifically, near a boundary with a vacuum region or a strong absorber, one would expect neutrons to enter these regions but few if any to return; this is where lower order approximations are least valid. On the other hand, in interior regions of moderately absorbing media, which may include most of the volume of a reactor, the flux distribution would be expected to be fairly isotropic and therefore a low order approximation would be valid. The  $P_1$  diffusion theory approximation fits the latter case; by defining the diffusion coefficient in terms of the transport cross section, the important effect of linearly anisotropic scattering in the laboratory is included in the formulation.

There are a number of specific situations for which the  $P_1$  equations are not adequate. Among these are the following:

- a) Diffusion theory is inappropriate for shielding design. We generally employ shields that are many mean free paths thick, composed of multiple layers of strongly absorbing materials, moderating materials, high- $Z$  materials for gamma ray attenuation, and rarefied materials such as air. The depth of penetration tends to make the angular flux distribution highly anisotropic, while the nature of the materials themselves requires a very detailed treatment of the neutron and gamma ray energy and angle dependence. Shields are therefore usually calculated using multi-group discrete-ordinates  $S_n$  transport codes such as TORT(3D), DORT(2D) or ANISN (1D), or using Monte Carlo

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codes such as MORSE or MCNP(3D).

- b) Diffusion theory does not work too well for small heterogeneous regions such as the basic PWR cell consisting of a  $\text{UO}_2$  fuel pin and water. Here, we usually employ local transport calculations to obtain homogeneous cell-averaged macroscopic cross sections that can then be used in a diffusion theory calculation of the entire fuel assembly. The thermal group cell problem is usually solved with either Integral Transport theory as in the THERMOS code, or with  $P_3$  or its equivalent, as in the GAMTEC code.
- c) Diffusion theory does not work for control rods or lumped absorbers. These problems are solved using a transport method, and the results are then used as a special extrapolation boundary condition for a diffusion calculation.
- d) Finally, diffusion theory is completely inadequate for designing very small high-leakage assemblies, i.e., weapons.

Note that the diffusion equation is a second-order differential equation in space and a first-order one in time. Hence we require two boundary conditions for each region in the problem, plus an initial condition. As formulated above, the equations are inhomogeneous when a source is present. The solution will consist of a particular solution corresponding to the source plus a transient solution corresponding to the initial condition. If the multiplication factor of the system is less than unity, i.e., if we produce less than one fission neutron per neutron absorbed, then the transient solution will die away with time leaving a steady state behavior corresponding to the particular solution, where all features of the solution are uniquely determined by the source distribution. On the other

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hand, if the multiplication factor is greater than or equal to unity, then the transient solution will increase without bound. When the multiplication factor is much greater than unity, the result is called an excursion and the behavior is independent of the source contribution. When the multiplication is exactly equal to unity, i.e., the reactor is critical, then the source simply keeps adding neutrons and each neutron present is replenished by fission.

When no source is present, the equations become homogeneous. The only possible steady state solution occurs when the multiplication factor is unity; otherwise the flux level either increases or decreases with time. This is a rather inconvenient situation with regard to reactor design because one rarely chooses a material composition and reactor size that are just exactly critical. To circumvent this difficulty, one usually converts the diffusion equation in the steady state to an eigenvalue or characteristic value problem by dividing the fission production term by a constant that we call  $k_{\text{eff}}$ , the effective multiplication factor. This is the effective criticality for a stationary system that is not exactly critical. One must find the value of  $k_{\text{eff}}$  as well as the corresponding flux solution, and since only two boundary conditions are available to solve for three unknowns, one of the unknowns must be left arbitrary. This, in fact, corresponds to the observation that a reactor can be critical and operate at an arbitrary power level from milliwatts to megawatts. The eigenvalue formulation of the diffusion equation in the one-speed approximation is

$$\begin{array}{ccc} \text{leakage} & \text{absorption} & \text{effective production} \\ -\nabla \cdot D(\vec{r}) \nabla \phi(\vec{r}) + \Sigma_a(\vec{r}) \phi(\vec{r}) & = & \frac{\nu \Sigma_f(\vec{r}) \phi(\vec{r})}{k_{\text{eff}}} \end{array} \quad (4.66)$$

Since we now have separate symbols for flux and current, we have

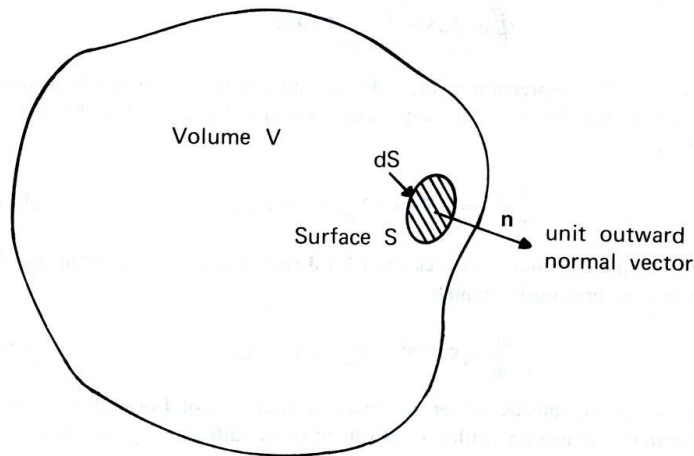
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dropped the subscript zero on the flux.

If we have a multi-region problem, a similar equation is used for each region, but the value of  $k_{\text{eff}}$  corresponds to the reactor as a whole and is therefore the same in each region. Hence, we have a second-order equation in each zone and need two boundary conditions for each zone. These boundary conditions are continuity of flux and continuity of current at each internal interface plus one boundary condition on each external surface such as zero current (symmetry), zero flux, or extrapolation to zero at an outer point. Current sources are not allowed interior to a region in diffusion theory, but may be placed in a problem as a boundary condition.

### 4.7\* Alternate Derivation of the Diffusion Equation

It is useful to derive the diffusion equation in an alternate manner using certain vector relationships that are commonly employed in diffusion theory proofs. We consider a neutron balance over a region having a volume  $V$  and a surface area  $S$ , as shown in Figure 4.7.



**Fig 4.7** Leakage from a Volume  $V$



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In deriving the leakage term in the Boltzmann equation, we made use of the directed flux along the direction  $\vec{\Omega}$  in  $d\Omega$ . The net neutron current density vector is simply the integral of this quantity over all angles, which we define to be the vector  $\vec{J}$ :

$$\vec{J} \equiv \int_{\text{all } \Omega} \vec{\Omega} \Phi(\vec{r}, \vec{\Omega}) d\Omega \quad (4.67)$$

In other words, there is a net flow or current of neutrons in some direction at each point in space. The component of this current that crosses any given surface  $dS$  is equal to the dot product of the vector current  $\vec{J}$  and the unit normal to the surface  $\vec{n}$ . Hence, the net leakage from the volume element is the integral of the current component over the entire surface of the region, or

$$[\text{net out - leakage}] = \iint_{\text{surface}} \vec{n} \bullet \vec{J} dS. \quad (4.68)$$

We complete the neutron balance over the region by adding in the other components such as isotropic sources and absorption. The resulting balance equation becomes

$$\begin{array}{cccc} \text{rate of change} & \text{source} & \text{fission} & \text{absorption} \\ \int_{\text{volume}} \frac{1}{v} \frac{\partial \phi}{\partial t} d\tau = \int_{\text{volume}} S d\tau + \int_{\text{volume}} \nu \Sigma \phi d\tau - \int_{\text{volume}} \Sigma_a \phi d\tau & & & \\ & \text{leakage} & & \\ & - \iint_{\text{surface}} \vec{n} \bullet \vec{J} dS. & & \end{array} \quad (4.69)$$

Now, we use the divergence theorem to convert the surface

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integral into a volume integral. The divergence theorem states that

$$\iint_{\text{surface}} \vec{n} \cdot \vec{J} \, dS = \int_{\text{volume}} \nabla \cdot \vec{J} \, dV.$$

Replacement of this expression in the balance equation leads to a similar volume integral in all terms. Therefore, the expression must also be satisfied in differential form, which is

$$\frac{1}{v} \frac{\partial \phi}{\partial t} = -\nabla \cdot \vec{J} - \sum_a \phi + S + v \sum_f \phi. \quad (4.70)$$

If we now assume the validity of Fick's law for  $\vec{J}$  from Eq. (4.62), we obtain the  $P_1$  equation derived previously, namely,

$$\frac{1}{v} \frac{\partial \phi}{\partial t} = \nabla \cdot D \nabla \phi - \sum_a \phi + S + v \sum_f \phi. \quad (4.71)$$

Note that we do not consider either the time rate of change of  $\vec{J}$  or current sources in our derivation, consistent with our treatment of the diffusion approximation to the Boltzmann equation.

### Problems

- 4.1 Show that the derivation of Fick's law is equally valid when the next term in the Taylor's series expansion is retained.
- 4.2 Show that, when a small amount of absorption is retained in the direct Fick's law derivation, the diffusion coefficient is given by the expression

$$D = \frac{\sum_s}{3 \sum_T^2}.$$

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### 4.3 Do the following:

- a) On polar graph paper plot  $P_0(\mu)$ ,  $P_1(\mu)$  and  $P_2(\mu)$  versus the polar angle  $\theta$ , where  $\mu = \cos\theta$ .
- b) On a separate sheet of polar graph paper plot the functions:
  1.  $\Phi(z_1, \mu) = 1/2 P_0(\mu) + 1/2 P_1(\mu)$ ;
  2.  $\Phi(z_2, \mu) = 1/2 P_0(\mu) + 1/3 P_1(\mu) + 1/3 P_2(\mu)$ ;
  3.  $\Phi(z_3, \mu) = 1/2 P_0(\mu) + 1/3 P_1(\mu) + 1/6 P_3(\mu)$ .These can be considered to be the angular fluxes at three points along the  $z$  axis.
- c) Based upon the above results, how many components would one need in order to approximate a parallel beam of neutrons traveling from left to right, where  $\theta = 0^\circ$ ? What does this say about the adequacy of using diffusion theory, which assumes that only the  $P_0(\mu)$  and  $P_1(\mu)$  components are present?

### 4.4 Prove that the first four Legendre polynomials are orthogonal over the range of $-1 < \mu < 1$ .

### 4.5\* Starting from the one-dimensional, steady-state, one-speed Boltzmann transport equation, derive the $P_3$ transport equations under the assumption that the source is isotropic and the scattering cross-section expansion contains only the terms $\Sigma_{s0}$ and $\Sigma_{s1}$ .

### 4.6\* At the symmetry plane located at $z = z_0$ in a one-dimensional problem, the angular flux is reflected in a mirror-like fashion such that

$$\Phi(z_0, \mu) = \Phi(z_0, -\mu)$$

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and

$$\frac{d\Phi(z,\mu)}{dz}\bigg|_{z=z_0} = -\frac{d\Phi(z,-\mu)}{dz}\bigg|_{z=z_0}.$$

- a) Prove that the above equations imply that the  $P_m$  flux components satisfy the expressions

$$\phi_m(z_0) = 0 \text{ for } m \text{ odd,}$$

and

$$\frac{d\phi_m}{dz}\bigg|_{z=z_0} = 0 \text{ for } m \text{ even.}$$

- b) Show that the above boundary conditions applied to the  $P_1$  equations are equivalent to the diffusion theory boundary conditions at a plane of symmetry.

**4.7\*** Derive the  $P_2$  transport equations and compare them to the  $P_1$  equations for the one speed, one-dimensional case. Assume a solution of the form  $\Phi_n(z) = A_n e^{kz}$  and use it to find the allowable values of  $k$ . Calculate the diffusion coefficient  $D$ . Comment on the general usefulness of the even-order expansions.

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## ANALYTICAL SOLUTIONS TO THE ONE-SPEED DIFFUSION EQUATION

Now that we have derived the diffusion equation in the one-speed approximation, we will seek analytic solutions to this equation for a variety of simple geometrical configurations. But first, we will generalize the boundary conditions to handle the two special situations of a vacuum boundary and a boundary near a source plane. The idea of a partial current is very useful here.

Next, we will look at problems containing neutron sources, placed either at interfaces or contained within one of the regions. Since these problems are inhomogeneous, complete solutions will be obtained whose behavior is dependent on the nature and location of the source.

In the absence of a source, the problem becomes homogeneous. If we seek steady state solutions, these will exist only for certain characteristic values of an extra parameter, called the effective multiplication factor, which must be introduced into the equations. In this case, solutions will be obtained which contain an arbitrary constant whose value must be specified externally.

Finally, we shall see that the analytic problem solution rapidly becomes unwieldy or impossible if there are more than a few spatial regions and spatial dimensions involved, even in the one-speed case. This leads us to Chapter 6, where numerical solutions to the few-group equations are discussed.

## NUCLEAR REACTOR THEORY AND DESIGN

### 5.1 Partial Currents and the Extrapolated Boundary Condition

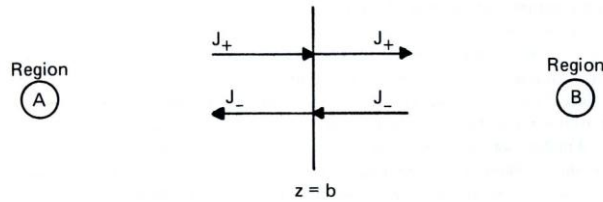
The angular flux in the one-dimensional  $P_1$  diffusion theory approximation is given by an expression that is derived in Section 4.4, namely,

$$\Phi(z, \mu) = \frac{\phi(z)}{2} + \frac{3\mu}{2} J(z). \quad (5.1)$$

The  $\phi_0$  component is called the total flux  $\phi(z)$ , and the  $\phi_1$  component is called the current  $J(z)$ . Consider a boundary between regions A and B as shown in Figure 5.1, and call all of the current traveling to the right  $J_+$  and all of the current traveling to the left  $J_-$ . Naturally, the positive components have a polar angle  $\theta$  between  $0^\circ$  and  $90^\circ$ , and the negative components have a polar angle between  $90^\circ$  and  $180^\circ$ . The corresponding values of  $\mu$  are 1 to 0 and 0 to -1, respectively.

We obtain the partial currents by integrating  $P_1(\mu)$  times the angular flux over the appropriate interval. Hence, the positive partial current to the right is

$$\begin{aligned} J_+(b) &= \int_0^1 \mu \Phi(b, \mu) d\mu \\ &= \int_0^1 \frac{\phi(b)}{2} \mu d\mu + \int_0^1 \frac{3J(b)}{2} \mu^2 d\mu \\ &= \frac{\phi(b)}{4} + \frac{J(b)}{2}. \end{aligned} \quad (5.2)$$



**Fig. 5.1** Partial Current Balance at a Region Interface



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Likewise, the negative partial current to the left is

$$\begin{aligned}
 J_{-}(b) &= \int_0^1 \mu \Phi(b, \mu) d\mu \\
 &= \int_0^1 \frac{\phi(b)}{2} \mu d\mu + \int_0^1 \frac{3J(b)}{2} \mu^2 d\mu \\
 &= \frac{\phi(b)}{4} - \frac{J(b)}{2}.
 \end{aligned} \tag{5.3}$$

We now use the one-dimensional form of Fick's law to replace  $J(b)$ , consistent with our  $P_1$  diffusion theory. Since

$$J(z) = -D \frac{d\phi}{dz}, \tag{5.4}$$

we obtain

$$J_{+}(b) = \frac{\phi(b)}{4} - \frac{D}{2} \frac{d\phi}{dz} \Big|_{z=b} \tag{5.5}$$

and

$$J_{-}(b) = \frac{\phi(b)}{4} + \frac{D}{2} \frac{d\phi}{dz} \Big|_{z=b}. \tag{5.6}$$

The above two equations are an *alternate form* of writing the boundary conditions at an interface. Specifically,  $J_{+}^A(b)$  must equal  $J_{+}^B(b)$  since neutrons leaving one region must enter the other. Similarly,  $J_{-}^A(b) = J_{-}^B(b)$ . If we write these expressions out, at the interface we obtain

$$\frac{\phi_A}{4} - \frac{D_A}{2} \frac{d\phi_A}{dz} = \frac{\phi_B}{4} - \frac{D_B}{2} \frac{d\phi_B}{dz} \tag{5.7}$$

and

$$\frac{\phi_A}{4} + \frac{D_A}{2} \frac{d\phi_A}{dz} = \frac{\phi_B}{4} + \frac{D_B}{2} \frac{d\phi_B}{dz}. \tag{5.8}$$

By adding the two expressions, we obtain

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$$\phi_A(b) = \phi_B(b). \quad (5.9)$$

By subtracting the two expressions, we obtain

$$-D_A \frac{d\phi_A}{dz} = -D_B \frac{d\phi_B}{dz} \quad (5.10)$$

or

$$J^A(b) = J^B(b).$$

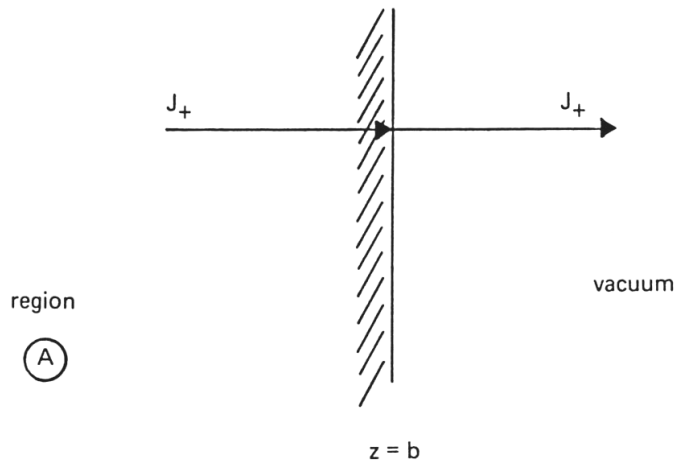
Hence, we have continuity of flux and continuity of current, as before.

**Extrapolation Distance.** When region B is a vacuum as shown in Figure 5.2, there is only an outward current,  $J_+^A(b)$ , and no return current, i.e.,  $J_-^A(b) = 0$ . Hence,

$$J_-^A(b) = 0 = \frac{\phi_A(b)}{4} + \frac{D_A}{2} \frac{d\phi}{dz} \Big|_{z=b}.$$

Solving for the slope at the boundary, we obtain

$$\frac{d\phi}{dz} \Big|_{z=b} = -\frac{\phi_A(b)}{2D_a} = -\frac{3\phi_A(b)}{2\lambda_{tr}^A}.$$

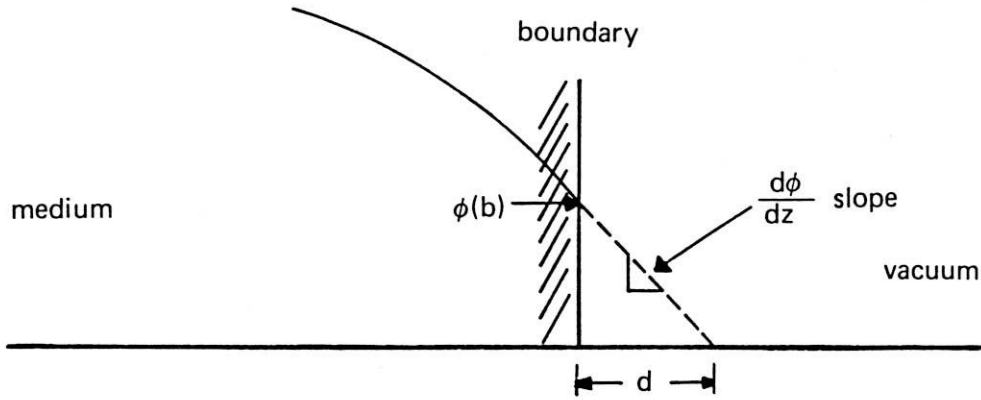


**Fig. 5.2** Partial Currents at a Vacuum Boundary

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From this expression we can define an extrapolation distance, called  $d$ , where the flux would go to zero if extrapolated linearly, as shown in Figure 5.3. This distance is

$$d = -\frac{\phi_A(b)}{d\phi_A/dz|_{z=b}} = \frac{2\lambda_{tr}^A}{3} = 0.667\lambda_{tr}^A. \quad (5.11)$$



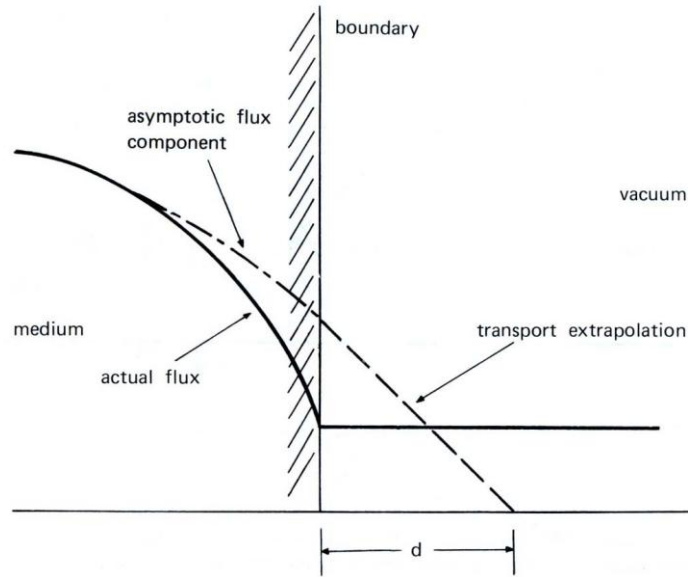
**Fig. 5.3** Extrapolation Distance Diagram

Since the  $P_1$  equations are only an approximation to the transport equation, the extrapolation distance is also only an approximation. The situation is sketched in Figure 5.4. The actual flux does not go to zero because the neutrons that leave the surface simply stream away (there is nothing to stop them). This is why we must do shielding calculations for reactor systems. The transport theory extrapolation distance is slightly larger than the diffusion theory value, and is given by the expression

$$d_{transport} = 0.7104\lambda_{tr}^A. \quad (5.12)$$

This is the value we use in elementary reactor theory. For strong absorption, or for curved boundaries with small radii, the correct value is somewhat smaller than that given above.

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**Fig. 5.4** Transport Theory Extrapolation Distance Diagram

**Additional Boundary Conditions.** For small reactors, where leakage is an important part of the total neutron balance, the transport theory-based extrapolation distance boundary condition given above is commonly used on the outer boundary. On the other hand, when the reactor is large, the extrapolation distance can often be ignored without significant error. This gives what is known as a zero-flux boundary condition, written as

$$\phi_A(b) = 0. \quad (5.13a)$$

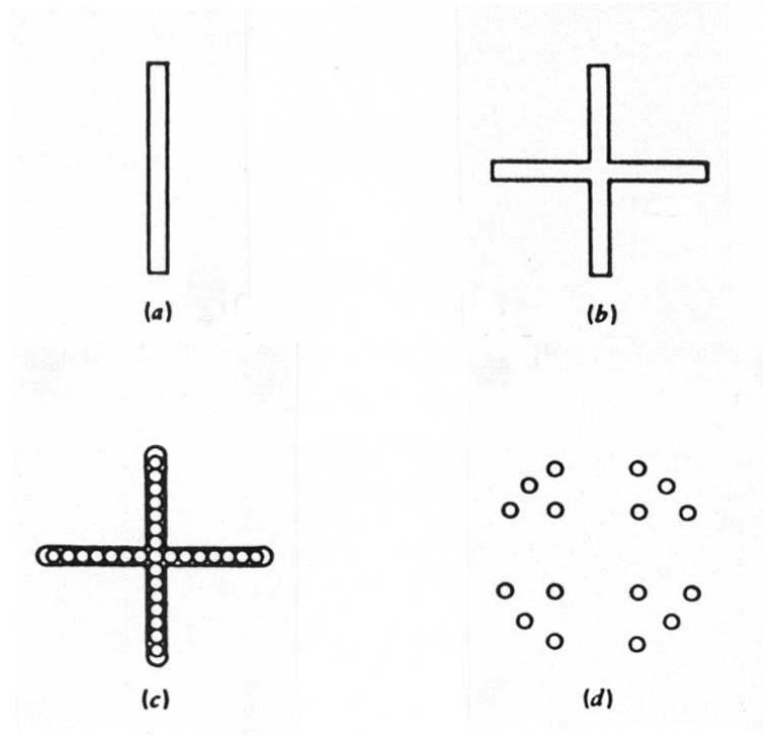
Furthermore, when a core possesses half or quarter-core symmetry, it becomes wasteful to treat the entire reactor when a symmetric portion will provide the complete solution. In this case, the internal symmetry planes can be represented by a zero-current boundary condition

$$\frac{d\phi_A}{dx}\bigg|_{x=b} = 0. \quad (5.13b)$$

One other common situation that involves a special boundary condition concerns the treatment of control rods in reactors. A

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number of different-shaped control rods are in current use, as illustrated in Figure 5.5. The slab-type control rod is typical of that found in a pool-type reactor such as the UVAR; these rods are made of boral, which is a boron-aluminum alloy. The cruciform-shaped control rod is an early design used in the Yankee PWR located at Rowe, Massachusetts; it is made of a silver, indium and cadmium alloy. The rodDED-cruciform shape is typical of that used in BWR's; the rods are usually filled with boron carbide. Finally, the rod cluster is typical of control rods in modern PWR's; the rods are usually filled with boron carbide.



**Fig. 5.5** Typical control rod geometries. (a) Thin slab. (b) Cruciform. (c) Rodded cruciform. (d) Control rod cluster.

Unfortunately, control rods cannot be represented accurately using diffusion theory. Instead, we must supply the medium *surrounding* the control rod with an *alternate* boundary condition

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that describes the fractional current flowing into the absorbing medium. This condition is called the "blackness" or absorption coefficient, and is given by the expression

$$\alpha = \frac{J_+^A(b) - J_-^A(b)}{J_+^A(b)} = \frac{J^A(b)}{J_+^A(b)}. \quad (5.13c)$$

Alpha is usually obtained from a separate transport theory calculation. A related boundary condition is called the "albedo" or reflection coefficient, which is defined as

$$\beta = \frac{J_-^A(b)}{J_+^A(b)} = 1 - \alpha. \quad (5.13d)$$

An even more convenient computational form of the blackness boundary condition is analogous to the extrapolation distance, and is given by the expression

$$C = \frac{J^A(b)}{\phi_A(b)}. \quad (5.13e)$$

A completely black control rod with  $\alpha = 1$  would have an extrapolation distance of  $d_r = 0.71 \lambda_{tr}$ , corresponding to a value of  $C = 0.469$ . As the control rod becomes gray, or less absorbing,  $d_r$  increases and  $C$  decreases. The amount of blackness depends upon the thickness of the rod, as well as on its material properties.

The control rod boundary condition is not commonly used in analytical calculations. But it is used in computer codes such as VENTURE, where the individual control rod regions are replaced by externally-supplied boundary conditions of the form given by Eq. (5.13e). The flux inside the rod region is set equal to zero, and the boundary condition is used to calculate the flux in the adjacent region. The absorption in the control rod is then obtained as the product of the control rod surface area and the current entering that surface as described by Eq. (5.13e). We

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are led to the important conclusion that neutron absorption in a control rod is proportional to the total surface area of the rod, as long as the rods are spaced sufficiently far apart that the presence of one rod does not shadow or depress the flux near another rod.

### 5.2 Source Plane Boundary Conditions.

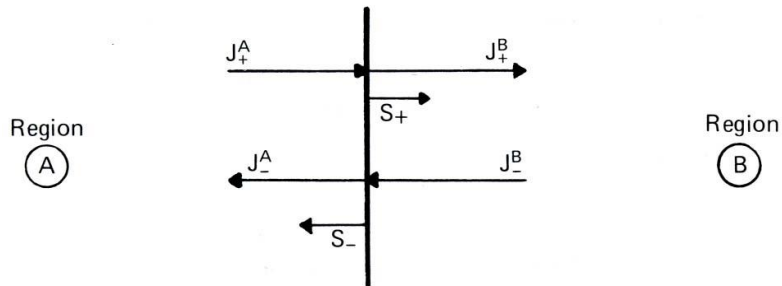
The partial currents form an alternate set of boundary conditions at an interface in lieu of continuity of flux and current. If we have an infinitely thin planar source located at the interface, then the boundary conditions are altered somewhat. If we denote the source strength to the right as  $S_+$  and to the left as  $S_-$ , as shown in Figure 5.6, then the general conditions become

$$J_+^A + S_+ = J_+^B \text{ and } J_-^B + S_- = J_-^A, \quad (5.14)$$

where

$$S_+ = \int_0^1 S(z, \mu) d\mu \text{ and } S_- = \int_{-1}^0 S(z, \mu) d\mu. \quad (5.15)$$

These conditions state that the current reaching the opposite region is augmented by the source. Note that the source need not be symmetric since it enters only as a boundary condition, but sources are usually isotropic.



**Fig. 5.6** Partial Currents in the Presence of a Source

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**Plane Source in an Infinite Medium.** A very simple example is an infinite medium having an infinite isotropic plane source, located at the origin, of strength  $S$  neutrons/cm<sup>2</sup>-s. The diffusion equation is

$$D \frac{d^2 \phi}{dx^2} - \Sigma_a \phi = 0, \quad (5.16)$$

or, defining  $L^2 \equiv D/\Sigma_a$ , where  $L$  is called the diffusion length,

$$\frac{d^2 \phi}{dx^2} - \frac{1}{L^2} \phi = 0. \quad (5.17)$$

We will attach a physical significance to  $L$  later. The above homogeneous equation has the general solution

$$\phi(x) = A_1 e^{-x/L} + A_2 e^{+x/L}, \quad (5.18)$$

where  $A_1$  and  $A_2$  are constants to be determined by the boundary conditions. Now, the flux must be finite as  $x \rightarrow \pm \infty$ , and we note that for  $x \rightarrow +\infty$ ,  $e^{x/L} \rightarrow \infty$ , while for  $x \rightarrow -\infty$ ,  $e^{-x/L} \rightarrow \infty$ . Thus, one of the constants is zero and the solution in each half plane must be of the form

$$\phi(x) = A e^{-|x|/L}. \quad (5.19)$$

The remaining constant  $A$  must be found by using a boundary condition at the source.

Since we have an isotropic source located on a plane of symmetry, we can heuristically say that the net current in each direction is one half of the source strength, or

$$\lim_{x \rightarrow 0^+} J(x) = \frac{S}{2} = \lim_{x \rightarrow 0^+} \left( -D \frac{d\phi}{dx} \right). \quad (5.20)$$

Performing the indicated operations, we obtain

$$\frac{S}{2} = \lim_{x \rightarrow 0^+} \left( \frac{DA}{L} \right) e^{-x/L} = \frac{DA}{L}.$$



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Hence, the constant is  $A = SL/2D$  and the full solution becomes

$$\phi(x) = \frac{SL}{2D} e^{-|x|/L}. \quad (5.21)$$

**General Interface conditions.** For the specific case of the planar source, we can also obtain a pair of general boundary conditions that are valid even when the source is not symmetric and when the problem does not contain spatial or material symmetry. Recall that the total current is given by the expression

$$J^A(b) \equiv J_+^A - J_-^A = -D_a \frac{d\phi_A}{dx} \Big|_{x=b}.$$

When we subtract the partial currents given by Eq. (5.14), with a source present, we obtain the relationship

$$J^A + (S_+ + S_-) = J^B. \quad (5.22)$$

Since  $S = S_+ + S_-$ , this expression states that the total current, which is a directed quantity, *jumps* at the interface by an amount equal to the total source strength. This is obvious in the symmetric problem: the current is equal to  $S/2$  directed to the left in region A and changes value to  $S/2$  directed to the right in region B as a result of the source of strength  $S$ .

We obtain the second general boundary condition by adding the partial currents, making use of the definitions of  $J_+$  and  $J_-$  in terms of the flux. Adding, one obtains the relationship

$$\frac{\phi_A(b)}{2} + (S_+ - S_-) = \frac{\phi_B(b)}{2}. \quad (5.23)$$

When the source is symmetric, so that  $S_+ = S/2$  and  $S_- = S/2$ , then the boundary condition is

$$\phi_A(b) = \phi_B(b),$$

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i.e., continuity of flux. When the source is asymmetric, there is a flux discontinuity equal to twice the difference between the partial sources in each direction.

The discontinuity is a mathematical phenomenon, caused by the truncation of the Boltzmann equation to a two-term expansion. In actual fact, the diffusion theory solution is not an adequate representation of the angular flux distribution near the source, at least not within a few mean free paths of the source plane. We consider this zone to be a transition region where the neutrons must undergo a few collisions before diffusion theory can be expected to be valid.

**Infinite Medium Plane Kernel.\*** If the source were placed at position  $x_0$  instead of at  $x = 0$ , then the solution would be translated to the form

$$\phi(x) = \frac{S_0 L}{2D} e^{-|x-x_0|/L}. \quad (5.24)$$

Notice that the diffusion theory solution indicates that the flux decreases by a factor of  $e$  every  $L$  centimeters from the source plane. Thus,  $L$  is called the relaxation length or diffusion length. By definition,

$$L = \sqrt{\frac{D}{\Sigma_a}} = \sqrt{\frac{l}{3\Sigma_{tr}\Sigma_a}}. \quad (5.25)$$

Hence, the diffusion length represents a type of geometrical mean between the mean free paths for absorption and scattering.

If there were two sources present, having different source strengths and locations, then the flux would be a superposition of the two solutions because the equations are linear. Hence, for sources at  $x_0$  and  $x_1$ ,

$$\phi(x) = \frac{S_0 L}{2D} e^{-|x-x_0|/L} + \frac{S_1 L}{2D} e^{-|x-x_1|/L}.$$

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The extension to a large number of sources is obvious. As a matter of fact, as the sources become a source distribution,  $S(x')$ , the superposition becomes an integral of the form

$$\phi(x) = \int_{\substack{\text{all space} \\ \text{containing sources}}} \frac{S(x')L}{2D} e^{-|x-x'|/L} dx' \quad (5.26)$$

$$= \int_{\text{all space}} S(x') G_{pl}(x' \rightarrow x) dx'.$$

The kernel is called the planar infinite medium Green's function, which is defined as

$$G_{pl}(x' \rightarrow x) \equiv \frac{L}{2D} e^{-|x-x'|/L}. \quad (5.27)$$

More will be said about Green's Functions shortly.

### 5.3 Two Region Planar Problem

Consider the two-region symmetric source problem shown in Figure 5.7. We need only consider half of the problem since, because of symmetry, the solution in the left-half plane will be a mirror image of the solution in the right-half plane. The source-free diffusion equation applies in both regions, which is written as

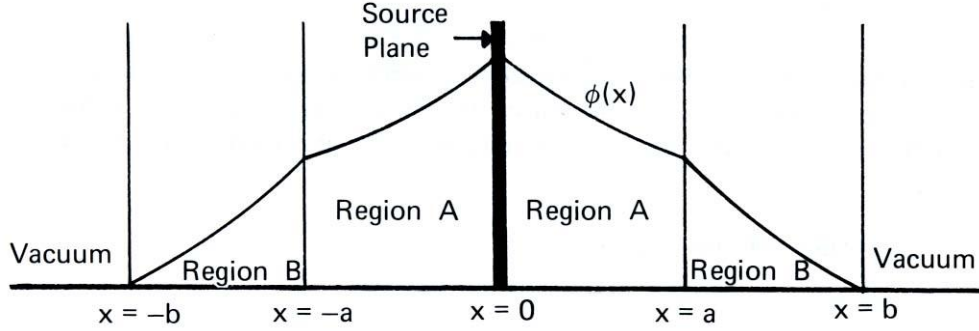
$$\frac{d^2 \phi}{dx^2} - \frac{1}{L^2} \phi = 0.$$

In finite geometry, the solutions can be written conveniently in terms of hyperbolic functions, namely,

$$\phi_A(x) = A_I \sinh \frac{x}{L_A} + C_I \cosh \frac{x}{L_A} \equiv A_I f_I(x) + C_I g_I(x) \quad (5.28)$$

and

$$\phi_B(x) = A_2 \sinh \frac{x}{L_B} + C_2 \cosh \frac{x}{L_B} \equiv A_2 f_2(x) + C_2 g_2(x). \quad (5.29)$$



**Fig. 5.7** Two Region Problem

We have four coefficients to be determined:  $A_1$ ,  $A_2$ ,  $C_1$ , and  $C_2$ . We have four boundary conditions, namely:

1. Source condition at  $x = 0$ ;  $\lim_{x \rightarrow 0} J^A(x) = S/2$ .
2. Flux continuity at the interface;  $\phi_A(a) = \phi_B(a)$ .
3. Current continuity at the interface;

$$-D_a \frac{d\phi_A}{dx} \Big|_{x=a} = -D_B \frac{d\phi_B}{dx} \Big|_{x=a}.$$

4. Flux is zero at the extrapolated outer boundary;  
 $\phi_B(b') = 0$ , where

$$b' = b + 0.71\lambda_{tr}^B.$$

Hence, the solution can be uniquely determined. Formally, the equations are best put into vector-matrix form in order to see the general nature of the solution. Inserting the boundary conditions leads to the following set of equations:

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$$\begin{bmatrix} -D_A f_1'(0) & -D_A g_1'(0) & 0 & 0 \\ f_1(a) & g_1(a) & -f_2(a) & -g_2(a) \\ -D_A f_1'(a) & -D_A g_1'(a) & D_B f_2'(a) & D_B g_2'(a) \\ 0 & 0 & f_2(b') & g_2(b') \end{bmatrix} \begin{bmatrix} A_1 \\ C_1 \\ A_2 \\ C_2 \end{bmatrix} = \begin{bmatrix} S/2 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \quad (5.30)$$

This equation is of the form

$$\underline{\underline{F}} \underline{\underline{a}} = \underline{\underline{s}}, \quad (5.31)$$

whose solution is

$$\underline{\underline{a}} = \underline{\underline{F}}^{-1} \underline{\underline{s}}, \quad (5.32)$$

subject to the condition that the determinant of  $\underline{\underline{F}}$  is not equal to zero so that the inverse exists. The extension to an n-region problem is obvious; the formulation is a 2n by 2n matrix problem to be solved for 2n coefficients using 2n boundary conditions. The detailed, step-by-step solution to the above problem is left as an exercise.

### 5.4 Point and Line Sources

**Point Source in an Infinite Medium.** Suppose we place an isotropic point source of strength S neutrons/s at the center of an infinite uniform medium and ask for the resulting flux as a function of position. The governing equation is simply

$$\nabla^2 \phi - \frac{1}{L^2} \phi = 0, \quad (5.33)$$

where, in spherical geometry with azimuthal and polar symmetry, the Laplacian operator is written as

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$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right). \quad (5.34)$$

The solution of the above problem is simplified greatly if a variable change is introduced of the form  $\omega = r\phi$ . Computing  $\nabla^2 \phi$ , one obtains

$$\begin{aligned} \nabla^2 \phi &= \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial}{\partial r} \left( \frac{\omega}{r} \right) \right] \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \left( -\frac{\omega}{r^2} + \frac{1}{r} \frac{\partial \omega}{\partial r} \right) \right] \\ &= \frac{1}{r^2} \left( -\frac{\partial \omega}{\partial r} + \frac{\partial \omega}{\partial r} + r \frac{\partial^2 \omega}{\partial r^2} \right) \\ &= \frac{1}{r} \frac{\partial^2 \omega}{\partial r^2}. \end{aligned}$$

Likewise, the second term becomes

$$\frac{1}{L^2} \phi = \frac{1}{L^2} \frac{\omega}{r}.$$

By canceling the factor  $1/r$ , we obtain the simpler equation

$$\frac{\partial^2 \omega}{\partial r^2} - \frac{1}{L^2} \omega = 0. \quad (5.35)$$

The solution to this equation is simply

$$\omega(r) = Ae^{-r/L} + Ce^{+r/L}, \quad (5.36)$$

or, in terms of the flux,

$$\phi(r) = \frac{Ae^{-r/L}}{r} + \frac{Ce^{+r/L}}{r}, \quad (5.37)$$

where A and C are coefficients to be determined by applying the

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boundary conditions.

There are two boundary conditions: (1) the flux must be finite as  $r \rightarrow \infty$ ; and (2) the source condition is obtained as  $r \rightarrow 0$ . The quantity  $e^{-r/L}/r$  is finite as  $r \rightarrow \infty$  because the exponential term goes to zero. On the other hand, the factor  $e^{+r/L}/r$  must be evaluated by using L'Hopital's rule to obtain

$$\lim_{r \rightarrow \infty} \left( \frac{e^{r/L}}{r} \right) = \lim_{r \rightarrow \infty} \left( \frac{de^{r/L}/dr}{dr/dr} \right) = \lim_{r \rightarrow \infty} \left( \frac{(1/L)e^{r/L}}{1} \right) = \infty.$$

Hence, the coefficient  $C = 0$ .

The source condition is

$$\lim_{r \rightarrow 0} 4\pi r^2 J(r) = S, \quad (5.38)$$

which states that the source neutrons give rise to a radial current. Since  $J(r) = -D d\phi/dr$ , we obtain

$$S = \lim_{r \rightarrow 0} 4\pi r^2 \left[ -DA \left( -\frac{e^{-r/L}}{rL} - \frac{e^{-r/L}}{r^2} \right) \right] = 4\pi DA. \quad (5.39)$$

Hence, the coefficient is

$$A = \frac{S}{4\pi D},$$

and the solution is

$$\phi(r) = \frac{S e^{-r/L}}{4\pi D r}. \quad (5.40)$$

Note that this solution is not finite at  $r = 0$ .

**Infinite Medium Point Kernel.\*** If the source is placed at position  $\bar{r}'$  rather than at  $\bar{r}$ , one can use the same solution provided that the distance from the source to the point at  $\mathbf{r}$  is properly computed. As shown in Figure 5.8 this involves a vector difference  $|\bar{r} - \bar{r}'|$ . For a unit source, the infinite medium point

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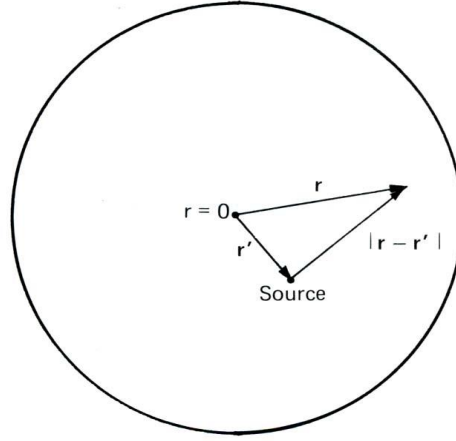
kernel can be written as

$$G_{pt}(r,0) = \frac{e^{-r/L}}{4\pi D r}, \quad (5.41)$$

which is a special case of the general infinite medium point kernel

$$G_{pt}(\vec{r},\vec{r}') = \frac{e^{-|\vec{r}-\vec{r}'|}}{4\pi D |\vec{r}-\vec{r}'|}. \quad (5.42)$$

Note that the vector quantities  $\vec{r}$  and  $\vec{r}'$  must be converted to the scalar variables  $r$ ,  $\theta$ , and  $\psi$  before evaluation of the kernel can be accomplished.

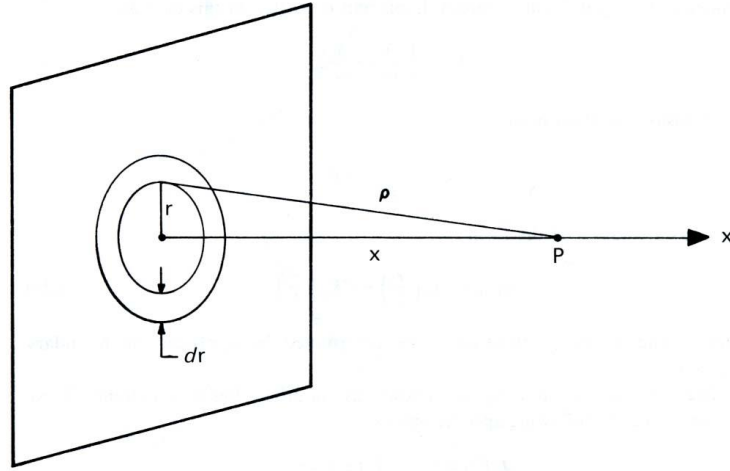


**Fig. 5.8.** Point Source at  $\vec{r}'$

To illustrate the use of the infinite medium point kernel (Green's function), we derive the flux that would be found at a distance  $x$  from an infinite plane source. Consider that we have a large number of point sources distributed in a plane such that the source strength is  $S = 1$  neutron/s-cm<sup>2</sup>. The flux at  $x$  is obtained by integrating over the source plane shown in Figure 5.9. In this case, the flux is given by the integral

$$\phi(x) = \int_0^\infty 2\pi r \left( \frac{e^{-\rho/L}}{4\pi D \rho} \right) dr. \quad (5.43)$$





**Fig. 5.9.** Point Source to Plane Source Conversion Diagram

To evaluate the integral, we make a variable change from  $r$  to  $\rho$ . Since  $r$ ,  $\rho$ , and  $x$  are related by the expression

$$\rho^2 = x^2 + r^2,$$

we can take the derivative to obtain

$$2\rho d\rho = 2r dr.$$

When  $r = 0$ ,  $\rho = x$ ; when  $r = \infty$ ,  $\rho = \infty$ . Hence, the integral becomes

$$\phi(x) = \int_x^\infty \frac{e^{-\rho/L}}{2D} d\rho = \frac{L}{2D} \int_x^\infty e^{-\rho/L} d\rho = \frac{L}{2D} e^{-x/L}. \quad (5.44)$$

But this is in fact the expression for the infinite medium plane kernel derived previously, i.e.,

$$G_{pl}(x, 0) = \frac{L}{2D} e^{-x/L}.$$

**Infinite Medium Line Kernel.\*** In the same fashion, the point kernel can be used to obtain a line kernel that can then be used to obtain an infinite-cylinder kernel, etc. Rather than do

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these exercises, we directly derive the line source solution in cylindrical geometry having no axial dependence and having azimuthal symmetry. The cylindrical geometry Laplacian is written in this case as

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right). \quad (5.45)$$

The diffusion equation is simply

$$\nabla^2 \phi - \frac{1}{L^2} \phi = 0,$$

which has a solution of the form

$$\phi(r) = AI_0\left(\frac{r}{L}\right) + CK_0\left(\frac{r}{L}\right), \quad (5.46)$$

where A and C are coefficients to be determined by applying the boundary conditions.

The functions  $I_0$  and  $K_0$  are known as modified Bessel functions. These functions have the following specific values:

$$I_0(0) = 1; \quad I_0(\infty) = \infty;$$

$$K_0(0) = \infty; \quad K_0(\infty) = 0.$$

Their derivatives obey the expressions

$$\frac{dI_0(x)}{dx} = I_1(x) \quad \text{and} \quad \frac{dK_0(x)}{dx} = -K_1(x),$$

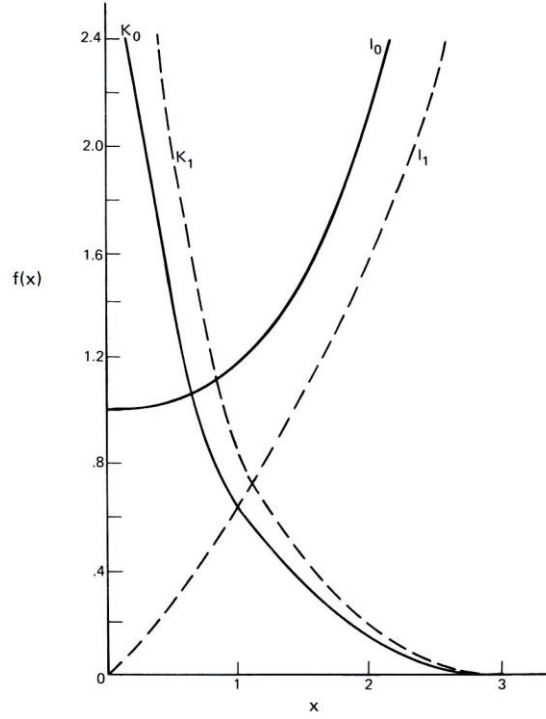
where  $I_1$  and  $K_1$  are also modified Bessel functions that have the specific values

$$I_1(0) = 0; \quad I_1(\infty) = \infty;$$

$$K_1(0) = \infty; \quad K_1(\infty) = 0.$$

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These functions are plotted in Figure 5.10.



**Fig. 5.10** Modified Bessel Functions I and K

We now apply the boundary conditions. Since the flux must be finite as  $r \rightarrow \infty$ , the coefficient  $A = 0$ , leaving the solution in the form

$$\phi(r) = CK_0\left(\frac{r}{L}\right). \quad (5.47)$$

If the source emits  $S$  neutrons/s-cm, the boundary condition is

$$\lim_{r \rightarrow 0} 2\pi J(r) = S. \quad (5.48)$$

The radial current in cylindrical geometry is

$$J(r) = -D \frac{d\phi}{dr} = \frac{CD}{L} K_1\left(\frac{r}{L}\right).$$

In the limit of small arguments, the  $K_1$  function can be approximated as

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$$\lim_{r \rightarrow 0} K_I\left(\frac{r}{L}\right) \approx \frac{L}{r}. \quad (5.49)$$

Hence, the source condition leads to

$$S = \lim_{r \rightarrow 0} 2\pi r \left(\frac{CD}{L}\right) \frac{L}{r} = 2\pi DC. \quad (5.50)$$

Solving for the coefficient C, we obtain the flux as a function of distance from a line source in the form

$$\phi(r) = \frac{S}{2\pi D} K_0\left(\frac{r}{L}\right). \quad (5.51)$$

The corresponding line kernel, when the source is located on the axis at  $r' = 0$ , is

$$G_l(r, 0) = \frac{I}{2\pi D} K_0\left(\frac{r}{L}\right). \quad (5.52)$$

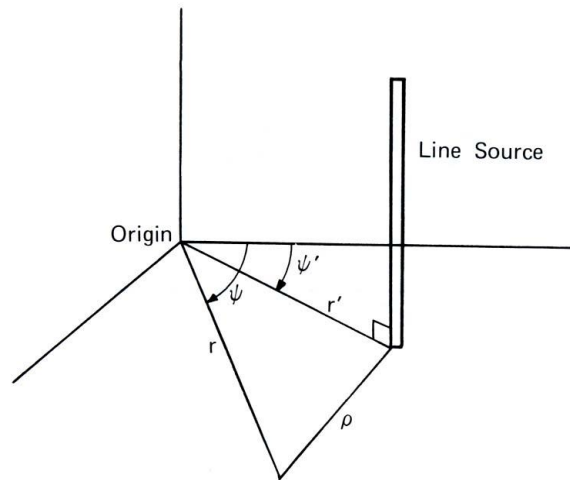
This is a simplification of the general line kernel, valid when the source is located at distance  $r'$  and angle  $\psi'$  from the origin of the coordinate system, namely (see Figure 5.11),

$$G_l(r, \psi, r', \psi') = \frac{I}{2\pi D} K_0\left(\frac{\rho}{L}\right), \quad (5.53)$$

where

$$\rho^2 = r^2 + r'^2 - 2r'r \cos(\psi - \psi').$$

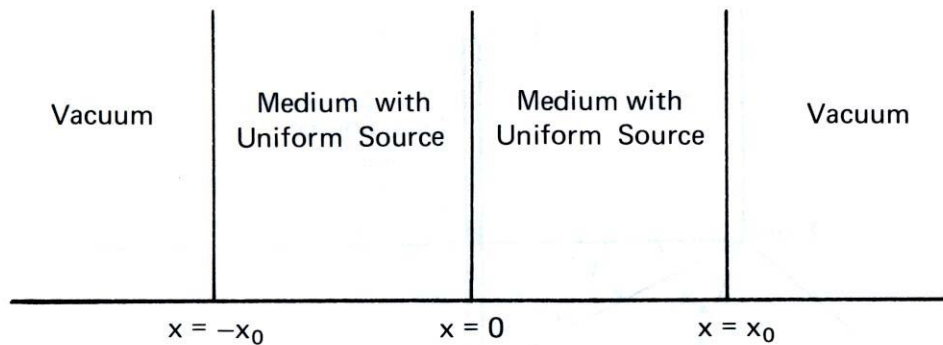
## NUCLEAR REACTOR THEORY AND DESIGN



**Fig. 5.11** Line Source Located at  $r', \psi'$  from the Origin

### 5.5 Solution to the Inhomogeneous Source Problem

Consider the case of a semi-infinite planar medium containing a spatially uniform isotropic source of strength  $S$  neutrons/cm<sup>3</sup>-s. The geometrical configuration is shown in Figure 5.12, where  $x_0$  is considered to be the extrapolated boundary.



**Fig. 5.12** Spatially Uniform Source in a Diffusing Medium

The differential equation in this case is the inhomogeneous equation

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$$D \frac{d^2 \phi}{dx^2} - \Sigma_a \phi + S = 0.$$

Dividing through by  $D$ , we obtain the form used previously, with the addition of a source component, namely,

$$\frac{d^2 \phi}{dx^2} - \frac{1}{L^2} \phi + \frac{S}{D} = 0. \quad (5.54)$$

The homogeneous solution to this problem is simply

$$\phi_h(x) = A \sinh\left(\frac{x}{L}\right) + C \cosh\left(\frac{x}{L}\right).$$

~~The coefficients  $A$  and  $C$  are determined by the boundary conditions. The particular solution is determined by the source term  $S$ .~~

We choose

$$\phi_p(x) = \frac{S}{\Sigma_a},$$

which obviously meets the condition when inserted into the differential equation.

The complete solution is the *sum* of the homogeneous and particular solutions, namely,

$$\phi(x) = \frac{S}{\Sigma_a} + A \sinh\left(\frac{x}{L}\right) + C \cosh\left(\frac{x}{L}\right). \quad (5.55)$$

The coefficients  $A$  and  $C$  are obtained by applying the boundary conditions to the *complete* solution. Making use of the symmetry of the problem, we see that there is no net current crossing the symmetry plane at  $x = 0$ . Hence  $d\phi/dx|_{x=0} = 0$ . Applying this boundary condition to the solution gives

$$\left[ \frac{A}{L} \cosh\left(\frac{x}{L}\right) + \frac{C}{L} \sinh\left(\frac{x}{L}\right) \right]_{x=0} = 0.$$

But since  $\cosh(0) = 1$  and  $\sinh(0) = 0$ , this implies that  $A = 0$ , leaving the solution

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$$\phi(x) = \frac{S}{\Sigma_a} + C \cosh\left(\frac{x}{L}\right).$$

The second boundary condition is that the flux must vanish at the extrapolated boundary  $x_0$ . This gives

$$0 = \frac{S}{\Sigma_a} + C \cosh\left(\frac{x_0}{L}\right) \quad \text{or} \quad C = -\frac{S}{\Sigma_a \cosh\left(\frac{x_0}{L}\right)}.$$

The complete solution can then be written as

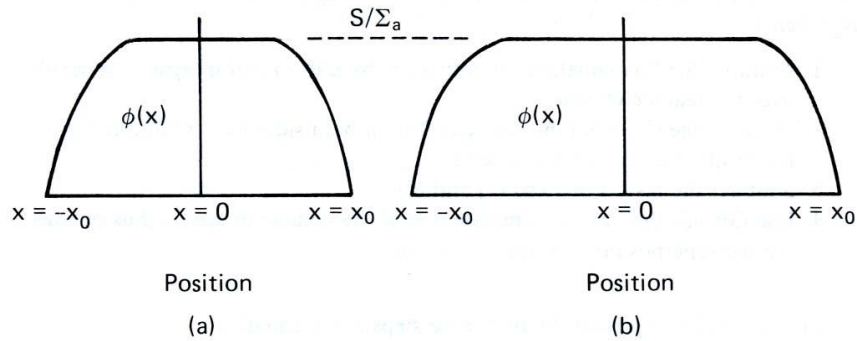
$$\phi(x) = \frac{S}{\Sigma_a} \left( 1 - \frac{\cosh(x/L)}{\cosh(x_0/L)} \right). \quad (5.56)$$

The solution is plotted in Figures 5.13a and 5.13b for small and large source regions, respectively.

As the medium gets larger, the second term in the brackets becomes of less importance near the center of the medium, leading to a much flatter flux distribution. In the limit, as the medium becomes infinite, the solution approaches the value

$$\lim_{x_0 \rightarrow \infty} \phi(x) = \frac{S}{\Sigma_a} = \text{constant} \quad (5.57)$$

which simply states that when there is no spatial leakage, the local absorption rate  $\Sigma_a \phi$  just equals the source rate  $S$ .



**Fig. 5.13** Flux Distribution in a Finite Slab Containing a Uniform Source

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### 5.6\* General Derivation of the Green's Function Superposition Integral

In the general case where the reactor properties and the source vary spatially, the diffusion equation must be written in the inhomogeneous form

$$-\nabla \cdot D \nabla \phi(\vec{r}) + \Sigma_a \phi(\vec{r}) = S(\vec{r}). \quad (5.58)$$

Since the left-hand side of the equation represents neutron losses due to leakage and absorption, we can define a single destruction operator  $L$  as

$$L \equiv (-\nabla \cdot D \nabla + \Sigma_a) \quad (5.59)$$

and put the diffusion equation in the form

$$L\phi(\vec{r}) = S(\vec{r}). \quad (5.60)$$

The Green's function is the flux solution to the same problem when the source term is replaced by a Dirac delta function. Hence, the Green's function satisfies the equation

$$LG(\vec{r}, \vec{r}') \equiv \delta(\vec{r} - \vec{r}'). \quad (5.61)$$

Now, in order to obtain the general superposition integral, we follow the procedure given below:

1. Multiply the flux equation on each side by  $G(\vec{r}, \vec{r}')$  and integrate the result over the reactor volume.
2. Multiply the Green's function equation on each side by  $\phi(\vec{r}')$  and integrate the result over the reactor volume.
3. Subtract the results of steps (1) and (2).
4. Use Green's theorem to eliminate one of the volume integrals, thus obtaining the superposition integral.



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The result of completing the first three steps is the equation

$$\int_{\text{reactor volume}} [G(\vec{r}, \vec{r}') L\phi(\vec{r}') - \phi(\vec{r}') LG(\vec{r}, \vec{r}')] d\vec{r}' =$$

$$(5.62)$$

$$\int_{\text{reactor volume}} G(\vec{r}, \vec{r}') S(\vec{r}') d\vec{r}' - \int_{\text{reactor volume}} \phi(\vec{r}') \delta(\vec{r} - \vec{r}') d\vec{r}'.$$

If the left-hand side of this equation can be shown to be identically zero, then the right-hand side will give the superposition integral. The absorption part of the left-hand side of the equation has an integrand that is

$$G(\vec{r}, \vec{r}') \Sigma_a(\vec{r}') \phi(\vec{r}') - \phi(\vec{r}') \Sigma_a(\vec{r}') G(\vec{r}, \vec{r}') = 0, \quad (5.63)$$

and therefore its integral is equal to zero. The leakage term is more complicated and requires Green's theorem, which states that for two arbitrary functions  $\psi_1$  and  $\psi_2$ ,

$$\int_{\text{volume}} \psi_1 \nabla \cdot D \nabla \psi_2 d\vec{r} = \oint_{\text{surface}} \vec{n} \cdot \psi_1 D \nabla \psi_2 dS - \int_{\text{volume}} \nabla \psi_1 \cdot D \nabla \psi_2 d\vec{r}, \quad (5.64)$$

where  $\vec{n}$  is the unit outward normal to the reactor surface. Green's theorem is obtained using the divergence theorem and the general expression for the derivative of a product of two functions. Specializing the theorem to the present case, we let  $\psi_1 = G$  and  $\psi_2 = \phi$  to obtain the expression

$$\int_{\text{reactor volume}} (G \nabla \cdot D \nabla \phi - \phi \nabla \cdot D \nabla G) d\vec{r} =$$

$$\oint_{\text{reactor surface}} \vec{n} \cdot (G D \nabla \phi - \phi D \nabla G) dS' \quad (5.65)$$

$$- \int_{\text{reactor volume}} [\nabla G \cdot D \nabla \phi - \nabla \phi \cdot D \nabla G] d\vec{r}'.$$

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The integrand of the volume integral on the right-hand side of Eq. (5.65) is symmetric and is therefore identically zero.

Furthermore, the boundary conditions on the (extrapolated) reactor surface  $\vec{R}$  are generally either

$$\phi(\vec{R}) = 0 \quad \text{and} \quad G(\vec{R}, \vec{r}') = 0,$$

or the symmetry conditions

$$\nabla \phi(\vec{R}) = 0 \quad \text{and} \quad \nabla G(\vec{R}, \vec{r}') = 0.$$

In either case, the surface integral vanishes because of the boundary conditions. Therefore, we have proved that in general

$$\int_{\text{reactor}} [G(\vec{r}, \vec{r}') L\phi(\vec{r}') - \phi(\vec{r}') LG(\vec{r}, \vec{r}')] d\vec{r}' = 0. \quad (5.66)$$

We are left with the expression

$$\int_{\text{reactor}} G(\vec{r}, \vec{r}') S(\vec{r}') d\vec{r}' - \int_{\text{reactor}} \phi(\vec{r}') \delta(\vec{r} - \vec{r}') d\vec{r}' = 0. \quad (5.67)$$

Making use of the fact that the integral of any function times the Dirac delta function is simply the integrand evaluated at the argument of the delta function, we obtain the Green's superposition integral in general form, namely,

$$\phi(\vec{r}) = \int_{\text{reactor volume}} G(\vec{r}, \vec{r}') S(\vec{r}') d\vec{r}'. \quad (5.68)$$

The kernel is oftentimes written in a slightly different notation, i.e.,

$$G(\vec{r}, \vec{r}') \equiv G(\vec{r}' \rightarrow \vec{r}), \quad (5.69)$$

giving the equivalent expression

$$\phi(\vec{r}) = \int G(\vec{r}' \rightarrow \vec{r}) S(\vec{r}') d\vec{r}'. \quad (5.70)$$

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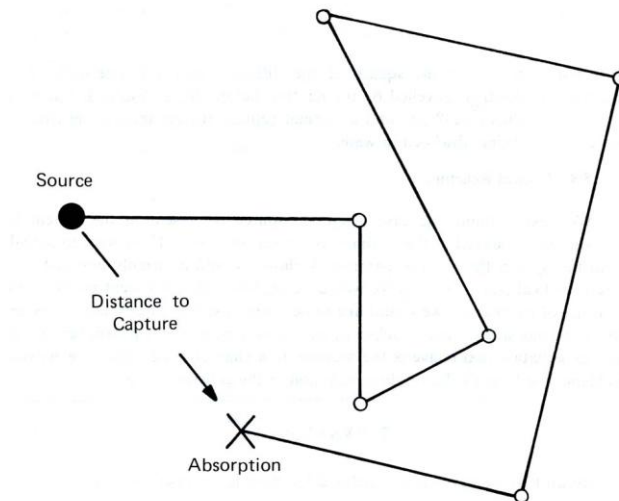
Note that, when the medium is *finite* or *non-uniform*, the kernel  $G(\vec{r}, \vec{r}')$  is *not equal* to any of the simple infinite media kernels defined previously.

### 5.7 Diffusion Length

You will recall that the flux from a point source in an infinite media was written in terms of the diffusion length  $L$  as

$$\phi(r) = \frac{S e^{-r/L}}{4\pi D r}. \quad (5.71)$$

The actual path traveled by a given neutron is relatively erratic as it leaves the source, since the direction of scattering at each point occurs in an arbitrary manner. One such path is shown in Figure 5.14, where the open circles represent scattering events. Remember, this is motion in three-dimensional space. One may ask the question, what is the mean-squared distance that the neutron travels from the point of emission to the point of absorption? Obviously, the mean distance is much less than the actual path length.



**Fig. 5.14** Path of a Neutron Emitted from a Point Source

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Consider a spherical shell of thickness  $dr$  about  $r$ . The number of absorptions/s in the shell is equal to

$$\left[ \frac{\text{absorptions}}{s} \right] = \sum_a \phi(r) 4\pi r^2 dr.$$

All neutrons from the source are eventually absorbed in the medium. Therefore, the integral of the absorption rate over all space is simply

$$\int_0^\infty \sum_a \phi(r) 4\pi r^2 dr = S, \quad (5.72)$$

which can be verified by direct calculation.

The probability that a neutron will be absorbed in the spherical shell is simply the ratio of the absorption rate in the shell to the total absorption rate over all space, or the expression

$$p(r)dr = \left[ \frac{\sum_a \phi(r) 4\pi r^2 dr}{S} \right]. \quad (5.73)$$

This probability is obviously normalized to unity. Therefore, the mean-square distance that a neutron travels before being absorbed is computed by taking the absorption-probability-weighted average of  $r^2$ . This has the value

$$\overline{r^2} = \frac{\int_0^\infty r^2 p(r) dr}{\int_0^\infty p(r) dr}. \quad (5.74)$$

If we insert the appropriate expressions, we obtain

$$\overline{r^2} = \frac{\sum_a}{D} \int_0^\infty r^3 e^{-r/L} dr. \quad (5.75)$$

The above integral can be evaluated by integrating by parts twice, giving the expression,

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$$\overline{r^2} = 6L^2. \quad (5.76)$$

This result states that the square of the diffusion length is one-sixth of the mean-square distance traveled by a slow neutron from its source before being absorbed. For water,  $L^2 = 8.1 \text{ cm}^2$ , thus  $\overline{r^2} \approx 49 \text{ cm}^2$  and a thermal neutron travels about 7 cm before being absorbed. A similar expression for fast neutrons states that the age  $\tau$  is one-sixth of the mean-square distance a fast neutron travels before reaching thermal energy.

### 5.8 Critical Reactors

We next examine the case where no source is present in the system but neutrons are produced in the medium as a result of fission. If we were to actually build this system the physical parameters chosen would invariably not lead to an exactly critical reactor so that we would be dealing with a transient problem. For purposes of calculation, we would like to deal with a steady state situation instead. This fictitious steady state is achieved by introducing an extra parameter  $\lambda$  into the balance equation that converts the problem to a characteristic value or eigenvalue problem. The form of the resulting equation in the general case is

$$\begin{array}{ccc} \text{leakage} & \text{absorption} & \text{effective} \\ & & \text{production} \end{array} \quad (5.77)$$

$$-\nabla \cdot D \nabla \phi + \Sigma_a \phi = \frac{\nu \Sigma_f \phi}{\lambda}.$$

Recall that we have already defined the destruction operator  $L$  as

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$$L \equiv (-\nabla \cdot D \nabla + \Sigma_a).$$

If we now define a corresponding production operator  $M$  as

$$M \equiv \nu \Sigma_f, \quad (5.78)$$

then the formulation is the generalized eigenvalue problem

$$L\phi = \frac{M\phi}{\lambda}. \quad (5.79)$$

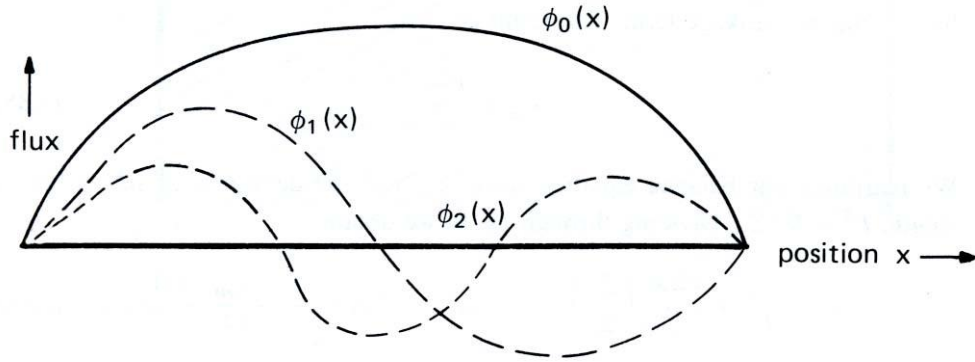
The object is to find *both*  $\lambda$  and the corresponding solution for the flux,  $\phi$ . If one notes that  $L\phi$  is the local volumetric destruction rate and  $M\phi$  is the local volumetric production rate, then integration of both sides of the equation over the reactor volume gives a physical interpretation of the eigenvalue  $k$  as

$$\lambda = \frac{\int_{\text{reactor}} M\phi \, dr}{\int_{\text{reactor}} L\phi \, dr} = \left[ \frac{\text{Total production rate}}{\text{Total destruction rate}} \right] \equiv k_{\text{eff}}, \quad (5.80)$$

where  $k_{\text{eff}}$  is the effective multiplication factor of the system. The system will be just exactly critical when  $k_{\text{eff}} = 1.0$ , i.e., when production just equals destruction.

Since the neutron density is positive everywhere, the flux is positive everywhere. Mathematically, however, the balance equation admits an infinite number of harmonic solutions corresponding to different allowed values of  $\lambda$ . If one appends an index to each of these solutions, then one can show that  $\lambda_0 > \lambda_1 > \lambda_2 > \dots \lambda_m$ , where the subscript  $m$  corresponds to the number of internal zero crossings that the corresponding flux solution makes with the axis. The solutions are called "lambda modes" and are pictured in Figure 5.15.

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**Fig. 5.15** Lambda Mode Flux Solutions

Roughly speaking, each harmonic corresponds to the flux solution in a smaller reactor (that is, the first harmonic is the solution obtained for either half of a symmetric system), and the value of  $\lambda$  is smaller because the smaller system has more leakage than the complete reactor. If the fundamental mode were just exactly critical, then each of the harmonic modes would be sub-critical and would represent a decaying transient solution in a real system. Therefore, the harmonics are not actually present in the steady state. Nonetheless, harmonics can be excited by fixed sources and can be excited in the transient state. An example of the latter case is a xenon-induced spatial power oscillation in a large high-power thermal reactor system.

For the present, we will only consider the fundamental mode solutions in various geometries.

### 5.9 Homogeneous Bare Critical Slab Reactor

The eigenvalue formulation for the homogenous bare slab is the equation

$$D\nabla^2\phi - \Sigma_a\phi + \frac{\nu\Sigma_f\phi}{k_{eff}} = 0. \quad (5.81)$$

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Since  $-D\nabla^2\phi$  represents leakage, we examine what the effective multiplication factor would be if the slab were infinite in extent so that there was no leakage. We call this multiplication factor "k-infinity," and obtain it from the above equation by ignoring the leakage term. The result is

$$k_{\infty} \equiv \frac{\nu \Sigma_f}{\Sigma_a}. \quad (5.82)$$

We rearrange our balance equation using  $k_{\infty}$  and the definition of the diffusion length,  $L^2 \equiv D/\Sigma_a$ . Dividing through by  $D$ , we obtain

$$\begin{aligned} \nabla^2\phi - \frac{\Sigma_a\phi}{D} + \frac{\nu\Sigma_f\phi}{k_{eff}D} \left( \frac{\Sigma_a}{\Sigma_a} \right) &= 0, \text{ or} \\ \nabla^2\phi + \left[ \frac{k_{\infty}/k_{eff} - 1}{L^2} \right] \phi &= 0. \end{aligned} \quad (5.83)$$

We define a new term to represent the square-bracketed quantity, namely, let

$$B^2 \equiv \frac{k_{\infty}/k_{eff} - 1}{L^2}. \quad (5.84)$$

Our balance equation becomes

$$\nabla^2\phi + B^2\phi = 0. \quad (5.85)$$

The quantity  $B^2$  is known as the material buckling. It is in fact the proportionality factor between the local flux and the curvature of the flux as represented by the second spatial derivative of the flux. The important thing to note is that  $B^2$  can either be a *positive* or a *negative* quantity depending upon whether or not the ratio  $k_{\infty}/k_{eff}$  is greater than or less than unity. Since the quantity  $-D\nabla^2\phi$  represents leakage, the quantity  $DB^2\phi$  must also represent leakage. Since  $\phi$  is positive

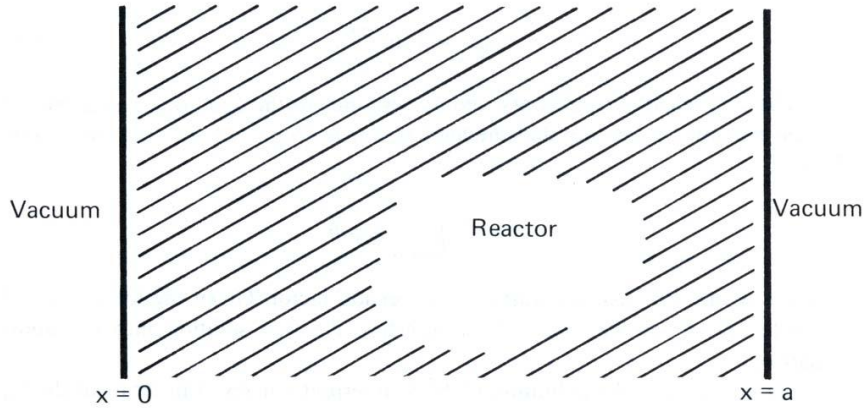


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everywhere, a region with a positive value of  $B^2$  must have a net out-leakage and must produce more neutrons than it consumes.

Furthermore if the diffusion coefficient is a function of position, then  $B^2$  must also vary as a function of position.

In the specific case of the bare homogeneous reactor, the quantity  $B^2$  turns out to be a positive constant, as will be seen shortly. Consider a slab of thickness  $a$  centimeters as shown in Figure 5.16, where  $a$  includes the extrapolation distances.



**Fig. 5.16** Bare Slab Reactor

The equation

$$\frac{d^2 \phi}{dx^2} + B^2 \phi = 0 \quad (5.86)$$

has the general solution

$$\phi(x) = A \sin Bx + C \cos Bx, \quad (5.87)$$

where the coefficients  $A$  and  $C$  are to be determined from the boundary conditions.

The boundary conditions are  $\phi(0) = \phi(a) = 0$ . Applying the boundary condition at  $x = 0$  gives

$$0 = A(0) + C(1).$$

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Therefore, the coefficient  $C = 0$  and the solution becomes

$$\phi(x) = A \sin Bx.$$

Applying the second boundary condition at  $x = a$  gives

$$0 = A \sin Ba.$$

This equation is satisfied in a non-trivial manner only if the geometric buckling is

$$B^2 = \left(\frac{n\pi}{a}\right)^2, \quad n = 1, 2, \dots \quad (5.88)$$

The fundamental-mode solution corresponds to  $n = 1$ , so that the final answer is

$$\phi(x) = A \sin \frac{\pi x}{a}. \quad (5.89)$$

The coefficient  $A$  is arbitrary and corresponds to the operating power level. It can be evaluated by noting that the local power is proportional to the fission rate. Thus,

$$P = \frac{1}{c} \int_{\text{reactor}} \Sigma_f \phi \, dx,$$

where  $c = 3.1 \times 10^{10}$  fissions/s-watt is a conversion factor. Given the total power  $P$ , the value of  $A$  can be obtained by inserting the flux solution into the above equation.

Let us return to the definition of  $B^2$  given by Eq. (5.84) to interpret our result in terms of the  $k_{\text{eff}}$  of the system. Solving for  $k_{\text{eff}}$ , we obtain

$$k_{\text{eff}} = \frac{k_{\infty}}{1 + L^2 B^2}. \quad (5.90)$$

Since  $k_{\infty}$  is the multiplication factor for an infinite system with no leakage and  $k_{\text{eff}}$  is the multiplication factor for a finite system, the factor  $1/(1 + L^2 B^2)$  represents a type of non-leakage

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probability that is denoted by the symbol  $L_T$ . Hence, in our simple model,

$$k_{eff} = k_{\infty} L_T. \quad (5.91)$$

Putting in the value of  $B^2$  for the slab, we have the relation

$$k_{eff} = \frac{k_{\infty}}{1 + L^2 \pi^2 / a^2}. \quad (5.92)$$

As the reactor becomes larger, the leakage becomes less important. Also note that the above expression represents a design choice. For a desired value of  $k_{eff}$ , which may be greater than unity to allow for eventual fuel burnup, insertion of control rods, poisoning, etc., the relation states that:

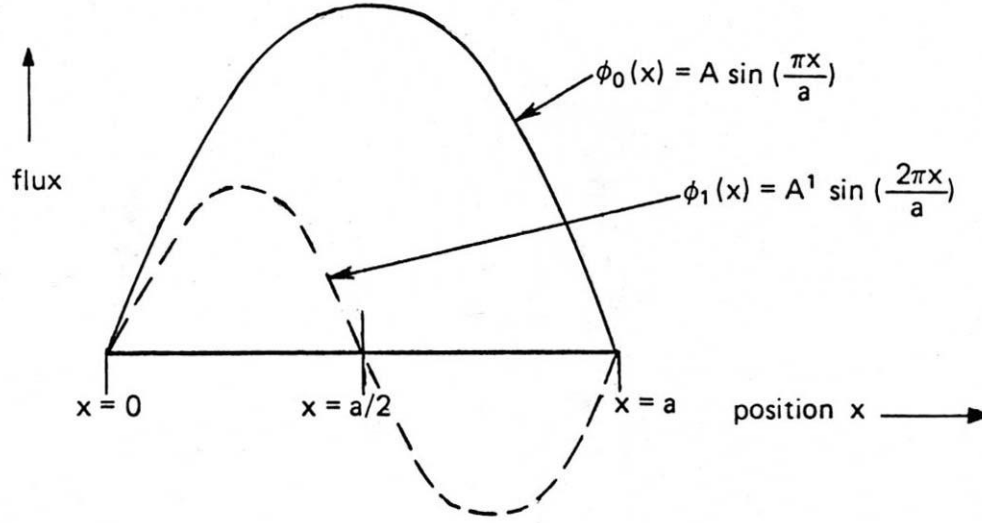
1. given the size  $a$ , there is a unique value of the material composition  $k_{\infty}$  which will produce the desired criticality;
2. given the composition  $k_{\infty}$ , there is a unique critical size for the system.

In this particular case, the first-harmonic solution is given when  $n = 2$ , and is

$$\phi_1(x) = A' \sin\left(\frac{2\pi x}{a}\right). \quad (5.93)$$

The solution is shown in Figure 5.17.

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**Fig. 5.17** Fundamental and First Harmonic Solutions for a Slab Reactor

If the fundamental-mode value of  $k_{eff}$  were exactly unity, then the criticality of the first-harmonic mode would be

$$k_{eff_1} = \frac{k_{\infty}}{1 + 4L^2\pi^2/a^2} = \frac{1 + L^2\pi^2/a^2}{1 + 4L^2\pi^2/a^2} < 1. \quad (5.94)$$

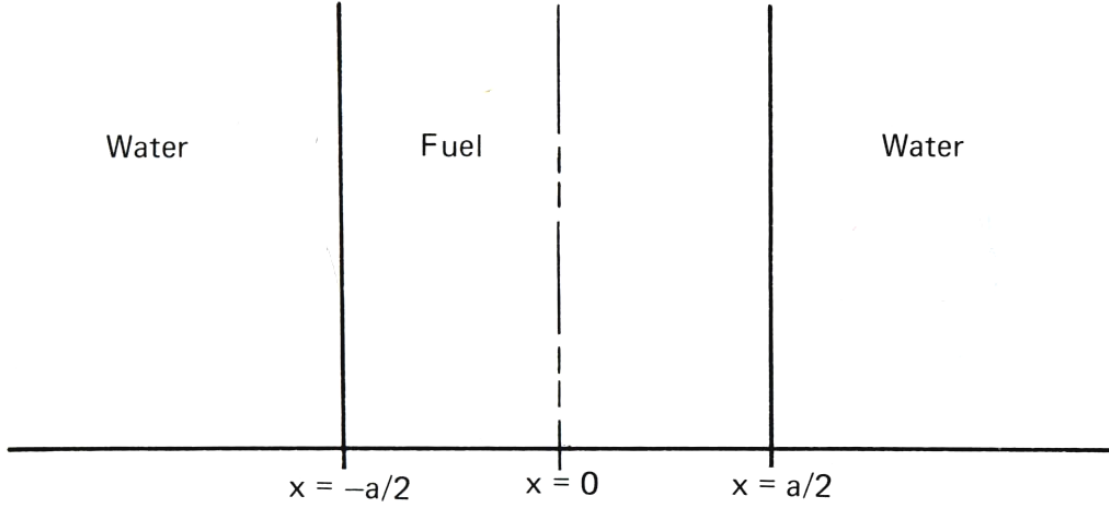
The amount of sub-criticality of the first harmonic decreases as the reactor becomes larger relative to the magnitude of the diffusion length!

### 5.10 Two Region Slab Reactor

Consider the case where the fuel region is surrounded by an infinitely large water region (reflector) on either side, as shown in Figure 5.18. We use the subscripts c for core and R for water. Note that since there is no fuel in the water region, its value of buckling is indeed negative and there is a net in-

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leakage into the water to supply the neutrons that are absorbed there.



**Fig. 5.18** Reflected Slab Reactor

The governing equations are

$$\nabla^2 \phi_c + B_c^2 \phi_c = 0, \quad \text{where } B_c^2 = \left[ \frac{\frac{k_{\infty c}}{k_{eff}} - 1}{L_c^2} \right], \quad (5.95)$$

and

$$\nabla^2 \phi_R + B_R^2 \phi_R = 0, \quad \text{where } B_R^2 = -\frac{1}{L_R^2}. \quad (5.96)$$

The general solutions are

$$\phi_c(x) = A_c \sin B_c x + C_c \cos B_c x \quad (5.97)$$

and

$$\phi_R(x) = A_R e^{-x/L_R} + C_R e^{+x/L_R}, \quad (5.98)$$

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respectively, where  $A_c$ ,  $C_c$ ,  $A_R$ , and  $C_R$  are coefficients to be determined. We have four boundary conditions, namely:

(1) at  $x=0$ ,

$$\left. \frac{d\phi_c}{dx} \right|_{x=0} = 0 \quad \text{because of symmetry.}$$

(2) at  $x=a/2$ ,

$$\phi_c\left(\frac{a}{2}\right) = \phi_R\left(\frac{a}{2}\right); \quad \text{continuity of flux.}$$

(3) at  $x=a/2$ ,

$$-D_c \left. \frac{d\phi_c}{dx} \right|_{x=a/2} = -D_R \left. \frac{d\phi_R}{dx} \right|_{x=a/2}; \quad \text{continuity of current.}$$

(4) at  $x=\infty$ ,

$$\lim_{x \rightarrow \infty} \phi_R(x) = 0; \quad \text{flux must be finite.}$$

Let us put these conditions into the vector-matrix format used previously. The result is

$$\begin{bmatrix} B_c & 0 & 0 & 0 \\ \sin\left(\frac{B_c a}{2}\right) & \cos\left(\frac{B_c a}{2}\right) & -e^{-a/2L_R} & -e^{+a/2L_R} \\ -D_c B_c \cos\left(\frac{B_c a}{2}\right) & D_c B_c \sin\left(\frac{B_c a}{2}\right) & \frac{-D_R}{L_R} e^{-a/2L_R} & \frac{D_R}{L_R} e^{+a/2L_R} \\ 0 & 0 & 0 & \lim_{x \rightarrow \infty} e^{+x/L_R} \end{bmatrix} \begin{bmatrix} A_c \\ C_c \\ A_R \\ C_R \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

(5.99)

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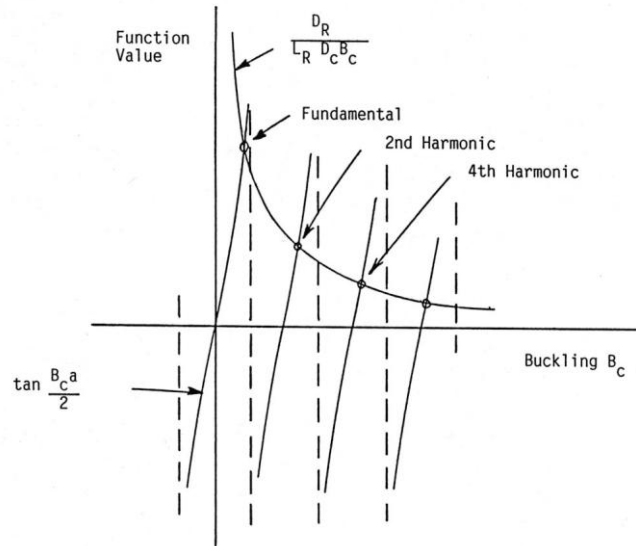
Obviously,  $A_c$  and  $C_R$  are both zero, so that the order of the system can be reduced. Contrary to the case where a source was present, this is the homogeneous equation

$$\underline{\underline{H}}\underline{\underline{a}} = \underline{\underline{0}}. \quad (5.100)$$

A nontrivial solution exists only when the determinant of  $\underline{\underline{H}}$  is identically zero. Setting  $|\underline{\underline{H}}| = 0$  gives the following transcendental equation, which can be solved for the critical value of  $B_c^2$ :

$$\tan\left(\frac{B_c a}{2}\right) = \frac{D_R}{L_R D_c B_c}. \quad (5.101)$$

We note that the transcendental equation also permits multiple solutions for the value of  $B_c^2$ , as can be seen by plotting the tangent function vs.  $B_c$ , as in Figure 5.19, and looking for the intersection with the right-hand side of the equation. The smallest value of  $B_c$  corresponds to the fundamental mode. Again, given the desired  $k_{eff}$  and the size  $a$ , we obtain the corresponding  $k_{\infty c}$  needed in the fuel region. Alternately, given  $k_{\infty c}$ , we find the dimension  $a$  for a desired  $k_{eff}$ .



**Fig. 5.19** Plot of Eq. (5.101) vs.  $B$

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### 5.11 One-Dimensional Bare Homogeneous Cylindrical Reactor

In cylindrical geometry, the Laplacian operator is

$$\nabla^2 \equiv \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r}.$$

Consider a bare cylindrical reactor with extrapolated radius  $R_0$  as shown in Figure 5.20. The reactor equation becomes

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + B^2 \phi = 0, \quad (5.102)$$

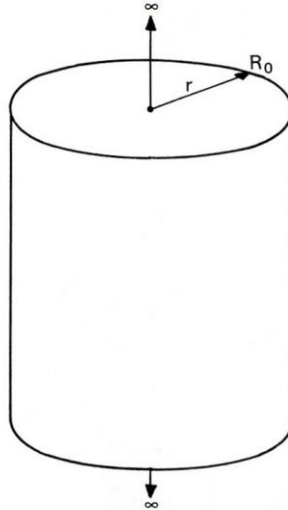
which is recognized to be Bessel's equation of order 0.

The general solution is of the form

$$\phi(r) = AJ_0(Br) + CY_0(Br), \quad (5.103)$$

where A and C are coefficients to be determined, and  $J_0$  and  $Y_0$  are Bessel functions of the first kind. The derivatives obey the relations

$$\frac{d}{dx}(J_0(x)) = -J_1(x) \quad \text{and} \quad \frac{d}{dx}(Y_0(x)) = -Y_1(x).$$



**Fig. 5.20** Bare Homogeneous Cylindrical Reactor



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Specific values of interest are the following:

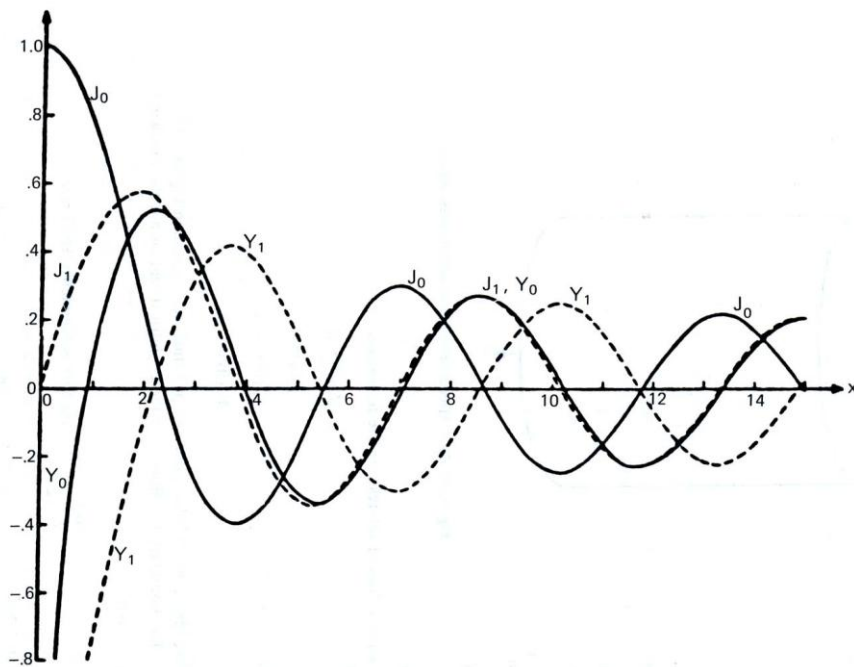
$$J_0(0) = 1;$$

$$J_1(0) = 0;$$

$$Y_0(0) = -\infty;$$

$$Y_1(0) = -\infty.$$

These functions all behave like damped sinusoids, as seen in Figure 5.21.



**Fig. 5.21** Bessel Functions J and Y of Orders 0 and 1

The boundary conditions for the cylindrical reactor are the following:

(1) at  $r = 0$ ,  $\frac{d\phi}{dr}\bigg|_{r=0} = 0$ ; the flux is symmetric and finite.

(2) at  $r = R_0$ ,  $\phi(R_0) = 0$ ; the flux vanishes at the extrapolated boundary.

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The first boundary condition gives

$$\frac{d\phi}{dr}/_{r=0} = 0 = -BAJ_1(0) - BCY_1(0).$$

Putting in values,

$$0 = BA(0) - BC(-\infty).$$

Therefore,  $C = 0$ , and the solution becomes

$$\phi(r) = AJ_0(Br). \quad (5.104)$$

Application of the second boundary condition gives

$$\phi(R_0) = 0 = AJ_0(BR_0).$$

This equation is satisfied only at the zeros of the  $J_0$  function, the first few of which are listed in Table 5.1.

**Table 5.1**  
Zeros of the  $J_0$  Bessel Function

$J_0$ function zero	Value of argument	Value of B
1	2.405	2.405/ $R_0$
2	5.520	etc.
3	8.654	
4	11.792	
5	14.931	

Therefore, the final solution is

$$\phi(r) = AJ_0\left(\frac{2.405r}{R_0}\right), \quad (5.105)$$

where the coefficient A corresponds to the power level of the reactor.

## NUCLEAR REACTOR THEORY AND DESIGN

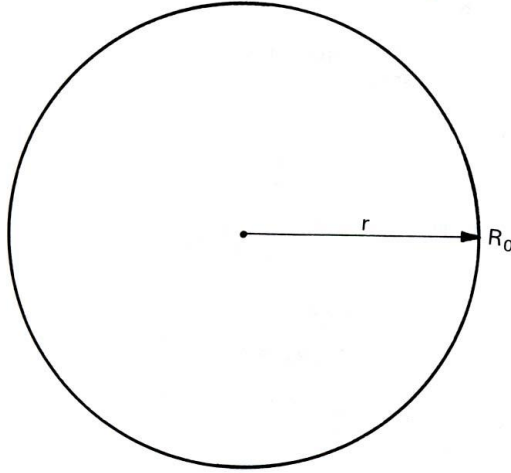
### 5.12 Bare Homogeneous Spherical Reactor

In spherical geometry, the Laplacian operator is

$$\nabla^2 \equiv \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right).$$

Consider a bare spherical reactor with extrapolated radius  $R_0$  as shown in Figure 5.22. The reactor equation can therefore be written as

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \phi}{\partial r} \right) + B^2 \phi = 0. \quad (5.106)$$



**Fig. 5.22** Bare Homogeneous Spherical Reactor

Using the variable change  $\omega = r\phi$ , as done previously, this equation can be converted to the form

$$\frac{\partial^2 \omega}{\partial r^2} + B^2 \omega = 0, \quad (5.107)$$

which has the solution

$$\omega(r) = A \sin Br + C \cos Br. \quad (5.108)$$

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Hence, substituting back, the flux solution is

$$\phi(r) = A \left[ \frac{\sin Br}{r} \right] + C \left[ \frac{\cos Br}{r} \right], \quad (5.109)$$

where A and C are coefficients to be determined using the boundary conditions.

Specific values of these functions that are of special interest are the following:

$$\lim_{r \rightarrow 0} \left[ \frac{\sin Br}{r} \right] = B; \quad \lim_{r \rightarrow 0} \left[ \frac{\cos Br}{r} \right] = \infty.$$

These functions, known as spherical Bessel functions, also behave like damped sinusoids. Their plots are similar to those obtained for the  $J_0$  and  $Y_0$  Bessel functions shown previously, as seen in Figure 5.23, where the following definitions have been used:

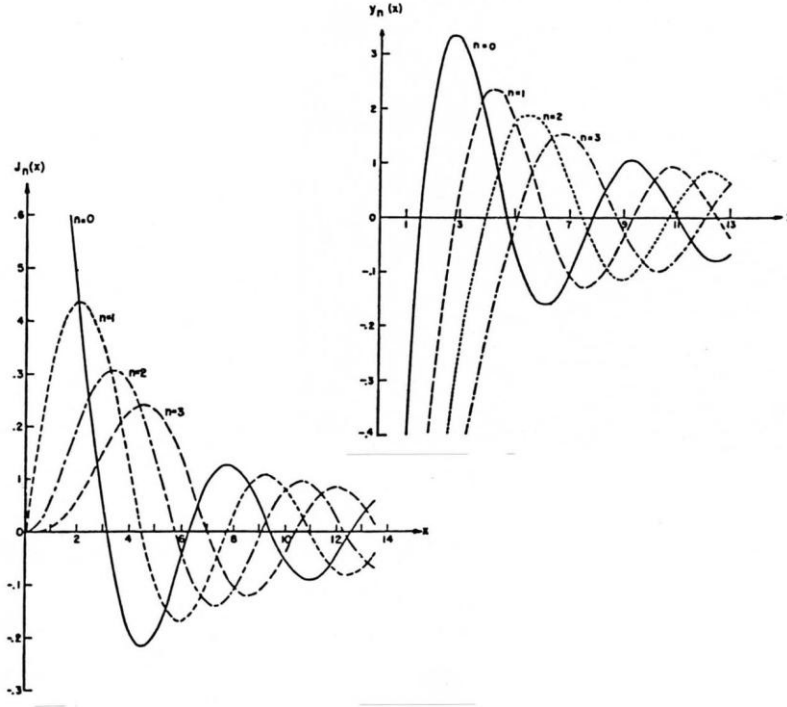
$$\begin{aligned} j_0(z) &= \frac{\sin z}{z}; \\ j_1(z) &= \frac{\sin z}{z^2} - \frac{\cos z}{z}; \\ j_2(z) &= \left( \frac{3}{z^2} - \frac{1}{z} \right) \sin z - \frac{3}{z^2} \cos z; \\ y_0(z) &= -j_{-1}(z) = -\frac{\cos z}{z}; \\ y_1(z) &= j_{-2}(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z}; \\ y_2(z) &= -j_{-3}(z) = \left( -\frac{3}{z^2} + \frac{1}{z} \right) \cos z - \frac{3}{z^2} \sin z. \end{aligned}$$

The boundary conditions for the spherical reactor are the following:

- (1) at  $r = 0$ ,  $\frac{d\phi}{dr}/_{r=0} = 0$ ; the flux is symmetric and finite.

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(2) at  $r = R_0$ ,  $\phi(R_0) = 0$ ; the flux vanishes at the extrapolated boundary.



**Fig. 5.23** Spherical Bessel Functions

The first boundary condition gives

$$\begin{aligned} \frac{d\phi}{dr}\bigg|_{r=0} = 0 &= \lim_{r \rightarrow 0} A \left[ \frac{B \cos Br}{r} - \frac{\sin Br}{r^2} \right] + \lim_{r \rightarrow 0} C \left[ \frac{-B \sin Br}{r} - \frac{\cos Br}{r^2} \right] \\ &= A(0) + C \left( \frac{-B^2}{2} \right). \end{aligned}$$

Application of the second boundary condition gives

$$\phi(R_0) = 0 = A \frac{\sin BR_0}{R_0}.$$

Therefore,  $C = 0$  and the solution becomes

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$$\phi(r) = \frac{A \sin Br}{r}. \quad (5.110)$$

This equation is satisfied only when  $B = n\pi/R_0$ ,  $n = 1, 2, \dots$ .

Therefore, the complete solution for the fundamental mode of the bare spherical reactor is

$$\phi(r) = \frac{A \sin(\pi r/R_0)}{r}, \quad (5.111)$$

where the coefficient  $A$  again corresponds to the operating power level of the reactor.

### 5.13 Comments on Multiregion One-Dimensional Reactors

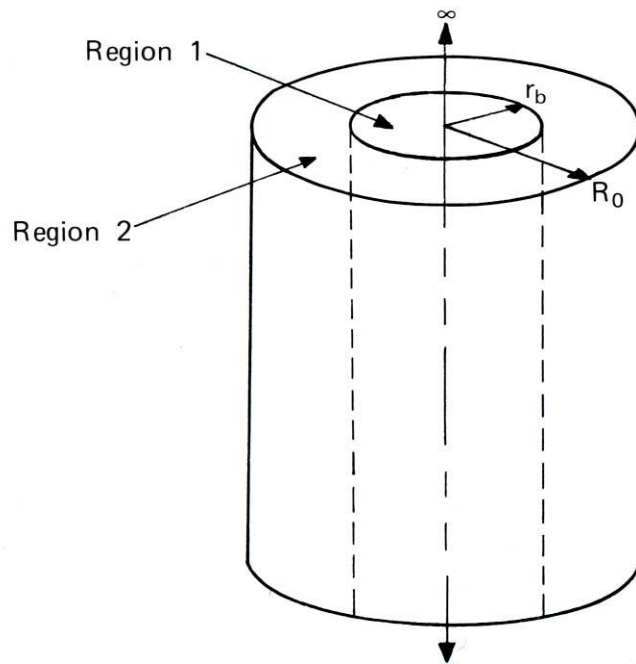
Extending the ideas already presented, we solve the problem of multi-region reactors by using the following series of steps:

1. determine whether  $B^2$  is positive or negative in each homogeneous region;
2. assume the correct type of general solution for the given geometry corresponding to the sign of the buckling term;
3. apply one boundary condition at each outer boundary (or at the center, if symmetry is present) and two boundary conditions of continuity at each interior interface;
4. put the resulting set of equations in vector-matrix form, with the coefficients in the vector;
5. set the determinant of the matrix equal to zero to obtain the transcendental critical equation;
6. solve for either the critical  $k_\infty$  in one region or the critical size of one of the dimensions, given the other parameters and the desired  $k_{\text{eff}}$  value;

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7. solve for all but one of the coefficients in terms of the last coefficient, which is arbitrary;
8. find the arbitrary normalization constant by setting the operating power level equal to the integral of the fission rate over the volume of the reactor.

As an example of the above procedure, consider the case of an infinitely long cylindrical reactor composed of an inner region with a  $k_{\infty 1} = 0.95$  and an outer region with a  $k_{\infty 2} = 1.05$ . Assuming that the outer extrapolated radius is fixed at  $r = R_0$ , we seek to locate the position of the inner boundary between regions,  $r = r_b$ , such that the reactor is critical with  $k_{\text{eff}} = 1.000$ . The situation is depicted in Figure 5.24.



**Fig. 5.24** Two Region Critical Cylindrical Reactor

As a first step, we calculate  $B^2$  for each region. For region 1,

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$$B_1^2 = \left[ \frac{k_{\infty 1} / k_{eff} - 1}{L_1^2} \right] = - \frac{0.05}{L_1^2} = - \kappa_1^2.$$

For region 2,

$$B_2^2 = \left[ \frac{k_{\infty 2} / k_{eff} - 1}{L_2^2} \right] = + \frac{0.05}{L_2^2}.$$

For a one-dimensional cylindrical system the diffusion equation for each region is of the form

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + B^2 \phi = 0.$$

Hence, the appropriate solution forms are

$$\phi_1(r) = A_1 I_0(\kappa_1 r) + C_1 K_0(\kappa_1 r) \quad (5.112)$$

and

$$\phi_2(r) = A_2 J_0(B_2 r) + C_2 Y_0(B_2 r). \quad (5.113)$$

Now, there are a total of five unknowns for this problem, namely,  $A_1$ ,  $C_1$ ,  $A_2$ ,  $C_2$ , and  $r_b$ . There are only four boundary conditions, hence one of the coefficients will be arbitrary. The boundary conditions are the following:

- (1) at  $r = 0$ ,  $\phi_1(0)$  is finite and symmetric, so that  $d\phi_1/dr|_{r=0} = 0$ ;
- (2) and (3), at  $r = r_b$ , we have continuity of flux and current so that

$$\phi_1(r_b) = \phi_2(r_b) \text{ and } -D_1 \frac{d\phi_1}{dr} \Big|_{r=r_b} = -D_2 \frac{d\phi_2}{dr} \Big|_{r=r_b};$$

- (4) at  $r = R_0$ , the flux vanishes at the extrapolated boundary so that



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$$\phi_2(R_0) = 0.$$

The condition of symmetry at the center of the core requires that the coefficient  $C_1 = 0$ . Hence, the solution in the center reduces to

$$\phi_1(r) = A_1 I_0(\kappa_1 r). \quad (5.114)$$

We put the remaining boundary condition equations into vector-matrix form. These are the following:

$$\begin{bmatrix} I_0(\kappa_1 r_b) & -J_0(B_2 r_b) & -Y_0(B_2 r_b) \\ D_1 \kappa_1 I_1(\kappa_1 r_b) & D_2 B_2 J_1(B_2 r_b) & D_2 B_2 Y_1(B_2 r_b) \\ 0 & J_0(B_2 R_0) & Y_0(B_2 R_0) \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ C_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}. \quad (5.115)$$

By setting the determinant of the coefficient matrix equal to zero, we obtain a transcendental equation to be solved for the critical radius  $r_b$ . This is of the form

$$\begin{aligned} & J_0(B_2 R_0) \{ I_0(\kappa_1 r_b) D_2 B_2 Y_1(B_2 r_b) + (Y_0(B_2 r_b) D_1 \kappa_1 I_1(\kappa_1 r_b)) \} \\ & = Y_0(B_2 R_0) \{ I_0(\kappa_1 r_b) D_2 B_2 J_1(B_2 r_b) + J_0(B_2 r_b) D_1 \kappa_1 I_1(\kappa_1 r_b) \}. \end{aligned} \quad (5.116)$$

The critical equation can most easily be solved graphically by plotting both the right- and left-hand sides as a function of the radius  $r_b$  on the same graph. The intersection of the curves at the smallest value of  $r_b$  is the critical radius.

Next, we solve for all but one of the coefficients in terms of one arbitrary coefficient, e.g.,  $A_1$ . This is a simple process of algebraic elimination. The coefficient values so derived can be placed into the expressions for  $\phi_1(r)$  and  $\phi_2(r)$ , which then contain only the single coefficient  $A_1$ .

Finally, we can find  $A_1$  by integrating the fission rate over

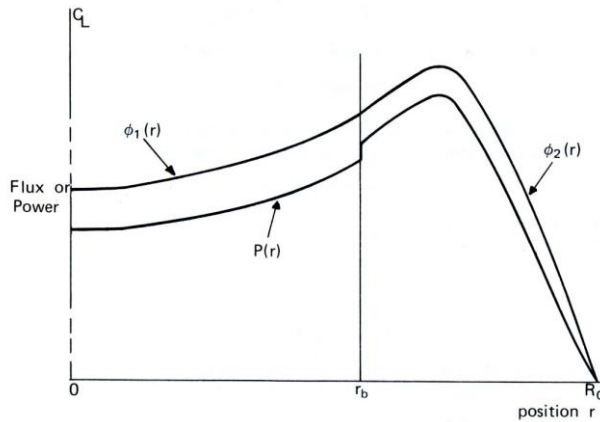
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the volume of the core and then setting the result equal to the total core power. For this particular case, the result is of the form

$$P \left( \frac{\text{total watts}}{\text{cm of height}} \right) = \frac{\int_0^{r_b} 2\pi r \Sigma_{f1} \phi_1(r) dr + \int_{r_b}^{R_0} 2\pi r \Sigma_{f2} \phi_2(r) dr}{3.1 \times 10^{10} (\text{fission/s} - \text{watt})}, \quad (5.117)$$

where  $\Sigma_{f1}$  and  $\Sigma_{f2}$  are the macroscopic fission cross sections in regions 1 and 2, respectively, and  $\phi_1$  and  $\phi_2$  are dependent upon  $A_1$ .

The flux solution and corresponding power distribution are plotted in Figure 5.25. Notice that the power distribution is discontinuous because of the change of  $\Sigma_f$  at the interface.



**Fig. 5.25** Flux and Power vs. Position in a Two Region Cylindrical Reactor

### 5.14 Multidimensional Reactors

As an example of a two-dimensional reactor system, we examine the bare, homogeneous, finite cylindrical reactor. In the general case, the directions  $r$  and  $z$  are not separable, which can be justified on physical grounds, but we assume separability here in order to examine the general form of the solution. In

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cylindrical geometry with azimuthal symmetry, the Laplacian is

$$\nabla^2 \equiv \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial z^2}.$$

Hence, our diffusion equation becomes

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{\partial^2 \phi}{\partial z^2} + B^2 \phi = 0. \quad (5.118)$$

Assume a separable solution of the form

$$\phi(r, z) = R(r)Z(z). \quad (5.119)$$

Insertion of this solution into the diffusion equation and division by  $RZ$  gives the separated equation

$$\left[ \frac{\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial R}{\partial r} \right)}{R} \right] + \left[ \frac{\frac{\partial^2 Z}{\partial z^2}}{Z} \right] + B^2 = 0. \quad (5.120)$$

Since  $R$  and  $Z$  are both independent, each of the bracketed terms must be a constant. We do not know the signs of the constants, but physically, since we do know that neutrons will leak out of the system in all directions, we guess that both will be negative corresponding to out-leakage. This assumption is subject to examination in terms of the ability of the separated solutions to meet the boundary conditions of the problem. The buckling equation with the above assumption becomes

$$-\alpha^2 - \beta^2 + B^2 = 0. \quad (5.121)$$

The separated differential equations become

$$\frac{1}{r} \frac{d}{dr} \left( r \frac{dR}{dr} \right) + \alpha^2 R = 0 \quad (5.122)$$

and

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$$\frac{d^2 Z}{dz^2} + \beta^2 Z = 0. \quad (5.123)$$

The boundary conditions are the following:

- (1)  $R(R_0) = 0$ , flux vanishes at the extrapolated boundary;
- (2)  $dR/dr|_{r=0} = 0$ , symmetry at the reactor centerline;
- (3)  $Z(Z_0/2) = 0$ , flux vanishes at the extrapolated boundary;
- (4)  $dZ/dz|_{z=0} = 0$ , symmetry.

The second boundary condition excludes the  $Y_0$  function, while the fourth excludes the sine function. Therefore, the final solution is of the form

$$\phi(r, z) = AJ_0(\alpha r) \cos(\beta z). \quad (5.124)$$

Since only the fundamental mode is present in a critical steady state reactor, the first boundary condition gives

$$\alpha = \frac{2.405}{R_0},$$

while the third gives

$$\beta = \frac{\pi}{Z_0}.$$

The complete solution is therefore

$$\phi(r, z) = AJ_0\left(\frac{2.405r}{R_0}\right) \cos\left(\frac{\pi z}{Z_0}\right). \quad (5.125)$$

The critical buckling, based upon both core geometry and material composition, then satisfies the expression

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$$B^2 = \left( \frac{2.405}{R_0} \right)^2 + \left( \frac{\pi}{Z_0} \right)^2 = \left[ \frac{k_\infty / k_{eff} - 1}{L^2} \right]. \quad (5.126)$$

Hence, the critical composition  $k_\infty$  can be obtained for fixed dimensions, or one of the dimensions can be obtained if the material composition and the other dimension are fixed, once a desired value of  $k_{eff}$  is chosen.

As before, the arbitrary constant  $A$  is determined from the desired power level by integration. In this case,

$$P = \frac{1}{c} \int_0^{R_0} \int_{-Z_0/2}^{+Z_0/2} \sum_f \phi(r,z) dz \, 2\pi r \, dr. \quad (5.127)$$

**Other Geometries.** Similar solutions can be obtained in other geometries, such as  $R\Theta$ ,  $XY$ ,  $XYZ$ ,  $R\Theta\Psi$ , etc. by appropriate specification of the Laplacian operator. Analytic solutions are usually only practical for a small number of dimensions or regions, since the algebra becomes unwieldy as the problem size increases. On the other hand, for a large number of small regions in a reactor, the solution may be approximately separable over each separate region, making analytic solutions to complicated problems feasible. A computer-based method of solution functions, which is a forerunner of the so-called "coarse-mesh" methods, has been developed by Bobone; the appropriate matching of solutions at interfaces and boundaries is handled automatically. In the usual case, however, the finite difference analog of the multi-region diffusion equation is solved numerically in an iterative fashion by computer.

**Effect of a Reflector.** If one puts a reflector material on the outside of a fuel region, the flux at the interface is increased over the value present without the reflector. This increases the fission rate near the interface with the net result that a smaller central core is necessary to achieve criticality.

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This effect is known as "reflector savings." Unfortunately, the concept does not include the moderating effect of the reflector, which is also significant, and therefore an analytical treatment will not be presented here.

### 5.15\* Diffusion Length Experiment

Recall that the flux distribution in a semi-infinite slab containing a planar source varies with distance as  $\phi(x) = (SL/2D)e^{-|x|/L}$ . This solution, when plotted on semi-logarithmic paper, is a straight line whose slope is equal to  $-1/L$ . Hence, a possible method of measuring  $L$  is to perform a source experiment and measure a quantity that is proportional to the local flux, such as the saturation activity of an indium foil.

Obviously, it is impossible to obtain a semi-infinite medium, but it is possible to approximate such a medium and correct for the effects of finite size. This experiment is called a Sigma Pile. One possible configuration is a rectangular parallelepiped, made of pure material such as graphite, which is placed on top of an essentially uniform planar source such as a small portion of a reactor. The experiment is shown in Figure 5.26.

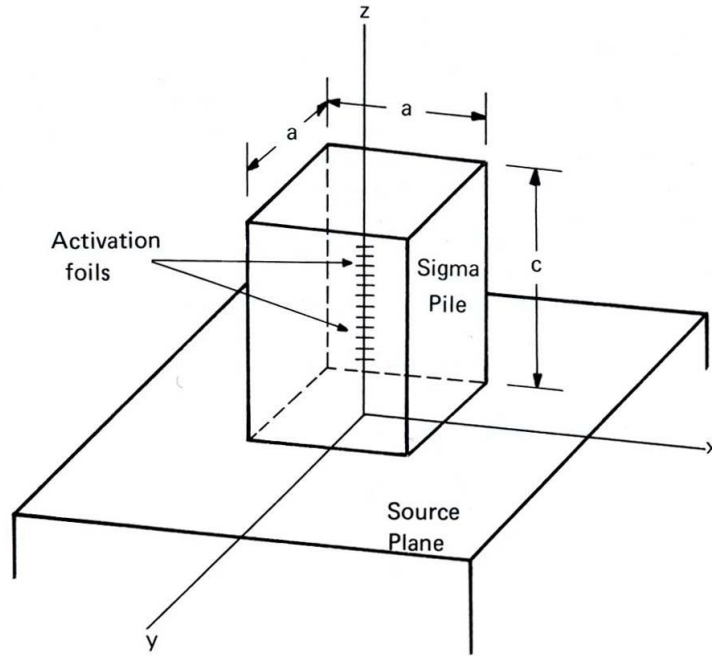
The diffusion equation in rectangular geometry is

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} - \frac{1}{L^2} \phi = 0. \quad (5.128)$$

We seek a solution by the process of separation of variables of the form

$$\phi(x,y,z) = X(x)Y(y)Z(z). \quad (5.129)$$

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**Fig. 5.26** Sigma Pile Experiment

When the assumed solution is substituted into the diffusion equation, the resulting separated expression is

$$\left[ \frac{1}{X} \frac{d^2 X}{dx^2} \right] + \left[ \frac{1}{Y} \frac{d^2 Y}{dy^2} \right] + \left[ \frac{1}{Z} \frac{d^2 Z}{dz^2} \right] - \frac{1}{L^2} = 0. \quad (5.130)$$

Each of the bracketed terms must be a constant in order to satisfy this equation.

Since the buckling of the system is negative, the total system has a net in-leakage. We examine the situation in each of the coordinate directions separately using physical reasoning. In both the  $x$  and  $y$  directions there are no sources but there is a leakage loss of neutrons across the outer surfaces. Net out-leakage implies that the buckling in each of these directions must be positive and the coefficients negative. On the contrary, in the  $z$  direction, neutrons enter from the source and leak out of the top surface; the source must supply this leakage, plus

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absorption in the medium and also the leakage out of the x and y directions. This implies a net in-leakage in the z direction so that the buckling is negative and the coefficient is positive. Since X, Y and Z are independent of one another, each of the terms of the separated equation must be equal to a constant whose sign has been determined above. The separated buckling equation becomes

$$-\alpha^2 - \beta^2 + \gamma^2 - \frac{1}{L^2} = 0, \quad (5.131)$$

which gives the three separate differential equations

$$\frac{d^2 X}{dx^2} + \alpha^2 X = 0, \quad (5.132)$$

$$\frac{d^2 Y}{dy^2} + \beta^2 Y = 0, \quad (5.133)$$

and

$$\frac{d^2 Z}{dz^2} - \gamma^2 Z = 0. \quad (5.134)$$

We need a total of six boundary conditions. These are the following:

- (1)  $X(a/2) = 0$ , flux vanishes at the extrapolated boundary;
- (2)  $dX/dx|_{x=0} = 0$ , symmetry about the centerline of the pile;
- (3)  $Y(a/2) = 0$ , flux vanishes at the extrapolated boundary;
- (4)  $dY/dy|_{y=0} = 0$ , symmetry about the centerline of the pile;
- (5)  $Z(c) = 0$ , flux vanishes at the extrapolated boundary;
- (6)  $-D dZ/dz|_{z=0} = S$ , source condition.

Boundary conditions (2) and (4) imply that only cosine solutions



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are present in the x and y directions. Boundary conditions (1) and (3) imply that solutions exist only for specific values of  $\alpha$  and  $\beta$ , namely,

$$\alpha = \frac{m\pi}{a}, m = 1, 3, 5, \dots \text{odd}$$

and

$$\beta = \frac{n\pi}{a}, n = 1, 3, 5, \dots \text{odd}.$$

All such even harmonics can be excited by the symmetric source, and can be present in the steady state. Hence, the constant  $\gamma$  must also be multi-valued and must obey the buckling equation

$$\gamma_{mn}^2 = \frac{1}{L^2} + \left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{a}\right)^2, m, n \text{ odd.} \quad (5.135)$$

The complete solution must therefore be of the form

$$\phi(x, y, z) = \sum_{m, n, \text{ odd}} Z_{mn}(z) \cos\left(\frac{m\pi x}{a}\right) \cos\left(\frac{n\pi y}{a}\right), \quad (5.136)$$

where the function Z is determined from the differential equation

$$\frac{d^2 Z_{mn}}{dz^2} - \gamma_{mn}^2 Z_{mn} = 0. \quad (5.137)$$

Application of boundary condition (5) leads to the form

$$Z_{mn}(z) = A_{mn} \sinh \gamma_{mn}(c - z), \quad (5.138)$$

and application of the source condition (6) leads to appropriate values for the constants  $A_{mn}$ , which will not be obtained here.

Experimentally, one puts activation foils at various positions along the z axis at a specific (x, y) location such as  $x = 0$  and  $y = 0$ . The approximate activation distribution for a long parallelepiped at a position not too near the outer surface

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is the exponential sum

$$A_{sat}(z) \approx C_{11}e^{-\gamma_{11}z} + C_{13}e^{-\gamma_{13}z} + C_{31}e^{-\gamma_{31}z} + \dots, \quad (5.139)$$

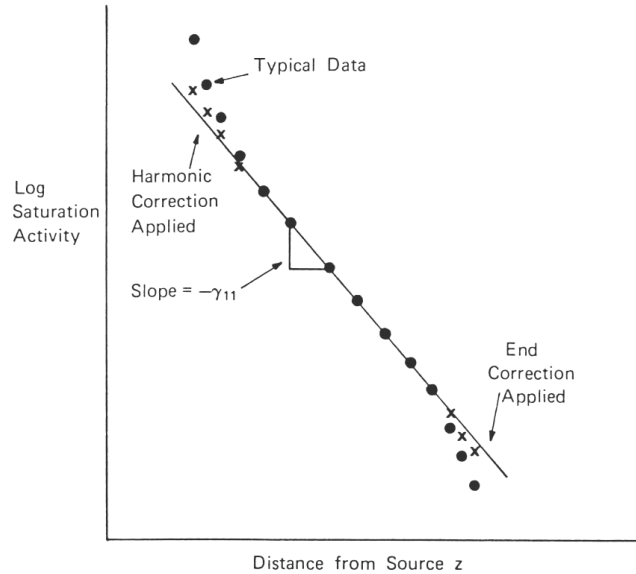
where  $C_{11}$ ,  $C_{13}$ ,  $\dots$  are coefficients that correspond to  $A_{11}$ , etc.

Since  $\gamma_{13}$  and  $\gamma_{31}$  are larger than  $\gamma_{11}$ , these exponentials decay more rapidly with distance from the source plane.

Therefore, not too near the source or the outer boundary the distribution is approximately

$$A_{sat}(z) \approx C_{11}e^{-\gamma_{11}z}. \quad (5.140)$$

The slope of the activation vs. distance curve is approximately  $-\gamma_{11}$ , which allows us to obtain an estimate of  $1/L^2$  from the buckling equation with  $m = n = 1$ . Typical experimental results are sketched in Figure 5.27.



**Fig. 5.27** Sigma (Exponential) Pile Data

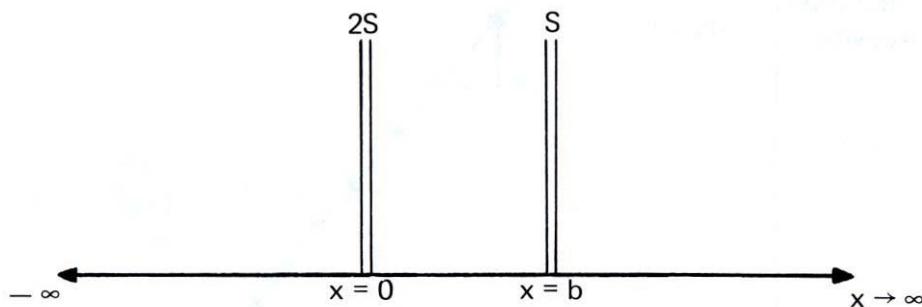
Two important points emerge from the foregoing analysis. First, under certain circumstances it is possible to obtain positive  $B^2$  type solutions (convex) for problems that are

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inherently of a negative  $B^2$  (concave) type. Second, harmonic flux solutions can be excited by suitable placement of neutron sources, and by analogy, placement of neutron sinks.

### Problems

- 5.1 Find the detailed flux solution for a point source of strength  $S$  neutrons/s located at the center of a sphere of radius  $R$ . The sphere is surrounded by a vacuum.
- 5.2 Complete the solution to the two region planar source problem described in Section 5.3.
- 5.3\* Consider an infinite medium containing two infinite source planes which emit neutrons isotropically and which are located perpendicular to the  $x$  axis a distance of  $b$  centimeters apart.



- a) If one of the sources is twice the strength of the other, calculate the flux distribution in the medium in terms of its diffusion coefficient  $D$  and its macroscopic absorption cross section  $\Sigma_a$ .
- b) If all of the material in the left-hand plane ( $x < 0$ ) is replaced with material that has a diffusion constant which is four times the value in the right-half plane, calculate the flux

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distribution.

- c) Sketch the results of parts a and b.

**5.4** A neutron current from a reactor is normally incident on a 50-cm slab of graphite. This current can be considered to be the partial current  $J_+(0)$ . For graphite, use  $D = 0.84$  cm and  $\Sigma_a = 2. \times 10^{-4}$  cm<sup>-1</sup>.

- a) Find the fraction of neutrons reflected by the slab, defined as  $J_-(0)/J_+(0)$ ;  
b) Find the fraction of neutrons transmitted through the slab, defined as  $J_+(50)/J_+(0)$ .

**5.5\*** The albedo, or reflection coefficient, of a scattering medium is defined as

$$\beta \equiv \frac{J^{out}}{J^{in}} = \frac{J_-}{J_+},$$

when the reflecting medium is located to the right of the source-containing medium. The albedo is used as a boundary condition to calculate the flux distribution in the source-containing region. In a similar manner, a quantity known as the blackness or absorption coefficient can be defined for an absorber region as

$$\alpha \equiv \frac{J}{J^{in}} = \frac{J_+ - J_-}{J_+} = 1 - \beta.$$

Consider an infinite medium with a spatially uniform unit source of thermal neutrons and constants  $D$  and  $\Sigma_a$ , containing a small sphere of radius  $R$  and known blackness  $\alpha$  (the fraction of incident current which is absorbed when the sphere is surrounded by vacuum).

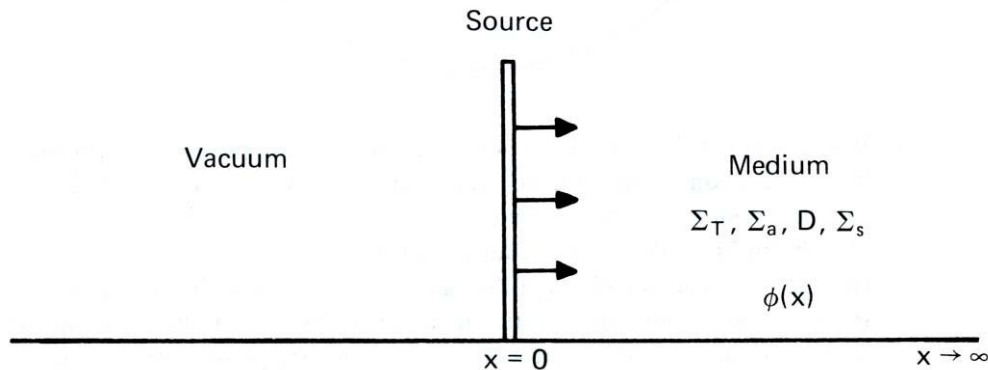
- a) Evaluate the flux outside the sphere as a function of  $L^2 = D/\Sigma_a$ ,  $R$  and  $\alpha$ , and find the rate at which

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neutrons are absorbed.

- b) Discuss the behavior of these results as the radius  $R$  approaches zero. In the limit, does taking  $\alpha = 1$  make any difference?
- c) Suppose there is no source in the medium, but that instead the sphere produces neutrons at the rate of  $S = 1/s$ . Find the flux distribution in general, and in the limit as  $R \rightarrow 0$ .
- d) Without detailed calculation, discuss the corresponding results for both an infinite plane and a line source and then sink of neutrons.
- e) What conclusions can you draw as to the appropriateness of using a point, line and plane as idealized neutron sources on the one hand, and as idealized sinks on the other?

**5.6** We wish to compute a realistic neutron flux distribution in the vicinity of a plane neutron source located at  $x = 0$  next to an infinite medium. This is an example of a medical physics application where the source is a beam from a reactor and the medium is a human patient.



We assume that the fast neutrons from the source are attenuated exponentially as they enter the medium and only enter the thermal flux distribution after a scattering

## NUCLEAR REACTOR THEORY AND DESIGN

event. Hence, the form of the source distribution is:

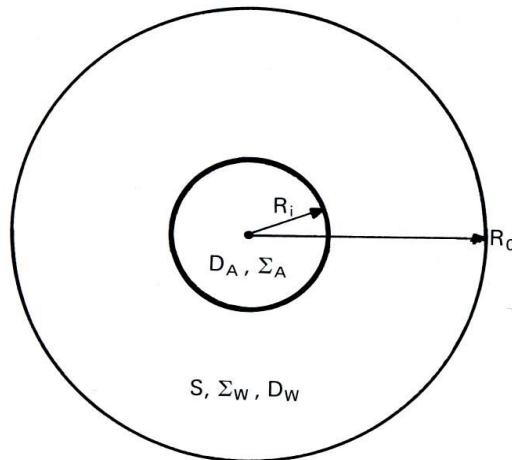
$$S(x) = \frac{\sum_s}{\sum_T} e^{-\sum_T x}.$$

- a) What is the total source strength  $S_0$ ?
- b) What is the particular solution to the diffusion equation?

Hint: Assume that the particular solution is proportional to the source.

- c) What are the boundary conditions?
- d) What is the complete solution for the flux?

**5.7\*** Consider a long cylindrical cell, which is one of many in a reactor. The cell consists of an outer region of radius  $R_0$  containing water, and an inner region of radius  $R_i$ , which for our purposes contains a strong neutron absorber. Assume that there is a spatially uniform neutron source of  $S$  neutrons/cm<sup>3</sup>-s in the water region only and none in the absorber region. Assume further that there is no net current crossing the outer boundary of the cell, and that the cell is very long compared to its diameter.



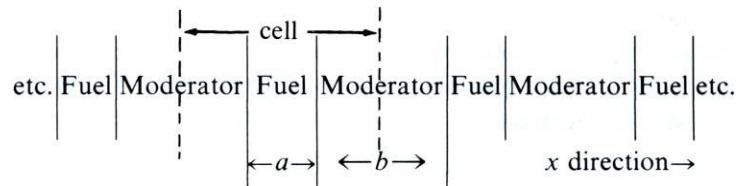
- a) If one-speed diffusion theory is considered to be

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applicable to this problem, obtain an expression for the neutron flux  $\phi(r)$  as a function of distance from the center of the cell.

- b) Sketch the flux solution as a function of  $r$ .
- c) Discuss the adequacy of using diffusion theory to solve this problem.
- d) If you want to homogenize the material properties of this cell into an equivalent uniform cell, what would be a reasonable way to proceed if you knew the original number densities in each region?

**5.8** Consider a slab-type reactor cell in a regular array, as shown below.



Consider that neutron slowing down occurs only in the moderator and that to a first approximation this acts as a spatially uniform source  $Q$  feeding the thermal flux group in the moderator region. There is no slowing down source in the fuel region. If one-speed diffusion theory is considered to be accurate for this problem, do the following:

- a) Sketch the thermal flux distribution in this array.
- b) Calculate the thermal flux distribution in a typical cell in this array.
- c) Calculate the disadvantage factor for this cell, defined as

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$$\zeta \equiv \frac{\bar{\phi}_M}{\phi_F}.$$

- d) If you wanted to homogenize the fuel and moderator into a single equivalent region, how would you do it? Explain.

**5.9\*** There is always a non-zero neutron population in reactors containing U-233, U-235, U-238, or Pu-239, even when the reactor is shut down, which is due to spontaneous fission. U-238 shows the greatest specific rate of spontaneous fission, i.e., it has the shortest half-life for spontaneous fission of those listed. Consider a homogeneous sub-critical bare slab of thickness  $2a$  containing only a slightly absorbing moderator and U-238. The spontaneous fission of the U-238 represents a volumetric neutron source of strength  $S$  neutrons/cm<sup>3</sup>-s. Assume that the fission neutrons are thermalized at their point of birth, i.e., ignore fast leakage and ignore any fission that might occur in U-238 from the absorption of fast neutrons from spontaneous fission. For both parts employ boundary conditions of zero flux at the slab surfaces.

- a) Show that the Green's function for the one group thermal diffusion operator for the slab is given by

$$G(x, x') = \begin{cases} \frac{-\sinh \eta(x' - a) \sinh \eta(x + a)}{\eta D \sinh 2\eta a} & \text{for } -a \leq x \leq x' \\ \frac{-\sinh \eta(x' + a) \sinh \eta(x - a)}{\eta D \sinh 2\eta a} & \text{for } x' \leq x \leq +a \end{cases},$$

where  $\eta = 1/L$ .

(Hint: Take the zero of the coordinate system at the center of the slab and initially work with

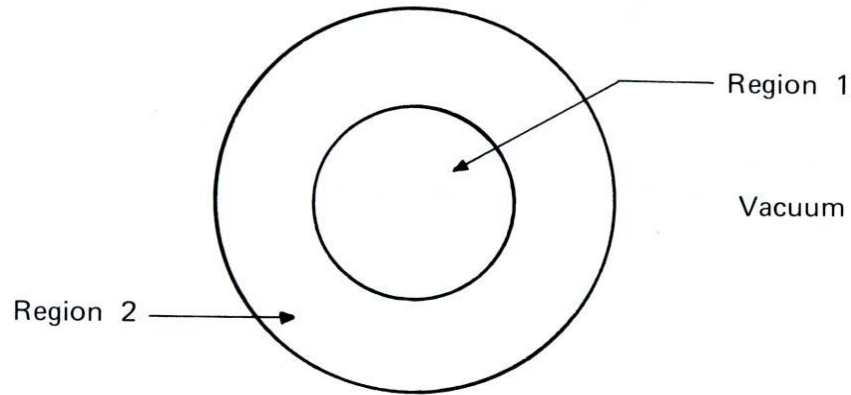


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exponentials rather than hyperbolic functions.)

- b) Use the Green's function to calculate the thermal flux resulting from the spontaneous fission source.

**5.10** Consider the two-region cylindrical reactor shown below, whose height is effectively infinite. Assume that one-group diffusion theory is adequate to represent the reactor.



You are given the following information for the two regions:

Property	Region 1	Region 2
Radius (cm)	$R$	$2R$
$k$ -infinity	$0.98$	$?$
Diffusion constant (cm)	$D$	$1.1D$
Absorption cross section ( $\text{cm}^{-1}$ )	$\Sigma_a$	$1.1\Sigma_a$
Prompt neutrons per fission	$\nu$	$\nu$
Extrapolation distance	$-$	negligible

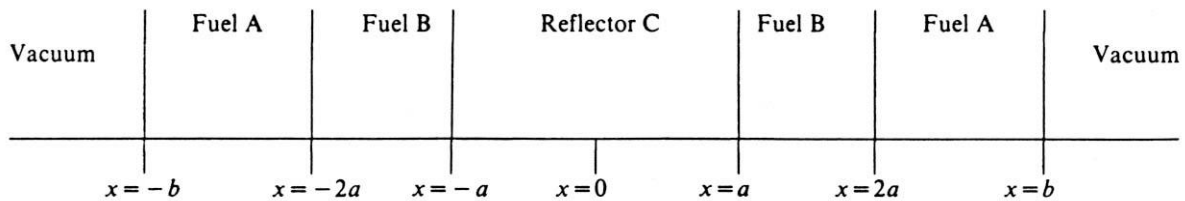
- a) If it is desired that the reactor be exactly critical with  $k_{\text{eff}} = 1.0$ , derive expressions which give the amount of fuel to be loaded into Region 2 in terms of the required macroscopic fission cross section  $\Sigma_f$ . You need not do all of the algebra,

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but must indicate the method of solution of your equations.

- b) Sketch the flux shape in the core as a function of position.
- c) Sketch the power profile in the core as a function of position.
- d) If the vacuum region were replaced with water, what would be the effect on the system? Do you think that one-group diffusion theory would still be adequate? Explain.

**5.11** Consider the following symmetric, three region, 1-dimensional slab reactor.



The value of the distance  $a$  is not specified as yet, but the extrapolated outer radius is  $x = \pm b$  and the properties of the three regions are:

$$[A] k_{\infty A} = 1.05; [B] k_{\infty B} = 1.25; [C] k_{\infty C} = 0.$$

All three regions have the same value of  $L^2$ .

- a) Set up the solution to the flux distribution problem (you need not do all of the algebra) if the value of  $k_{\text{eff}}$  which is desired is  $k_{\text{eff}} = 1.15$ .
- b) Set up the solution to the problem if the desired  $k_{\text{eff}} = 1.00$ .
- c) Sketch qualitatively the flux distributions obtained in parts a and b.

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- 5.12** You are given a bare slab reactor of half-width  $l$ , describable by one-group diffusion theory. Consider that the material properties are  $D$ ,  $\Sigma_a$  and  $\nu\Sigma_f$ . The flux at each outer boundary extrapolates linearly to zero at a distance  $X_L$  from the surface.
- a) Find the critical ( $k_{\text{eff}} = 1$ ) flux solution in this core.
  - b) What is the value of the flux at the surface relative to that in the center?
  - c) What is the leakage per unit surface area from the core?

## References

- S. Glasstone and M. C. Edlund**, *The Elements of Nuclear Reactor Theory*, (D. Van Nostrand, Princeton, NJ 1952), Chapter 5.
- M. Abramowitz and I. A. Stegun**, *Handbook of Mathematical Functions*, NBS Applied Mathematics Series, (USGPO, Washington, D.C., 1964).
- R. Bobone**, "The Method of Solution Functions: A Computer-Oriented Solution of Boundary Value Problems as Applied to Nuclear Reactors," *Nucl. Sci. Eng.*, **29**, (1967) 337.



## FEW-GROUP EQUATIONS AND NUMERICAL SOLUTION METHODS

In Chapter 5 we examined in some detail the analytic solutions to both the one-speed source problem and the critical reactor problem. We now consider a more realistic and practical treatment that includes energy-dependent effects for a system composed of many spatial regions.

To this end the treatment starts with a description of the static energy-dependent neutron balance equation. This equation is first discretized into the standard few-group diffusion theory equations; these equations are then converted to a finite difference form for one-dimensional geometries. At this point, the spatial flux solution can be obtained iteratively; simple proofs of convergence are given. Finally, the one-speed and two-group solutions are compared.

### 6.1 Energy-Dependent Diffusion Equation

Recall that the one-speed transport equation contained two different physical deficiencies: namely, that (1) no energy was transferred in a scattering collision; and (2) all fission neutrons were born at a single energy. We know that in a thermal reactor, the majority of absorption reactions occur at an energy that is a fraction of an electron volt, while all fission neutrons appear at energies of the order of a million electron volts. The fast neutrons moderate down to thermal energies by virtue of the energy transferred in scattering collisions.

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Hence, these features must be included in the balance equations if realistic computational results are to be achieved.

In order to include the energy dependence in our calculations, we now must consider the neutron balance in  $dE$  about  $E$ , as well as the balance in  $d\Omega$  about  $\vec{\Omega}$  and in  $dr$  about  $\vec{r}$ . In the case of the fission term, we must integrate the fission rate over all energies and angles to obtain the total number of fission reactions, and then distribute those fission neutrons isotropically according to the spectrum distribution  $\chi(E)$ . In the case of the inscattering term, we must consider neutrons of any energy  $E'$  and angle  $\vec{\Omega}'$  that can enter the energy  $E$  at angle  $\vec{\Omega}$ , which means that this term contains an integral over  $E'$  as well as over  $\vec{\Omega}'$ . The angular energy-dependent flux is written as

$$\Phi(\vec{r}, E, \vec{\Omega}) \frac{\text{neutrons}}{\text{cm}^2 \cdot \text{s} \cdot \text{eV} \cdot \text{sr}}$$

The energy-dependent, steady state Boltzmann transport equation can be written as follows, when fission is isotropic:

$$\text{leakage} \quad \text{absorption and} \\ \text{outscatter}$$

$$\begin{aligned} & \vec{\Omega} \cdot \nabla \Phi(\vec{r}, E, \vec{\Omega}) + \sum_T(\vec{r}, E) \Phi(\vec{r}, E, \vec{\Omega}) \\ & \quad \text{source} \quad \quad \quad \text{inscatter} \quad \quad \quad (6.1) \\ & = S(\vec{r}, E, \vec{\Omega}) + \int_0^\infty \int_0^{4\pi} \sum_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(\vec{r}, E', \vec{\Omega}') d\Omega' dE' \\ & \quad \quad \quad \text{fission} \\ & + \frac{\chi(E)}{4\pi} \int_0^\infty \int_0^{4\pi} \nu \sum_f(\vec{r}, E') \Phi(\vec{r}, E', \vec{\Omega}') d\Omega' dE'. \end{aligned}$$

The in-scattering term is not really as formidable as it seems at

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first, because the amount of energy transfer and the angular direction change that occur in a scattering collision are uniquely related to one another by the conservation laws. One of the integrations over angle which is necessary in deriving the  $P_n$  equations becomes trivial and leads to a scattering transfer cross section of the form  $\sum_{sn}(\vec{r}, E' \rightarrow E)$ , for order  $n = 0, 1, 2, \dots$ .

The energy-dependent diffusion equation can be derived from the transport equation in the same manner as the one-speed diffusion equation was derived. The result is simply

$$\begin{aligned}
 & \text{leakage} \quad \text{absorption and} \\
 & \quad \text{outscatter} \\
 & -\nabla \cdot D(\vec{r}, E) \nabla \phi(\vec{r}, E) + \sum_T(\vec{r}, E) \phi(\vec{r}, E) \\
 & \quad \text{source} \quad \text{inscatter} \quad (6.2) \\
 & = S(\vec{r}, E) + \int_0^\infty \sum_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E') dE' \\
 & \quad \text{fission} \\
 & + \chi(E) \int_0^\infty \nu \sum_f(\vec{r}, E') \phi(\vec{r}, E') dE',
 \end{aligned}$$

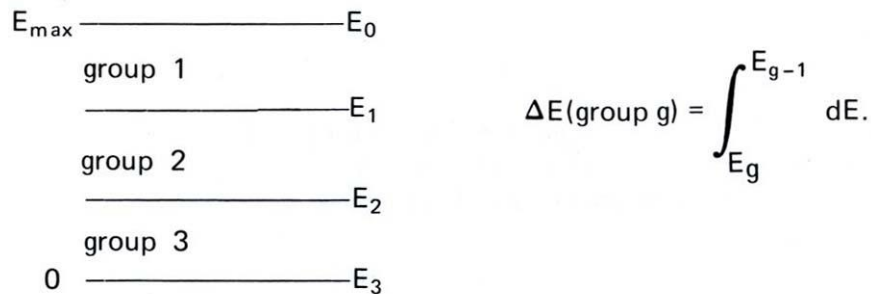
where the energy-dependent flux is  $\phi(\vec{r}, E)$  neutrons/cm<sup>2</sup>-s-eV. The in-scattering integral is actually fairly complicated to evaluate because the energy transfer for scattering species having a mass of  $A > 1$  is a discontinuous process. This subject will be treated in detail in the section on neutron slowing down theory in Chapter 11.

### 6.2 Few-Group Diffusion Equations

Assuming that we know all of the material properties of the

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system, the few-group equations can be obtained for each homogeneous region of the reactor by discretizing the energy-dependent diffusion equation over energy. One chooses important energy intervals called groups and simply averages the balance equation over each of these energy regions to obtain a set of few-group equations that approximates the basic features of the original energy-dependent equation. The energy groups are numbered from  $g = 1$  for the highest energy, to  $g = G$  for the lowest energy. For thermal reactors one often takes  $G = 3$ , where group 1 is usually chosen to include the entire fission spectrum region (say from  $E_{\max} = 10$  MeV down to 100 keV), group 2 is chosen to include the slowing down and resonance region (say 100 keV down to 0.6 eV), and group 3 is chosen to include the thermalization region (say from 0.6 eV down to 0). More groups are chosen if other important energy-dependent features must be described with accuracy. For example, a three-group structure is shown in Figure 6.1.



**Fig. 6.1** Few Group Energy Structure

In order to obtain the few-group equations, the following steps are required:

1. Express all integrals over the full energy range as the sum of integrals over the groups. This is done for both the in-scatter and fission terms;



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2. Integrate the energy-dependent diffusion equation over group  $g$ , term by term. Do this separately for  $g = 1, G$ ;
3. Replace each of the resulting integrals with the product of the average group flux and the average group cross section.

The equation for the  $g$ th group becomes the following for each homogeneous spatial region in the reactor:

$$\begin{aligned}
 & \text{leakage} \quad \text{absorption and} \\
 & \quad \text{outscatter} \\
 & \int_{E_g}^{E_{g-1}} -D(E) \nabla^2 \phi(E) dE + \int_{E_g}^{E_{g-1}} \Sigma_T(E) \phi(E) dE \\
 & \quad \text{source} \quad \text{inscatter} \\
 & = \int_{E_g}^{E_{g-1}} S(E) dE + \int_{E_g}^{E_{g-1}} \left[ \sum_{g'=1}^G \int_{E_{g'}}^{E_{g'-1}} \Sigma_s(E' \rightarrow E) \phi(E') dE' \right] dE
 \end{aligned} \tag{6.3}$$

Note that the in-scattering term contains a double integral because the scattering transfer cross section is a function of the two variables  $E$  and  $E'$ , whereas the fission term contains the product of two single integrals.

In order to simplify the equations further, we must make a number of definitions of average quantities. Let the group flux be given by the expression

$$\phi_g(\vec{r}) \equiv \int_{E_g}^{E_{g-1}} \phi(\vec{r}, E) dE. \tag{6.4}$$

The group flux has units of (neutrons/cm<sup>2</sup>-s), whereas the energy-dependent flux has units of (neutrons/cm<sup>2</sup>-s-eV). Furthermore, let the following cross-section averages be defined, where the spatial dependence is implied:

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$$\sum_{sg \rightarrow g} \phi_{g'} \equiv \int_{E_g}^{E_{g+1}} \int_{E_{g'}}^{E_{g'+1}} \sum_s (E' \rightarrow E) \phi(E') dE' dE.$$

$$\sum_{Tg} \phi_g \equiv \int_{E_g}^{E_{g+1}} \sum_T (E) \phi(E) dE,$$

$$D_g \nabla^2 \phi_g \equiv \int_{E_g}^{E_{g+1}} D(E) \nabla^2 \phi(E) dE,$$

(6.5)

$$\nu \sum_{fg} \phi_g \equiv \int_{E_g}^{E_{g+1}} \nu \sum_f (E) \phi(E) dE,$$

$$\sum_{fg} \phi_g \equiv \int_{E_g}^{E_{g+1}} \sum_f (E) \phi(E) dE,$$

Finally, let the source and group spectra be defined as

$$S_g \equiv \int_{E_g}^{E_{g+1}} S(E) dE,$$

and

$$\chi_g \equiv \int_{E_g}^{E_{g+1}} \chi(E) dE. \tag{6.6}$$

It should be noted that proper averages for the group cross sections can only be obtained if a detailed energy spectrum, appropriate to the problem at hand, is available beforehand for use in the averaging process. This implies that fine-mesh, zero-dimensional calculations must be done first for each different material region in the reactor in order to obtain an acceptable weighting function. It also implies that a few-group library suitable for thermal reactor calculations would not be usable for fast reactor calculations, and vice versa.

When the group averages are inserted, the equation for the  $g$ th energy group becomes simply

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*leakage   absorption and outscatter   source   in scatter   fission*

$$-D_g \nabla^2 \phi_g + \sum_{Tg} \phi_g = S_g + \sum_{g'=1}^G (\sum_{sg \rightarrow g} \phi_{g'}) + \chi_g \sum_{g'=1}^G (\nu \sum_{fg} \phi_{g'}). \quad (6.7)$$

Note that, by definition

$$\sum_{Tg} = \sum_{ag} + \sum_{g'=1}^G \sum_{sg \rightarrow g'}. \quad (6.8)$$

Therefore, the within-group scattering term,  $\sum_{sg \rightarrow g}$ , appears on both sides of Eq. (6.7) and cancels out in agreement with the one-speed situation. In the few-group structure pictured in Figure 6.1, where  $G = 3$ , the scattering includes down-scatter only because neutrons always lose energy in scattering collisions. This implies that

$$\sum_{sg \rightarrow g} = 0 \quad \text{for } g' > g.$$

Neutrons that scatter out of one group reappear in a lower energy group. Hence, the three-group equations can be written explicitly as

$$-D_1 \nabla^2 \phi_1 + \sum_{a1} \phi_1 + \sum_{s1 \rightarrow 2} \phi_1 + \sum_{s1 \rightarrow 3} \phi_1 = S_1 + \chi_1 [\nu \sum_{f1} \phi_1 + \nu \sum_{f2} \phi_2 + \nu \sum_{f3} \phi_3],$$

$$-D_2 \nabla^2 \phi_2 + \sum_{a2} \phi_2 + \sum_{s2 \rightarrow 3} \phi_2 = S_2 + \sum_{s1 \rightarrow 2} \phi_1 + \chi_2 [\nu \sum_{f1} \phi_1 + \nu \sum_{f2} \phi_2 + \nu \sum_{f3} \phi_3],$$

and

$$-D_3 \nabla^2 \phi_3 + \sum_{a3} \phi_3 = S_3 + \sum_{s1 \rightarrow 3} \phi_1 + \sum_{s2 \rightarrow 3} \phi_2 + \chi_3 [\nu \sum_{f1} \phi_1 + \nu \sum_{f2} \phi_2 + \nu \sum_{f3} \phi_3]. \quad (6.9)$$

The few-group equations can be put into a very compact form

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by introducing vectors and matrices. One makes the following definitions to put the equations in a commonly used notation: For  $G = 3$ ,

$$\underline{\phi} \equiv \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix}, \underline{S} \equiv \begin{bmatrix} S_1 \\ S_2 \\ S_3 \end{bmatrix}, \underline{\chi} \equiv \begin{bmatrix} \chi_1 \\ \chi_2 \\ \chi_3 \end{bmatrix}, \underline{F} \equiv \begin{bmatrix} \nu \Sigma_{f1} \\ \nu \Sigma_{f2} \\ \nu \Sigma_{f3} \end{bmatrix}, \underline{\Sigma}_f \equiv \begin{bmatrix} \Sigma_{f1} & 0 & 0 \\ 0 & \Sigma_{f2} & 0 \\ 0 & 0 & \Sigma_{f3} \end{bmatrix}, \quad (6.10)$$

$$\underline{H} \equiv \begin{bmatrix} (\Sigma_{a1} + \Sigma_{s1 \rightarrow 2} + \Sigma_{s1 \rightarrow 3}) & 0 & 0 \\ -\Sigma_{s1 \rightarrow 2} & (\Sigma_{a2} + \Sigma_{s2 \rightarrow 3}) & 0 \\ -\Sigma_{s1 \rightarrow 3} & -\Sigma_{s2 \rightarrow 3} & \Sigma_{a3} \end{bmatrix}, \underline{D} \equiv \begin{bmatrix} D_1 & 0 & 0 \\ 0 & D_2 & 0 \\ 0 & 0 & D_3 \end{bmatrix}.$$

The diagonal terms in the  $\underline{H}$  matrix are often referred to as the removal cross sections,  $\Sigma_{rg}$ . With the above definitions, the few-group equations for each homogeneous spatial region in the reactor reduce to the relatively simple vector-matrix form

$$\begin{array}{ccccccc} \text{leakage} & \text{absorption} & \text{and scattering} & & \text{fission} & \text{source} & \\ -\underline{D} \nabla^2 \underline{\phi} & + & \underline{H} \underline{\phi} & = & \underline{\chi} \underline{F}^T \underline{\phi} & + \underline{S}, & \end{array} \quad (6.11)$$

which must be solved subject to the appropriate boundary conditions at each internal interface and each external boundary.

Leakage in directions not included in the spatial calculation is specified externally by supplying a group-dependent buckling term  $B_g^2$ . Since leakage is proportional to  $D_g B_g^2 \phi_g$ , the product  $D_g B_g^2$  acts like a fictitious macroscopic absorption cross section that can be added to the regular  $\Sigma_{ag}$  term to increase the effective losses in the system. Note that we allow the value of  $B_g^2$  to be either positive or negative so that in-leakage as well as out-leakage can be treated separately in each

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energy group. These values can be included in the  $\underline{H}$  matrix.

In the specific case where out-scattering goes only to the next lowest group, the scattering transfer terms can be designated by the letter E and the absorption terms can be designated by the letter A, where both are vectors of length G. This leads to the commonly used DEAF $\chi$ B<sup>2</sup> notation for specifying few-group reactor properties, which is often seen in the literature.

### 6.3 Finite Difference Few-Group Equations in One Dimension

We have derived the multi-group form of the diffusion equation. Unfortunately, it is still a second-order partial differential equation in space that must be solved by applying suitable boundary conditions. For the most part analytic solutions are not feasible, so we turn to an approximate method called Finite Difference.

For relatively small problems, we may consider solving for all of the group fluxes simultaneously. However, for most practical-sized problems, we actually solve for the flux in one group at a time, starting with the fastest group and working down. The solution is usually iterative, because we need to know some information about the fluxes in the lower groups in order to properly include the fission contribution. What is normally done is to construct an effective group source that contains the actual source, plus fission, plus down-scattering from the groups above. The equation that we use is the one-group form,

$$\text{leakage removal} \quad \text{effective source} \tag{6.12}$$

$$-\nabla \cdot D \nabla \phi + \sum_r \phi = S.$$

When the problem is further restricted to be one dimensional,

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then the equation we treat is

$$-\frac{1}{r^k} \frac{d}{dr} \left[ r^k D(r) \frac{d}{dr} \phi(r) \right] + \Sigma_r(r) \phi(r) = S(r), \quad (6.13)$$

where the one-dimensional Laplacian has been written out explicitly. By appropriately choosing the integer  $k$  we can solve the following problems:

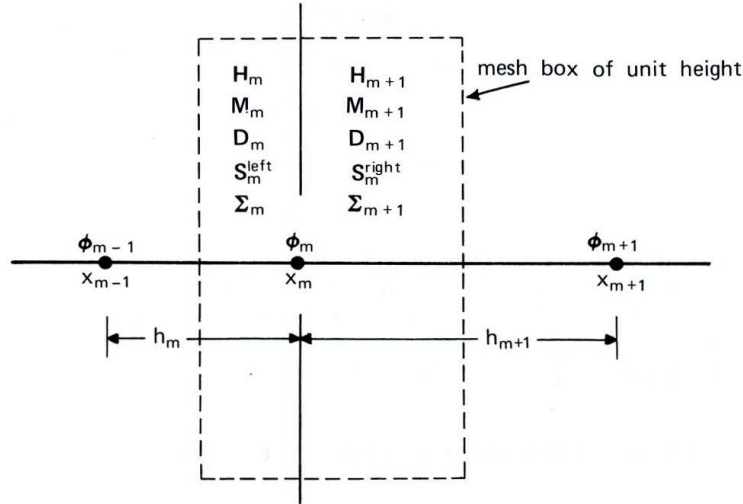
$k = 0;$     slab  
 $k = 1;$     cylinder,  
 $k = 2;$     sphere.

**Edge-Centered Method.** There are a variety of ways to convert the above equation to finite difference form. The method illustrated here for  $k = 0$  is called "mesh box integration." Consider the spatial diagram shown in Figure 6.2 for an interior set of mesh points, where the index  $m$  represents the  $m$ th mesh point,  $h_m$  represents the mesh spacing between points  $m$  and  $m - 1$ , and  $D_m$  and  $\Sigma_m$  represent the material properties in the region between  $m$  and  $m - 1$ . For convenience we assume that the material properties are different in the region between mesh points  $m$  and  $m + 1$  so that we have an interface between regions. By allowing material property changes at each mesh point the formulation becomes extremely flexible. The present form is called an "edge-centered" method because the fluxes are calculated on the region interfaces. This is in contrast to a "mesh-centered" method where the fluxes are calculated in the centers of the regions. We will come back to this point later.

The finite difference equations are formed by integrating the diffusion equation over the volume of the mesh box, term by term. For the slab geometry case this is just the integral with respect to  $x$  from one-half of a mesh space to the left of the point to one-half of a mesh space to the right of the point. We

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allow the flux at mesh point  $m$  to be constant over this range thus giving continuity of flux at the interfaces automatically; the plot of the flux is therefore a histogram, as shown in Figure 6.3 for one of the energy groups. Unfortunately, the flux is discontinuous at the mesh box centers!



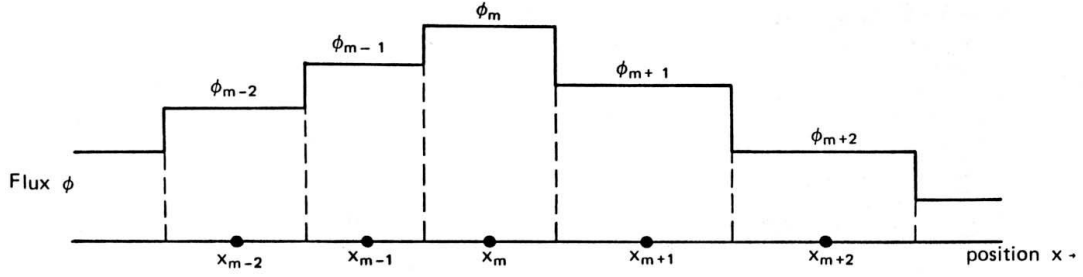
**Fig. 6.2** Edge-Centered Mesh Box for Slab Geometry

We also need an approximation to the first derivative of the flux. We use the simplest approximation possible, by assuming that the flux varies linearly between mesh points; this is known as the first forward difference. Let

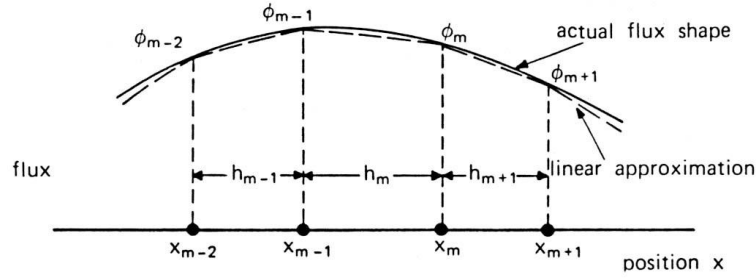
$$\frac{d\phi}{dx}\bigg|_{x_m - h_m/2} \approx \frac{\phi_m - \phi_{m-1}}{h_m} \quad \text{and} \quad \frac{d\phi}{dx}\bigg|_{x_m + h_{m+1}/2} \approx \frac{\phi_{m+1} - \phi_m}{h_{m+1}}. \quad (6.14)$$

This approximation is illustrated in Figure 6.4. Should we require higher-order accuracy, then we will have to use more spatial points in the approximation or allow the flux to vary within the mesh interval. The latter case is an example of a "course-mesh" method.

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**Fig. 6.3** Histogram Representation of the Flux



**Fig. 6.4** Linear Approximation of  $\frac{d\phi}{dx}$

Integrating the leakage term, we obtain

$$\begin{aligned}
 & - \int_{x_m^- h_m/2}^{x_m^+ h_{m+1}/2} \frac{d}{dx} \left( D(x) \frac{d\phi}{dx} \right) dx \\
 & = \lim_{\varepsilon \rightarrow 0} \left\{ -D_m \int_{x_m^- h_m/2}^{x_m^- \varepsilon} \frac{d}{dx} \left( \frac{d\phi}{dx} \right) dx - D_{m+1} \int_{x_m^+ \varepsilon}^{x_m^+ h_{m+1}/2} \frac{d}{dx} \left( \frac{d\phi}{dx} \right) dx \right\} \\
 & = \lim_{\varepsilon \rightarrow 0} \left\{ -D_m \frac{d\phi}{dx} \Big|_{x_m^- h_m/2}^{x_m^- \varepsilon} - D_{m+1} \frac{d\phi}{dx} \Big|_{x_m^+ \varepsilon}^{x_m^+ h_{m+1}/2} \right\} \\
 & = \lim_{\varepsilon \rightarrow 0} \left\{ +D_m \left( \frac{\phi_m - \phi_{m-1}}{h_m} \right) - D_m \frac{d\phi}{dx} \Big|_{x_m^- \varepsilon} + D_{m+1} \frac{d\phi}{dx} \Big|_{x_m^+ \varepsilon} - D_{m+1} \left( \frac{\phi_{m+1} - \phi_m}{h_{m+1}} \right) \right\}.
 \end{aligned} \tag{6.15}$$



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The two middle terms on the right-hand side of the equation represent continuity of current as  $\varepsilon \rightarrow 0$ ; hence, they cancel each other leaving

$$\begin{aligned}
 - \int_{x_m - h_m/2}^{x_m + h_{m+1}/2} \frac{d}{dx} \left( D(x) \frac{d\phi}{dx} \right) dx &= - \frac{D_m}{h_m} \phi_{m-1} + \left[ \frac{D_m}{h_m} + \frac{D_{m+1}}{h_{m+1}} \right] \phi_m - \frac{D_{m+1}}{h_{m+1}} \phi_{m+1} \\
 &+ O(h).
 \end{aligned} \tag{6.16}$$

For uniform spacing and constant material properties, the order of accuracy is  $h^2$ . Using Taylor series expansions for the flux at  $x_{m+1}$  in terms of the flux at  $x_m$ , we can show quite generally that the odd-order derivatives of the flux cancel when the second spatial derivative is formed, leading to the foregoing result.

The removal term integrates to the following form:

$$\begin{aligned}
 \int_{x_m - h_m/2}^{x_m + h_{m+1}/2} \Sigma_r(x) \phi(x) dx &= \Sigma_m \phi_m \int_{x_m - h_m/2}^{x_m} dx + \Sigma_{m+1} \phi_m \int_{x_m}^{x_m + h_{m+1}/2} dx \\
 &= \left[ \frac{h_m \Sigma_m + h_{m+1} \Sigma_{m+1}}{2} \right] \phi_m.
 \end{aligned} \tag{6.17}$$

while the source term becomes

$$\int_{x_m - h_m/2}^{x_m + h_{m+1}/2} S(x) dx = \left[ h_m S_m^{left} + h_{m+1} S_m^{right} \right] \equiv S_m. \tag{6.18}$$

The final result is obtained by combining all of the above terms, giving the 3-point difference equation

$$\begin{aligned}
 - \frac{D_m}{h_m} \phi_{m-1} + \left[ \frac{D_m}{h_m} + \frac{h_m \Sigma_m}{2} + \frac{D_{m+1}}{h_{m+1}} + \frac{h_{m+1} \Sigma_{m+1}}{2} \right] \phi_m \\
 - \frac{D_{m+1}}{h_{m+1}} \phi_{m+1} &= S_m.
 \end{aligned} \tag{6.19}$$

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**Other One-Dimensional Geometries\*.** The corresponding equation for an arbitrary value of the spatial index  $k$  can be derived in an analogous but slightly more complicated manner by applying the integral operator

$$\int_{r_m-h_m/2}^{r_m+h_{m+1}/2} r^k dr$$

to the diffusion equation. The result of this derivation is the following 3-point difference equation:

$$\begin{aligned} & - \left[ \left( r_m - \frac{h_m}{2} \right)^k \frac{D_m}{h_m} \right] \phi_{m-1} + \left[ \left( r_m - \frac{h_m}{2} \right)^k \frac{D_m}{h_m} + \left( r_m + \frac{h_{m+1}}{2} \right)^k \frac{D_{m+1}}{h_{m+1}} \right. \\ & + \left. \left( \frac{r_m^{k+1} - \left( r_m - \frac{h_m}{2} \right)^{k+1}}{k+1} \right) \Sigma_m + \left( \frac{\left( r_m + \frac{h_{m+1}}{2} \right)^{k+1} - r_m^{k+1}}{k+1} \right) \Sigma_{m+1} \right] \phi_m \\ & - \left[ \left( r_m + \frac{h_{m+1}}{2} \right)^k \frac{D_{m+1}}{h_{m+1}} \right] \phi_{m+1} \\ & = S_m^{left} \left[ \frac{r_m^{k+1} - \left( r_m - \frac{h_m}{2} \right)^{k+1}}{k+1} \right] + S_m^{right} \left[ \frac{\left( r_m + \frac{h_{m+1}}{2} \right)^{k+1} - r_m^{k+1}}{k+1} \right] \equiv S_m . \end{aligned} \quad (6.20)$$

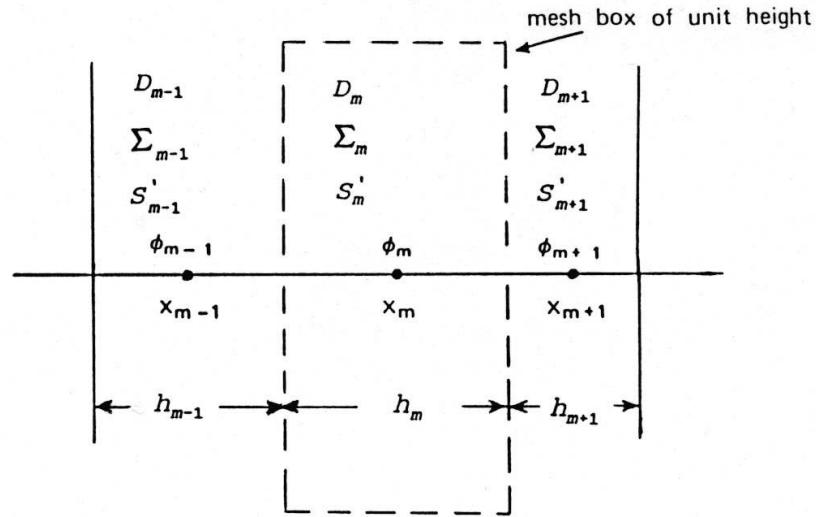
The above expression can be simplified somewhat. Whenever  $r_m \gg h_m$ , which is true after the first five or ten mesh points from the center of a cylinder or sphere, the relationship is reduced to

$$\begin{aligned} & - \left[ r_m^k \frac{D_m}{h_m} \right] \phi_{m-1} + \left[ r_m^k \left( \frac{D_m}{h_m} + \frac{D_{m+1}}{h_{m+1}} + \frac{h_m \Sigma_m}{2} + \frac{h_{m+1} \Sigma_{m+1}}{2} \right) \right] \phi_m \\ & - \left[ r_m^k \frac{D_{m+1}}{h_{m+1}} \right] \phi_{m+1} \approx \left[ r_m^k \left( S_m^{left} \frac{h_m}{2} + S_m^{right} \frac{h_{m+1}}{2} \right) \right] = S_m . \end{aligned} \quad (6.21)$$

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After removal of the common factor  $r_m^k$ , this is identical to the expression for the slab reactor.

**Mesh-Centered Method.** A "mesh-centered" mesh box is shown in Figure 6.5. In this model, the flux is also assumed to be constant within each mesh box, so it has a histogram appearance similar to that shown in Figure 6.3. The primary difference is that the flux discontinuities now occur at the region interfaces. We simply *ignore* this fact!



**Fig. 6.5** Mesh-Centered Mesh Box for Slab Geometry

The derivation proceeds in the same manner as before, except that we must now postulate temporary flux values on the interfaces,  $\phi_{m-1/2}$  and  $\phi_{m+1/2}$ , that can be used to satisfy continuity of current. Specifically, for the left-hand interface we have the derivative approximations,

$$\frac{d\phi}{dx}\bigg|_{x_{m-1}+h_{m-1}/2} \approx \frac{\phi_{m-1/2} - \phi_{m-1}}{h_{m-1}/2}$$

and

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$$\frac{d\phi}{dx}\bigg|_{x_m-h_m/2} \approx \frac{\phi_m - \phi_{m-1/2}}{h_m/2}. \quad (6.22)$$

For continuity of current, we set

$$D_{m-1} \frac{d\phi}{dx}\bigg|_{x_{m-1}+h_{m-1}/2} = D_m \frac{d\phi}{dx}\bigg|_{x_m-h_m/2}, \quad (6.23)$$

and solve for  $\phi_{m-1/2}$  in terms of  $\phi_{m-1}$  and  $\phi_m$ , etc.

When all of the volume integrations have been performed, the leakage integral is found to contain both  $\phi_{m-1/2}$  and  $\phi_{m+1/2}$ . We replace these values with those obtained from the continuity expression. The result is also a 3-point difference equation, but the coefficients now contain contributions from both adjacent mesh boxes, i.e., we have the expression

$$\begin{aligned} & -\frac{D_m}{h_m} \left[ \frac{2}{1 + \frac{D_m h_{m-1}}{D_{m-1} h_m}} \right] \phi_{m-1} \\ & + \left[ \frac{D_m}{h_m} \left( \frac{2}{1 + \frac{D_m h_{m-1}}{D_{m-1} h_m}} \right) + \Sigma_m h_m + \frac{D_m}{h_m} \left( \frac{2}{1 + \frac{D_m h_{m+1}}{D_{m+1} h_m}} \right) \right] \phi_m \\ & - \frac{D_m}{h_m} \left[ \frac{2}{1 + \frac{D_m h_{m+1}}{D_{m+1} h_m}} \right] \phi_{m+1} = S'_m h_m \equiv S_m. \end{aligned} \quad (6.24)$$

**Coupling Coefficients.** All of the one-dimensional formulations lead to a 3-point equation of the form

$$-a_m \phi_{m-1} + b_m \phi_m - c_m \phi_{m+1} = S_m. \quad (6.25)$$

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The coefficients in this equation, namely  $a_m$ ,  $b_m$  and  $c_m$ , are called "coupling coefficients" because they couple the flux at point  $m$  to its nearest neighbors. In all of the finite-difference applications it is found that  $a_{m+1} = c_m$ , which means that only half of the coefficients need to be stored during a computation. Since the coefficients only depend upon the mesh spacings and material properties of the regions, they need be calculated only once for each flux computation, even if the solution procedure is iterative.

The so-called "nodal" methods also lead to an equation of the form of Eq. (6.25). However, the nodal coupling coefficients do not contain simple ratios of  $D/h$  values, but instead are obtained in a semi-empirical manner, e.g., by using a Green's function technique. Other than that, the properties of the coefficients are similar to those of the finite-difference coefficients. On the other hand the "coarse-mesh" methods lead to coupling coefficients that are dependent on the flux solution itself so that the coefficients must be modified during an iterative solution. Also, in general,  $a_{m+1} \neq c_m$ , which means that all coefficients must be stored during a computation. The higher accuracy that is achieved using fewer mesh points more than pays for the cost of the extra effort required per mesh point.

In some situations, the finite-difference equations are derived in the complete few-group form. In this case, the 3-point difference equation has the form

$$-\underline{\underline{A}}_m \phi_{m-1} + \underline{\underline{B}}_m \phi_m - \underline{\underline{C}}_m \phi_{m+1} = \underline{\underline{S}}_m. \quad (6.26)$$

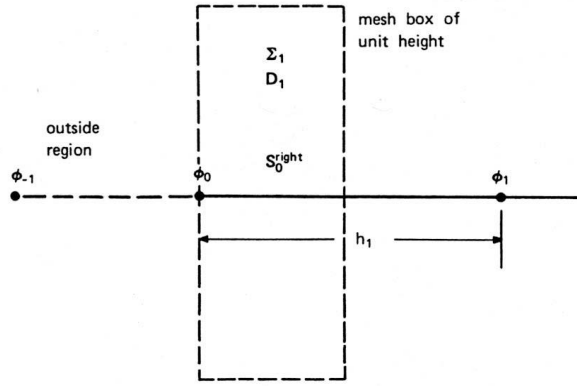
Here, the matrices  $\underline{\underline{A}}_m$ ,  $\underline{\underline{B}}_m$ , and  $\underline{\underline{C}}_m$  are the coefficients of the equation obtained from the mesh box integration.  $\underline{\underline{A}}_m$  and  $\underline{\underline{C}}_m$ , which correspond to the discretized leakage terms, contain the diffusion coefficients and the mesh spacing and happen to be diagonal matrices. In fact,  $\underline{\underline{A}}_{m+1} = \underline{\underline{C}}_m$  in slab geometry. The

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matrix  $\underline{\underline{B}}_m$  corresponds to the reaction rate and leakage terms and therefore contains the diffusion coefficients, absorption and scattering cross sections, and the mesh spacing values.

### 6.4 Specification of Boundary Conditions

The material regions end at either boundary, so that we only obtain 2-point difference equations there. This implies that the flux is zero at fictitious mesh points outside of the reactor, i.e.,  $\phi_{-1} = \phi_{M+1} = 0$ , where M is the total number of mesh spaces used. At the left boundary, the mesh box structure is as shown in Figure 6.6 for mesh point  $m = 0$ .



**Fig. 6.6** Edge-Centered Boundary Mesh Box for Slab Geometry

As before, we integrate the diffusion equation over the mesh box, term by term. The leakage formulation in this case is

$$\begin{aligned}
 - \int_0^{h_1/2} \frac{d}{dx} \left( D(x) \frac{d\phi(x)}{dx} \right) dx &= - \left[ D_1 \frac{d\phi}{dx} \right]_0^{h_1/2} \\
 &= - D_1 \left( \frac{\phi_1 - \phi_0}{h_1} \right) + D_1 \frac{d\phi}{dx} \Big|_{x=0}.
 \end{aligned} \tag{6.27}$$

Likewise, the removal and source terms give the following results when integrated over the mesh box volume:

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$$\int_0^{h_1/2} \sum_r(x) \phi(x) dx = \frac{\sum_l h_l \phi_0}{2}, \quad (6.28)$$

and

$$\int_0^{h_1/2} S(x) dx = \frac{S_0^{right} h_l}{2} \equiv S_0. \quad (6.29)$$

There are three different boundary conditions that are normally applied to this problem. These are the following:

1.  $\phi_0 = 0$ , or zero flux condition;
2.  $d\phi_0/dx = 0$ , or symmetry condition;
3.  $d\phi_{g0}/dx = K_g \phi_{g0}$ , or extrapolation distance condition, where  $K_g$  is the reciprocal of the distance to where the group  $g$  flux goes to zero.

However, only the symmetry condition can be used at  $r = 0$  in 1-D curved geometries.

Specification of the three possible boundary conditions proceeds as follows:

1. *Zero flux condition* - We set the coefficient of  $\phi_0$ , i.e.,  $K$  equal to a very large value. One physical interpretation of this procedure is that the mesh spacing distance to the outside point  $\phi_{-1}$  is very small, so that the flux  $\phi_0$  approaches the value  $\phi_{-1}$ , which is zero;
2. *Symmetry condition* - At a symmetry boundary there is no net current of neutrons. We set the value of  $K$  equal to zero, which eliminates the external leakage. This is equivalent to having the flux go to zero at a very large distance from the boundary;

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3. *Extrapolation condition* - We set the value of  $1/K_g$  equal to the extrapolation distance, which can be taken to be  $0.71 \lambda_{\text{trg}}$ , for example.

The complete equation therefore becomes the two-point expression,

$$\left[ K_l D_l + \frac{D_l}{h_l} + \frac{h_l \Sigma_l}{2} \right] \phi_0 - \frac{D_l}{h_l} \phi_l = S_0. \quad (6.30)$$

Similar expressions are obtained for the mesh-centered and coarse-mesh formulations.

The corresponding appropriate boundary conditions can also be applied at the mesh point  $m = M$ . Since the finite difference equations are identical at large distances from the origin for slab, cylindrical, and spherical geometry, the above equation can be applied directly. Different boundary conditions can be applied at the outer boundary and at the inner boundary.

### 6.5 Direct Solution of the Source Problem

Consider the one-group one-dimensional finite difference form derived above for the spatial mesh given in Figure 6.2. The complete set of equations representing the fluxes in the group at all of the spatial mesh points can be put into vector-matrix form. Define a flux and a source vector, respectively, as

$$\underline{\psi} \equiv \begin{bmatrix} \phi_0 \\ \phi_l \\ \cdot \\ \cdot \\ \cdot \\ \phi_M \end{bmatrix} \quad \text{and} \quad \underline{S} \equiv \begin{bmatrix} S_0 \\ S_l \\ \cdot \\ \cdot \\ \cdot \\ S_M \end{bmatrix} \quad (6.31)$$



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The resulting finite difference equation is in the form of a source problem

$$\underline{\underline{G}}\psi = \underline{S}, \quad (6.32)$$

where the coefficients of the spatial flux values can be put into a matrix which has non-zero values only on the main diagonal and on the diagonals just above and below the main diagonal. We call this a tri-diagonal matrix, and recognize that we need only store  $3(M+1)$  coefficient values in the three vectors  $\underline{a}$ ,  $\underline{b}$ , and  $\underline{c}$ .

The  $\underline{\underline{G}}$  matrix is written as

$$\underline{\underline{G}} \equiv \begin{bmatrix} b_0 & -c_0 & 0 & & & & \\ -a_1 & b_1 & -c_1 & 0 & & & \\ 0 & -a_2 & b_2 & -c_2 & 0 & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & & 0 & & 0 & -a_{M-1} & b_{M-1} & -c_{M-1} \\ & & & & & 0 & -a_M & b_M \end{bmatrix}$$

(6.33)

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To obtain the flux solution we must, in effect, invert the  $\underline{\underline{G}}$  matrix, which results in the form

$$\underline{\psi} = \underline{\underline{G}}^{-1} \underline{S}. \quad (6.34)$$

The basic solution procedure is Gaussian elimination, but since the system matrix is tri-diagonal and contains mostly zeros, a simpler solution procedure is possible. This procedure is called Crout's method or the Forward Elimination, Backward Substitution (FEBS) method. In this procedure, we simply ignore all non-zero terms. The object is to reduce Eq. (6.32) to the equivalent bi-diagonal form,

$$\underline{\underline{P}} \underline{\psi} = \underline{p}, \quad (6.35)$$

where

$$\underline{\underline{P}} = \begin{bmatrix} 1 & -P_0 & 0 & & & & \\ 0 & 1 & -P_1 & 0 & & & 0 \\ & 0 & 1 & -P_2 & 0 & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & & 0 & & & 0 & 1 & -P_{M-1} \\ & & & & & & 0 & 1 \end{bmatrix}.$$

(6.36)

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Once we have obtained this form, we can solve recursively from the bottom up for all of the fluxes, i.e.,

$$\phi_M = p_M,$$

and

$$\phi_m = P_m \phi_{m+1} + p_m, \quad \text{for } m = (M-1), 0. \quad (6.37)$$

Since there are only two terms in the first row of the G matrix, the first row values of  $P_o$  and  $p_o$  are simply

$$P_o = c_o / b_o$$

and

$$p_o = S_o / b_o.$$

For the second row, we divide by the leading coefficient  $a_1$ , and then add rows one and two. Next, we divide the result term-by-term by the new diagonal coefficient to obtain the following form, which is, in fact, a recursion for all of the other rows, namely,

$$P_m = c_m / (b_m - a_m P_{m-1}) \quad (6.38)$$

and

$$p_m = (S_m + a_m p_{m-1}) / (b_m - a_m P_{m-1}), \quad \text{for } m = 1, M. \quad (6.39)$$

We find all of the  $P$ 's and  $p$ 's in this manner starting at  $m = 0$  going forward, and then find the  $\phi$ 's starting at  $m = M$  going backward.

This relatively simple procedure is very commonly used in the case of two and three-dimensional problems, as a part of the overall iterative sweep. In these cases, it is referred to as line relaxation. We will return to this point later.

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**Matrix Form\*.** The FEBS procedure also works in matrix form. In the formulation given by Eq. (6.26), the corresponding vector-matrix equivalent of Eq. (6.32) contains a block tri-diagonal  $\underline{\underline{G}}$  matrix of order  $(M+1)G$ . For 3 energy groups, the form of this matrix is as shown below, where the x's represent nonzero values:

$$\underline{\underline{G}} = \begin{bmatrix} \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix} \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} & 0 & \\ \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix} \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix} \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} & & \\ \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix} \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix} \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} & & \\ & 0 & \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix} \\ & & \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{bmatrix} \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \end{bmatrix} \end{bmatrix}.$$

(6.40)

Assume that a relationship exists between adjacent flux vectors of the form

$$\underline{\phi}_m = \underline{\underline{P}}_m \underline{\phi}_{m+1} + \underline{p}_m, \quad (6.41)$$

where the matrix  $\underline{\underline{P}}_m$  and the vector  $\underline{p}_m$  are as yet undetermined. The object is to try to find the values of  $\underline{\underline{P}}_m$  and  $\underline{p}_m$  for  $m = 0, M$ . In this regard, insert the above expression into the equation for the  $m$ th mesh point to obtain the equation

$$-\underline{\underline{A}}_m [\underline{\underline{P}}_{m-1} (\underline{\underline{P}}_{m-1} \underline{\phi}_{m+1} + \underline{p}_{m-1}) + \underline{p}_{m-1}] + \underline{\underline{B}}_m [\underline{\underline{P}}_m \underline{\phi}_{m+1} + \underline{p}_m] - \underline{\underline{C}}_m \underline{\phi}_{m+1} = \underline{S}_m. \quad (6.42)$$

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This expression can be separated into two component equations. Combine the terms in  $\underline{\phi}_{m+1}$  to obtain the equation

$$\left[ -\underline{A}_{m=m-1} \underline{P}_m + \underline{B}_{m=m} - \underline{C}_{m=m} \right] \underline{\phi}_{m+1} = \underline{0}. \quad (6.43)$$

Combine the terms in  $\underline{p}_m$  to obtain the equation

$$\left[ -\underline{A}_{m=m-1} \underline{P}_{m-1} + \underline{B}_{m=m} \right] \underline{p}_m - \underline{A}_{m=m} \underline{p}_{m-1} = \underline{S}_m. \quad (6.44)$$

Since  $\underline{\phi}_{m+1}$  is not a null vector, the bracketed term in the first equation gives a recursion relationship for  $\underline{P}_m$  in terms of  $\underline{P}_{m-1}$ , namely,

$$\underline{P}_m = [\underline{B}_{m=m} - \underline{A}_{m=m} \underline{P}_{m-1}]^{-1} \underline{C}_{m=m}. \quad (6.45)$$

At the left-hand boundary of the core,  $\underline{P}_0$  is uniquely determined to be

$$\underline{P}_0 = \underline{B}_{0=0}^{-1} \underline{C}_{0=0}.$$

We also obtain a recursion relationship for the vector  $\underline{p}_m$  in terms of  $\underline{p}_{m-1}$ , i.e.,

$$\underline{p}_m = [\underline{B}_{m=m} - \underline{A}_{m=m} \underline{P}_{m-1}]^{-1} [\underline{S}_m + \underline{A}_{m=m} \underline{p}_{m-1}]. \quad (6.46)$$

At the left-hand boundary,  $\underline{p}_0$  is uniquely determined to be

$$\underline{p}_0 = \underline{B}_{0=0}^{-1} \underline{S}_0.$$

Note that the same inverse matrix appears in both recursions so that it only needs to be computed once for each value of  $m$ . Evaluation of these recursion relations completes the forward elimination sweep.

When all of the  $\underline{P}_m$ 's and  $\underline{p}_m$ 's are known, the backward substitution sweep is performed starting at the right-hand side of the core at mesh point  $m = M$ . The flux at  $m = M$  is obtained from the substitution

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$$\underline{\phi}_M = \underline{p}_M.$$

Continuing the recursion back to  $m = 0$ , the flux at successive points is obtained as

$$\underline{\phi}_m = \underline{P}_m \underline{\phi}_{m+1} + \underline{p}_m, \quad (6.47)$$

completing the solution. This solution procedure is used in the 1-D computer program RAUMZEIT.

### 6.6\* Iterative Solution of the Source Problem

In its most general form, the source problem can still be written as the vector-matrix equation

$$\underline{\underline{G}}\psi = \underline{S}. \quad (6.48)$$

For normal two-dimensional diffusion theory calculations, the  $\underline{\underline{G}}$  matrix can be as big as order 100,000, while the number of nonzero elements in any given row can be less than 100. Therefore, an iterative approach is the only practical method of solution. Furthermore, the properties of the  $\underline{\underline{G}}$  matrix are not difficult to determine because there are few nonzero terms.

There are a number of iterative schemes available, but we concentrate on a single scheme in order to illustrate the nature of the solution. This method involves partitioning the  $\underline{\underline{G}}$  matrix into one part that is easy to invert and a second part that is not. For example, we first operate on both sides of the source problem by the transformation operator  $\underline{\underline{F}}$  that normalizes all of the equations such that the terms along the main diagonal are unity. Hence, we obtain the modified equation

$$\underline{\underline{F}}\underline{\underline{G}}\psi = \underline{\underline{F}}\underline{S}. \quad (6.49)$$

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We define a modified source vector as

$$\underline{\underline{k}} \equiv \underline{\underline{F}}\underline{\underline{S}}, \quad (6.50)$$

and furthermore partition the  $\underline{\underline{F}}\underline{\underline{G}}$  matrix into the identity matrix  $\underline{\underline{I}}$  minus a new matrix  $\underline{\underline{R}}$  that contains just zeros along its main diagonal, i.e., let

$$(\underline{\underline{I}} - \underline{\underline{R}}) = \underline{\underline{F}}\underline{\underline{G}}. \quad (6.51)$$

Under these conditions, the modified source problem takes the form

$$(\underline{\underline{I}} - \underline{\underline{R}})\underline{\underline{\psi}} = \underline{\underline{k}}. \quad (6.52)$$

Next, bring the vector  $\underline{\underline{R}}\underline{\underline{\psi}}$  to the right-hand side of the equation to obtain the form

$$\underline{\underline{\psi}} = \underline{\underline{R}}\underline{\underline{\psi}} + \underline{\underline{k}}. \quad (6.53)$$

A straightforward method of successive approximations is to add an iteration index as a bracketed superscript to the value of  $\underline{\underline{\psi}}$  and generate an improved solution on the left-hand side of the equation by inserting a trial solution on the right-hand side of the equation. Use of the improved solution on the right-hand side of the equation leads to a still better value on the left-hand side, and so on. The  $i$ th iterate is generated using the formula

$$\underline{\underline{\psi}}^{(i)} = \underline{\underline{R}}\underline{\underline{\psi}}^{(i-1)} + \underline{\underline{k}}. \quad (6.54)$$

Let the initial arbitrary guess be  $\underline{\underline{\psi}}^{(0)}$ , which may conveniently be taken to be the null vector  $\underline{\underline{0}}$ . We begin the iteration process with  $\underline{\underline{\psi}}^{(0)}$  and continue to insert the left-hand result into the right-hand side of the equation until the solution "converges". The solution is said to converge if the

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difference between the true solution  $\underline{\psi}$  and the  $j$ th iterate  $\underline{\psi}^{(j)}$  is less than a given error, or flux convergence criterion  $\varepsilon_f$ , in some sense. Using the Euclidean  $l_2$  norm (square root of the sum of the squares of the point-wise deviations), this expression can be written as

$$\|\underline{\psi}^{(j)} - \underline{\psi}\| < \varepsilon_f. \quad (6.55)$$

A more practical test is to compare the last iterate to the next-to-last iterate, since the true solution is unknown.

The iteration scheme will converge if the spectral radius  $\mu$  of the  $\underline{\underline{R}}$  matrix, which is defined as the absolute value of the largest eigenvalue of the  $\underline{\underline{R}}$  matrix, satisfies the expression

$$\mu(\underline{\underline{R}}) < 1.$$

Formally, the eigenvalues are obtained by setting  $|\underline{\underline{R}} - \mu \underline{\underline{I}}| = 0$ . The speed of convergence increases as  $\mu(\underline{\underline{R}})$  decreases. A rough proof of this statement proceeds as follows: Let the initial guess be  $\underline{\psi}^{(0)} = \underline{0}$ . Then, the results for the first  $j$  iterations can be written as

$$\begin{aligned} \underline{\psi}^{(1)} &= \underline{k}, \\ \underline{\psi}^{(2)} &= \underline{\underline{R}}\underline{\psi}^{(1)} + \underline{k} = (\underline{\underline{I}} + \underline{\underline{R}})\underline{k}, \\ \underline{\psi}^{(3)} &= (\underline{\underline{I}} + \underline{\underline{R}} + \underline{\underline{R}}^2)\underline{k}, \\ &\vdots \\ &\vdots \\ &\vdots \\ \underline{\psi}^{(j)} &= (\underline{\underline{I}} + \underline{\underline{R}} + \underline{\underline{R}}^2 + \dots + \underline{\underline{R}}^{j-1})\underline{k}. \end{aligned} \quad (6.56)$$

The term in the brackets is the matrix form of a geometric series. Summing this series by adding the rest of the terms out to  $\infty$  (i.e., multiply by  $(\underline{\underline{I}} - \underline{\underline{R}}^j)(\underline{\underline{I}} - \underline{\underline{R}}^j)^{-1}$  and expand the second expression in series) leads to a closed expression for the  $j$ th



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iterate, namely,

$$\underline{\psi}^{(j)} = \underline{\mathbf{I}}(\underline{\mathbf{I}} - \underline{\mathbf{R}})^{-1}(\underline{\mathbf{I}} - \underline{\mathbf{R}}^j) \underline{\mathbf{k}}. \quad (6.57)$$

But the exact solution is

$$\underline{\psi} = (\underline{\mathbf{I}} - \underline{\mathbf{R}})^{-1} \underline{\mathbf{k}}. \quad (6.58)$$

Hence, convergence occurs if and only if the factor  $\underline{\mathbf{R}}^j \underline{\mathbf{k}}$  approaches the null vector  $\underline{\mathbf{0}}$  in some sense. The fractional error is given by the equation

$$\left[ \begin{array}{c} \text{fractional error} \\ \text{for the } j\text{th} \\ \text{iterate} \end{array} \right] = \frac{\|\underline{\psi}^{(j)} - \underline{\psi}\|}{\|\underline{\psi}\|} = \frac{\|\underline{\mathbf{R}}^j \underline{\psi}\|}{\|\underline{\psi}\|} \leq [\mu(\underline{\mathbf{R}})]^j. \quad (6.59)$$

Therefore, if the spectral radius of  $\underline{\mathbf{R}}$  is less than unity, then  $\mu(\underline{\mathbf{R}})$  to the  $j$ th power approaches zero and convergence is assured. Proof that the matrix  $\underline{\mathbf{R}}$  is indeed possessed of a spectral radius that is less than unity is beyond the scope of this treatment. However, for the diffusion equations in multi-group form,  $\underline{\mathbf{R}}$  belongs to a class of matrices known as an "S-matrix" that does possess the required properties.

The partitioning could have been done in other ways, for example, let  $\underline{\mathbf{FG}}$  be taken to be

$$\underline{\mathbf{FG}} = \underline{\mathbf{V}} - \underline{\mathbf{Q}}, \quad (6.60)$$

where  $\underline{\mathbf{V}}$  is easy to invert. Substitution into the original source problem then gives the expression

$$\underline{\mathbf{V}}\underline{\psi} = \underline{\mathbf{Q}}\underline{\psi} + \underline{\mathbf{k}}$$

or

$$\underline{\psi} = \underline{\mathbf{V}}^{-1} \underline{\mathbf{Q}}\underline{\psi} + \underline{\mathbf{V}}^{-1} \underline{\mathbf{k}}. \quad (6.61)$$

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The iteration scheme becomes

$$\underline{\underline{\psi}}^{(j)} = \underline{\underline{V}}^{-1} \underline{\underline{Q}} \underline{\underline{\psi}}^{(j-1)} + \underline{\underline{V}}^{-1} \underline{\underline{k}}. \quad (6.62)$$

The important thing to notice is that the convergence properties of this problem depend on the spectral radius of  $\underline{\underline{V}}^{-1} \underline{\underline{Q}}$ , which could conceivably be smaller than the spectral radius of  $\underline{\underline{R}}$ , so that the problem posed in this form could converge faster.

**Multidimensional Problems.** The commonly used multidimensional geometries are XY, R $\theta$ , RZ, XYZ, R $\theta$ Z and HEXZ. With the exception of the hexagonal geometries, these coordinate systems are composed of orthogonal components. The corresponding finite-difference equations, as obtained by mesh-box integration, contain independent leakage contributions from each coordinate direction of the same type as are obtained in the one-dimensional case. We are led to 5-point equations in 2D and 7-point equations in 3D, which couple all of the nearest neighbors of a given mesh point in a given energy group.

Consider one of the 5-point formulations, for example, in XY geometry. Using any type of consistent ordering, it is not possible to put all of the adjacent mesh point fluxes next to one another. For example, if we list all of the x-fluxes for the first y-point, and then all of the x-fluxes for the second y-point, etc, we obtain a 5-stripe  $\underline{\underline{G}}$  matrix.

The three center stripes correspond to the x-direction while the upper and lower stripes correspond to the y-direction. The span between the sets of stripes represents the number of x-points in any given row. The order of the matrix for each group is NX by NY.

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$$\underline{\underline{G}} = \begin{bmatrix} & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \end{bmatrix} \cdot$$

(6.63)

The 7-point equations in XYZ geometry produce a  $\underline{\underline{G}}$  matrix of the form,

$$\underline{\underline{G}} = \begin{bmatrix} & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \end{bmatrix} \cdot$$

(6.64)

In this case, the center stripes correspond to the x-direction, the next stripes above and below correspond to the y-direction, and the upper and lower stripes correspond to the z-direction. The span between the central and upper-middle stripes represents

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the number of x-points in a row, while the span between the upper-middle and upper stripes represents the number of y-points in a row. The order of the matrix for each group is NX by NY by NZ.

We search for computationally efficient methods of finding the flux solution vector  $\underline{\psi}$ . We recognize that we only want to work with and store non-zero elements in the  $\underline{\underline{G}}$  matrix. One attractive procedure, known as the Gauss-Seidel method, involves partitioning the  $\underline{\underline{G}}$  matrix into several pieces. For example let's call the central three stripes  $\underline{\underline{D}}$ , the upper triangular portion  $\underline{\underline{U}}$ , and the lower triangular portion  $\underline{\underline{L}}$ . We then have the problem

$$(\underline{\underline{U}} + \underline{\underline{L}} + \underline{\underline{D}})\underline{\psi} = \underline{\underline{S}}. \quad (6.65)$$

We now add an iteration index i. Assume that all of the  $\underline{\underline{U}}$  components are known in terms of the old fluxes at step i. Therefore, we have the problem

$$\underline{\underline{D}}\underline{\psi}^{(i+1)} = \underline{\underline{S}} - \underline{\underline{L}}\underline{\psi}^{(i+1)} - \underline{\underline{U}}\underline{\psi}^{(i)}. \quad (6.66)$$

The problem is split in this somewhat unusual manner to emphasize the fact that we invert only a portion of the  $\underline{\underline{G}}$  matrix at a time by FEBS, corresponding to a single line in the x-direction. This is called a line-relaxation. Once this portion is available, we use it as a known function of the new fluxes to compute the portion of  $\underline{\underline{L}}\underline{\psi}^{(i+1)}$  needed to invert the next line by FEBS, etc., until all lines are solved. Symbolically, the solution is of the form

$$\underline{\psi}^{(i+1)} = (\underline{\underline{D}} + \underline{\underline{L}})^{-1}\underline{\underline{S}} - (\underline{\underline{D}} + \underline{\underline{L}})^{-1}\underline{\underline{U}}\underline{\psi}^{(i)}, \quad (6.67)$$

where we recognize that the inverse was computed in a series of steps. This iteration procedure converges approximately twice as fast as those methods that are based on using old flux values in

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both the  $\underline{\underline{L}}$  and  $\underline{\underline{U}}$  terms.

An even better procedure is known as the method of successive over-relaxation (SOR). This procedure is similar to the Gauss-Seidel method, but also includes a flux extrapolation that accelerates convergence. It is, in effect, a two-step method. The first step is given by Eq. (6.67), but the values thus obtained are referred to as the intermediate flux estimate  $\underline{\psi}^{(i+1/2)}$ . The second step then gives the new fluxes according to the equation

$$\underline{\psi}^{(i+1)} = \beta \underline{\psi}^{(i+1/2)} + (1 - \beta) \underline{\psi}^{(i)}. \quad (6.68)$$

Beta is known as the over-relaxation coefficient, and has a value between 1 and 2. When  $\beta = 1$  we have the ordinary Gauss-Seidel method. A good value for the UVAR reactor is  $\beta = 1.6$ .

It should be noted that  $\beta$  is obtained automatically in computer codes such as EXTERMINATOR and VENTURE. Periodically, the ordinary  $k_{\text{eff}}$  computation is interrupted, all sources are set to zero, and the convergence of the iterative flux solution towards the null vector is observed. An optimum value of  $\beta$  is estimated from an appropriate norm of the flux error vector, and then the original computation is resumed using the new  $\beta$ . When  $\beta$  is chosen near the optimum value, a considerable speedup in convergence is usually obtained.

### 6.7 Iterative Solution of the Critical Reactor Problem

Consider now that there is no external source present so that the reactor equations become homogeneous. As in the one-speed case we introduce a characteristic value into the equations and convert the problem to a static eigenvalue problem of the form

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$$\begin{array}{cc} \text{destruction} & \text{production} \\ \underline{\underline{L}}\phi & = \frac{1}{\lambda} \underline{\underline{M}}\phi. \end{array} \quad (6.69)$$

We define the terms appearing on the left-hand side of the equation as the loss matrix operator  $\underline{\underline{L}}$ , i.e.,

$$\underline{\underline{L}} \equiv (-\underline{\underline{D}}\nabla^2 + \underline{\underline{H}}), \quad (6.70)$$

and further define the fission terms as the production matrix  $\underline{\underline{M}}$ , i.e.,

$$\underline{\underline{M}} \equiv \chi \underline{\underline{F}}^T. \quad (6.71)$$

This is an example of what is known as a generalized eigenvalue problem because there is an operator on either side of the equation. The  $\underline{\underline{L}}$  operator contains the leakage and absorption plus scattering terms while the  $\underline{\underline{M}}$  operator contains the fission terms. Formally, the problem can be put into the form

$$\underline{\underline{M}}^{-1} \underline{\underline{L}}\phi = \frac{1}{\lambda} \phi, \quad (6.72)$$

which is an ordinary eigenvalue problem. The values of  $1/\lambda$  can therefore be identified with the infinite number of characteristic values of the matrix operator  $\underline{\underline{M}}^{-1} \underline{\underline{L}}$ .

As before, we discretize the problem over space by integrating over a mesh box. In this case we put all of the group spatial fluxes into a single supervector  $\underline{\psi}$ , to obtain the discretized eigenvalue problem:

$$\underline{\underline{L}}'\underline{\psi} = \frac{\underline{\underline{M}}'\underline{\psi}}{\lambda}. \quad (6.73)$$

Both  $\underline{\underline{L}}'$  and  $\underline{\underline{M}}'$  are of order  $(M+1)G$  by  $(M+1)G$  for a one-dimensional problem, where  $M$  is the number of mesh spaces and  $G$  is the number of groups. Note that the number of values of  $\lambda$  is

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now  $M+1$  instead of infinity, which is one of the effects of approximating a continuous problem by a discretized problem. For an accurate solution one hopes that the largest values of  $\lambda$ , corresponding to the fundamental mode and the first few harmonics, are adequately represented by the choice of an appropriate spatial mesh.

For the reactor eigenvalue problem we must do two things:

1. Find the largest value of  $\lambda_0 = k_{\text{eff}}$  and the corresponding fundamental mode solution  $\underline{\psi}_0$ .
2. Show that convergence of the iterative solution leads to the fundamental mode solution.

We will first discuss the nature of the iterative scheme used to solve the eigenvalue problem, which corresponds to what is known as the "outer iteration." Let an outer iteration index  $i$  be added to the equations as a bracketed subscript such that an improved value of the flux is calculated on the left-hand side of the equation using an earlier approximation on the right-hand side, i.e.,

$$\underline{L}\underline{\psi}_{(i)} = \frac{\underline{M}'\underline{\psi}_{(i-1)}}{\lambda_{(i-1)}}. \quad (6.74)$$

The iterative scheme that we employ is the following, as illustrated in Figure 6.7. These steps are:

- a. Make a guess for the flux solution, e.g., let  $\underline{\psi}_{(0)}$  arbitrarily be taken to be uniform over the core. This can be accomplished using the unity vector  $\underline{1}$  which is a vector having 1's in every location.

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- 1) SET VARIABLE DIMENSIONS
- 2) READ MACROSCOPIC SIGMAS, GEOMETRY
- 3) FINITE - DIFFERENCE CONSTANTS  
(OUTER ITERATION LOOP)
- 4) FISSION SOURCE  
(ENERGY GROUP LOOP)
- 5) INSCATTER SOURCE  
(INNER ITERATION LOOP)
- 6) LINE OVERRELAXATION
- 7) NEW FLUXES
- 8) EIGENVALUE
- 9) CONVERGENCE TEST

**Fig. 6.7** Structure of a Multi-group Calculation

- b. Compute the corresponding eigenvalue  $\lambda_{(0)}$  by inserting the guess into both sides of the balance equation. Since  $\lambda$  is a single number, we must treat the balance equations correspondingly. The most physically meaningful reduction is to compute the total production rate and the total destruction rate by summing over all groups and over all mesh points. Mathematically, this can be written in very compact form using the inner product definition

$$(\underline{u}, \underline{v}) = \underline{u}^T \underline{v} = \sum_{i=1}^n u_i v_i = \text{a number.}$$

In our case, we take the inner product with the unity vector  $\underline{1}$ , to obtain

$$\lambda_{(0)} = \frac{(\underline{M}' \underline{\psi}_{(0)}, \underline{1})}{(\underline{L} \underline{\psi}_{(0)}, \underline{1})} = \left[ \frac{\text{Total production rate}}{\text{Total destruction rate}} \right] = k_{\text{eff}(0)}. \quad (6.75)$$



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Note that the leakage part of the loss operator is only composed of leakage over the outer boundaries, and is therefore usually summed separately. Naturally, since  $\underline{\psi}_{(0)}$  does not give a consistent result on both sides of the balance equation,  $\lambda_{(0)}$  is only a first guess as to the true criticality  $k_{\text{eff}}$ , and we must compute successive values of  $\lambda_{(i)}$ . There is also a second way to obtain the value of  $\lambda_{(i)}$ , which is based on saving the total production integral

$$P_{(i)} = (\underline{M}' \underline{\psi}_{(i)}, \underline{1}). \quad (6.76)$$

- c. Use the values of  $\lambda_{(0)}$  and  $\underline{\psi}_{(0)}$  to obtain an effective fission source vector, defined as

$$\underline{S}_{(0)} = \frac{\underline{M}' \underline{\psi}_{(0)}}{\lambda_{(0)}}. \quad (6.77)$$

Actually, we only use the fission source for one group at a time when the group fluxes are obtained separately, as in the multidimensional case.

- d. If one inserts this source vector into the eigenvalue problem given by Eq. (6.74), one obtains, in fact, a source problem of the form

$$\underline{L}' \underline{\psi}_{(1)} = \underline{S}_{(0)}. \quad (6.78)$$

Formally, the solution for  $\underline{\psi}_{(1)}$  is

$$\underline{\psi}_{(1)} = \underline{L}^{-1} \underline{S}_{(0)}, \quad (6.79)$$

where the inversion can be done in two ways:

1. direct inversion using the FEBS method;
2. iteratively, by guessing  $\underline{\psi}_{(1)}^{(0)}$  and iterating to

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convergence where  $\underline{\psi}_{(l)}^{(j)} \rightarrow \underline{\psi}_{(1)}$  on the  $j$ th inner iteration.

When the group fluxes are obtained separately we must add the scattering source to the fission source and do the inversion symbolized by Eq. (6.79) one group at a time. Down-scattering contributions are calculated using the newest group flux values.

- e. Compute  $\lambda_{(1)}$  as done in step b. Alternately compute  $\lambda_{(1)}$  from the integral production rate according to the formula

$$\lambda_{(i)} = \lambda_{(i-1)} \frac{P_{(i)}}{P_{(i-1)}}. \quad (6.80)$$

- f. Check for convergence; that is, check for consistency between the production and loss vector in the balance equation by comparing the eigenvalue  $\lambda_{(1)}$  to the eigenvalue produced in the previous step, namely  $\lambda_{(0)}$ . We ask that the fractional change in the eigenvalue be less than a convergence criterion  $\varepsilon_\lambda$ , that is,

$$\left[ \frac{\text{Fractional}}{\text{change in } \lambda} \right] = \frac{|\lambda_{(1)} - \lambda_{(0)}|}{\lambda_{(1)}} \leq \varepsilon_\lambda. \quad (6.81)$$

If this condition is satisfied, we have solved the problem and our last computed flux is the solution that is desired. If not, then another iteration is required. Actually, this test is not always guaranteed to produce success, especially when the sequence of  $\lambda_{(i)}$  values oscillates about the true value. A more restrictive additional test is usually performed on successive flux solutions, and requires that

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$$\left[ \begin{array}{c} \text{Maximum} \\ \text{relative flux} \\ \text{change} \end{array} \right] \leq \varepsilon_{\phi}. \quad (6.82)$$

The completion of steps c through f comprises one outer iteration. If convergence is not attained, then  $\underline{\psi}_{(1)}$  is used to compute a new source and steps c through f are repeated, as many times as necessary, until convergence is reached on the  $i$ th outer iteration giving the solution  $\underline{\psi}_{(i)}$ . In most multidimensional computer codes, convergence is also accelerated by performing what is known as a source extrapolation.

Since the problem is homogeneous, the normalization of the flux is arbitrary. Therefore, we must specify the operating power level of the system and scale the flux solution so that the integrated fission rate gives the specified total power. If we define the matrix  $\underline{\Sigma}_f$  to be the mesh-box integrated matrix of fission cross sections, define  $P$  as the power in watts and let  $c = 3.1 \times 10^{10}$  fissions/s-watt, then the normalization factor is

$$N_{(i)} \equiv \frac{Pc}{b(\underline{\Sigma}_f \underline{\psi}_{(i)}, 1)}. \quad (6.83)$$

where  $b$  is an appropriate factor that depends on the problem geometry. The inner product in the denominator, times  $b$ , is equal to the total fission rate in the reactor. The properly scaled flux solution is therefore

$$\underline{\psi}_{(i)}^{scaled} = N_{(i)} \underline{\psi}_{(i)}. \quad (6.84)$$

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### 6.8\* Convergence of the Outer Iteration to the Fundamental Mode Solution

In the previous section we described an iterative method for solving the reactor eigenvalue problem. We finally show that the solution that is obtained is indeed equal to the fundamental mode solution. To illustrate this proof, we work with a much simpler problem that contains all of the essential features of the reactor eigenvalue problem.

Consider the ordinary eigenvalue problem

$$\underline{\underline{A}}\underline{x} = \lambda\underline{x}, \quad (6.85)$$

where  $\underline{\underline{A}} = \underline{\underline{A}}^T$  is a symmetric system matrix (not an essential requirement). By assigning an iteration index  $i$  as a bracketed subscript, the iteration procedure used previously can be written as

$$\underline{x}_{(i)} = \frac{\underline{\underline{A}}\underline{x}_{(i-1)}}{\lambda_{(i-1)}}. \quad (6.86)$$

One finds the new value of the vector  $\underline{x}_{(i)}$  by operating on the previous value  $\underline{x}_{(i-1)}$  by the system matrix  $\underline{\underline{A}}$ . At each step, the value of  $\lambda_{(i-1)}$  is estimated using the solution obtained previously. One estimate is obtained by taking inner products with the unit vector, i.e.,

$$\lambda_{(i-1)} = \frac{(\underline{\underline{A}}\underline{x}_{(i-1)}, \underline{1})}{(\underline{x}_{(i-1)}, \underline{1})}. \quad (6.87)$$

A somewhat better variational estimate, corresponding to a type of least-squares analysis, is obtained by taking the Rayleigh Quotient, giving

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$$\lambda_{(i-1)} = \frac{(\underline{\underline{A}}\underline{x}_{(i-1)}, \underline{x}_{(i-1)})}{(\underline{x}_{(i-1)}, \underline{x}_{(i-1)})}. \quad (6.88)$$

In either event, if the initial guess is the vector  $\underline{x}_{(0)}$ , succeeding iterates are obtained by successively operating on  $\underline{x}_{(0)}$  by the system matrix  $\underline{\underline{A}}$ . The result of the first  $i$  iterates is the following:

$$\begin{aligned} \underline{x}_{(1)} &= \frac{\underline{\underline{A}}\underline{x}_{(0)}}{\lambda_{(0)}}; \\ \underline{x}_{(2)} &= \frac{\underline{\underline{A}}}{\lambda_{(1)}} \left( \frac{\underline{\underline{A}}\underline{x}_{(0)}}{\lambda_{(0)}} \right); \\ &\vdots \end{aligned} \quad (6.89)$$

$$\underline{x}_{(i)} = \frac{\underline{\underline{A}}^i \underline{x}_{(0)}}{\prod_{k=0}^{i-1} [\lambda_{(k)}]}.$$

Since  $\lambda$  is of the order of magnitude of unity, the  $\prod$  product in the denominator is also of a magnitude near unity.

Now, the system matrix  $\underline{\underline{A}}$  is of the order  $n$  and admits  $n$  exact eigenvalues and their corresponding eigenvectors. Let these exact equations be written as

$$\underline{\underline{A}}\underline{e}_j = \lambda_j \underline{e}_j; \quad j = 0, \dots, (n-1), \quad (6.90)$$

where  $\underline{e}_j$  are unit vectors. For a symmetric matrix, the eigenvectors are orthogonal, i.e.,

$$(\underline{e}_j, \underline{e}_k) = \delta_{jk}, \quad (6.91)$$

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where  $\delta_{jk}$  is the Kroniker delta. By operating on the equation by  $\underline{\underline{A}}$  successively, we further show that

$$\begin{aligned}\underline{\underline{A}}(\underline{\underline{A}}\underline{e}_j) &= \underline{\underline{A}}(\lambda_j \underline{e}_j) = \lambda_j^2 \underline{e}_j, \\ \underline{\underline{A}}^3 \underline{e}_j &= \lambda_j^3 \underline{e}_j, \\ &\vdots \\ \underline{\underline{A}}^i \underline{e}_j &= \lambda_j^i \underline{e}_j.\end{aligned}\tag{6.92}$$

We now expand the initial guess  $\underline{x}_{(0)}$  in a power series in terms of the eigenvectors of  $\underline{\underline{A}}$ , namely,

$$\underline{x}_{(0)} = \sum_{k=0}^{n-1} a_k \underline{e}_k.\tag{6.93}$$

The coefficients  $a_k$  can be considered to be known because they can be obtained by taking the inner product of the above expression with respect to  $\underline{e}_j$  to obtain

$$a_k = (\underline{e}_k, \underline{x}_{(0)}).\tag{6.94}$$

Insert the expansion into the expression for the  $i$ th iterate and make use of the expression derived above for the  $i$ th power of the system matrix  $\underline{\underline{A}}$ . The result is

$$\underline{x}_{(i)} = \frac{\sum_{k=0}^{n-1} a_k \underline{\underline{A}}^i \underline{e}_k}{\prod_{k=0}^{i-1} [\lambda_{(k)}]} = \frac{\sum_{k=0}^{n-1} a_k \lambda_k^i \underline{e}_k}{\prod_{k=0}^{i-1} [\lambda_{(k)}]}.\tag{6.95}$$

Factor out the fundamental mode eigenvalue  $\lambda_0$ , and write the term containing the fundamental mode eigenvector separately

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from the rest of the summation. The resulting form is

$$\underline{x}_{(i)} = \frac{\lambda_0^i}{\prod_{k=0}^{i-1} [\lambda_{(k)}]} \left[ a_0 \underline{e}_0 + \sum_{k=1}^{n-1} a_k \left( \frac{\lambda_k}{\lambda_0} \right)^i \underline{e}_k \right]. \quad (6.96)$$

Since  $\lambda_0$  is the largest eigenvalue of the reactor problem, the ratio

$$\frac{\lambda_k}{\lambda_0} < 1; k = 1, \dots, (n-1). \quad (6.97)$$

In the limit as  $i \rightarrow \infty$  (convergence),

$$\lim_{i \rightarrow \infty} \left\{ \frac{\lambda_k}{\lambda_0} \right\}^i \rightarrow 0; k = 1, \dots, (n-1). \quad (6.98)$$

Hence, all terms in the square brackets except the first tend to vanish leaving

$$\underline{x}_{(i)} \rightarrow \left[ \frac{\lambda_0^i}{\prod_{k=0}^{i-1} [\lambda_{(k)}]} \right] a_0 \underline{e}_0 = [\text{constant}] \underline{e}_0, \quad (6.99)$$

where the factor

$$\frac{\lambda_0^i}{\prod_{k=0}^{i-1} [\lambda_{(k)}]} \approx \text{order of } 1$$

and

$$\lambda_{(i)} \rightarrow \lambda_0.$$

We have proved that a power iteration scheme of the type used in the above discussion converges to the fundamental mode

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solution. As before, the scaling of the solution is found to be arbitrary and is usually obtained by specifying the reactor power. From a physical viewpoint, we can postulate that the iteration process consists of sweeping out the contributions of the higher harmonic modes in the initial flux guess until only the fundamental mode remains. Naturally, since the values of  $\lambda$  lie in the sequence  $\lambda_0 > \lambda_1 > \lambda_2 > \dots > \lambda_{n-1}$ , the highest harmonic terms are eliminated first until the final convergence depends only upon the ratio of the first-harmonic mode eigenvalue to the fundamental mode eigenvalue. This ratio is called the "dominance ratio," i.e.,

$$\left[ \begin{array}{c} \textit{Dominance} \\ \textit{Ratio} \end{array} \right] \equiv \frac{\lambda_1}{\lambda_0}. \quad (6.100)$$

Physically, the closer the first harmonic mode is to being critical, the longer one must iterate to obtain convergence. One can demonstrate this fact numerically by solving the eigenvalue problem for a series of similar but successively longer cores. It has already been shown in Chapter 5 that the eigenvalue separation between modes decreases as a core gets larger.

### 6.9 Qualitative Comparison Between One-Speed and Two-Group Solutions

We have shown that the one-speed equation is amenable to analytic solution for a variety of reactor configurations, subject only to the validity of spatial flux separability. For the one-dimensional case, separability is not a problem and solutions can be generated for a reactor having any number of homogeneous regions by suitably satisfying the boundary conditions at each interface.

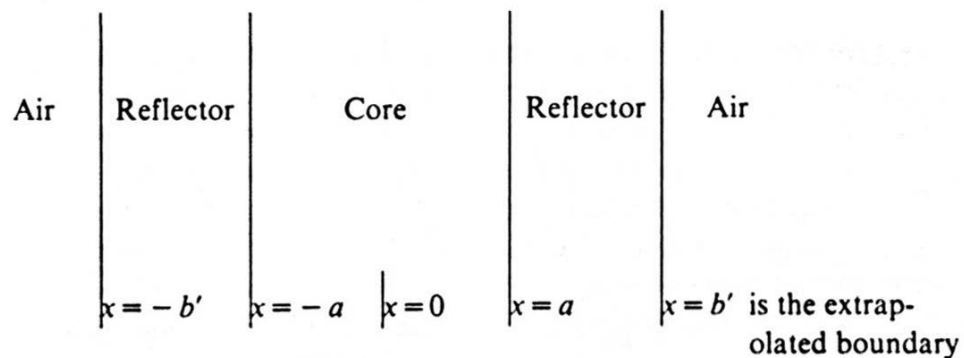
In the case of the few-group diffusion equations, we have



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adopted an approach of seeking numerical solutions to the finite difference analog of the diffusion equations. As a matter of fact, analytic solutions are still possible for the two-group case, but the amount of effort required for anything beyond a two-region, one-dimensional system is prohibitive. Suffice it to say that the numerical solutions have been verified against the analytic solutions, and against experiments, so that one can have confidence in the numerical results, subject only to the validity of diffusion theory itself.

Perhaps the best way to gain an appreciation for the differences between one-speed and few-group flux solutions is to compare the flux shapes and eigenvalues (criticality) obtained in similar problems. In such comparisons, the differences can be explained in terms of the physical processes that occur and the ability of the reactor model to represent these processes. We illustrate the nature of this comparison for the simple case of the bare, homogeneous reflected reactor shown in Figure 6.7.

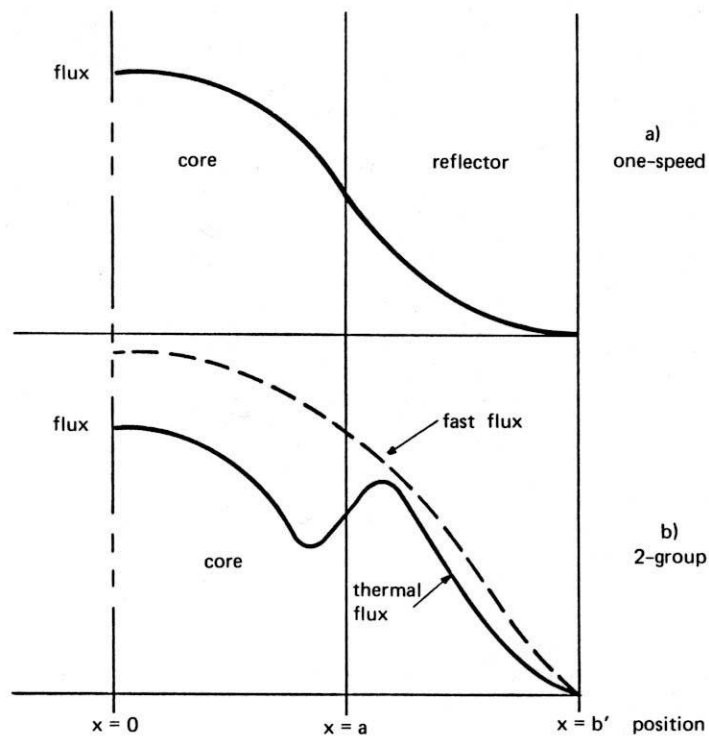


**Fig. 6.7** One-Dimensional Reflected Reactor

The flux shape obtained for the one-speed formulation is shown in Figure 6.8(a), while the flux shapes for the two-group representation are shown in Figure 6.8(b). There are several differences worth noting. First, we compare the thermal flux in the two-group situation with the one-speed flux, remembering that

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the fission rate is essentially proportional to the thermal flux. In the one-speed model, the flux decreases with distance from the core boundary with a concave curvature suggesting out-leakage. In the two-group case, there is what is known as a "reflector peak" with a curvature at the core boundary that suggests a net in-leakage of thermal neutrons. This is, in fact, caused by the superposition of two separate effects: the reflector peak is the sum of neutrons that were thermal in the core and diffuse out into the reflector, plus neutrons that have diffused out of the core as fast neutrons and have subsequently thermalized in the reflector. Since the one-speed model is unable to treat neutron moderation, the reflector peak is absent there.



**Fig. 6.8** Comparison of One-Speed and Two-Group Solutions for the Bare Homogeneous Reflected Slab Reactor

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The phenomenon of flux peaking in moderator regions is not limited to reflector-fuel interfaces. One sees "water gap peaking" in places where control rods have been withdrawn leaving a water-filled region between fuel assemblies or fuel rods. Such peaking can lead to local hot spots because the fission rate in the fuel next to the water region may be higher than in the rest of the fuel bundle. Oftentimes, this peaking is sufficiently large that it must be recognized in the design and corrective action taken. Possible alternatives are the use of control rod followers to keep water out of the gap, the use of fixed poisons, or the use of lower enrichments in the adjacent fuel rods.

The second major observation is that the magnitude of the fast flux distribution is much greater than the magnitude of the thermal flux distribution. Of course, the shape is also different because fission neutrons are only born in regions containing fuel and can only enter non-fueled regions by diffusion. The magnitude difference can be explained qualitatively as follows. Since neutrons are born fast and are absorbed at thermal energies, the scattering (moderation) rate of fast neutrons must be comparable to the absorption rate of thermal neutrons, i.e., for two groups,

$$\Sigma_{s1 \rightarrow 2} \phi_1 \approx \Sigma_{a2} \phi_2.$$

But  $\Sigma_{s1 \rightarrow 2} < \Sigma_{a2}$  because the fission cross section in fueled regions is large. Hence,  $\phi_1 > \phi_2$ . Ratios of 2 to 10 are commonly observed between the fast group flux and the thermal group flux in typical thermal reactor calculations. Finally, it should be noted that the few-group calculations generally predict a different value of  $k_{\text{eff}}$  than the one-speed calculation because the thermal flux distribution is represented more accurately. Referring to Figure 6.8, the thermal flux is higher at the reflector interface than in the one-speed case, which leads to more fissions in the core and a greater  $k_{\text{eff}}$ .

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### Problems

- 6.1** Use an available one-dimensional, two-group computer program to obtain  $k_{\text{eff}}$  and the two-group flux solution for a cylindrical model of the UVAR swimming pool reactor, where the core dimensions are taken as the following: Equivalent radius is 15 cm. This is a circle having the same area as the actual square core; Equivalent height of the bare core is 67 cm. The actual core is 59.7 cm high and is reflected. Using the concept of reflector savings, the equivalent bare core is about 7 cm longer, and this is the value to be used in calculating the transverse buckling  $B_z^2$ . For two-groups, a different  $B^2$  should really be used for each group. Use a mesh spacing of approximately  $\frac{1}{2}$  cm in the core and 1 cm in the reflector. Appropriate two-group constants are the following:

Core	Reflector
$D_1 = 1.36$	$D_1 = 1.27$
$D_2 = 0.192$	$D_2 = 0.146$
$\Sigma_{a1} = 0.00242$	$\Sigma_{a1} = 0.000468$
$\Sigma_{a2} = 0.0909$	$\Sigma_{a2} = 0.0197$
$\Sigma_{s1 \rightarrow 2} = 0.0344$	$\Sigma_{s1 \rightarrow 2} = 0.085$
$\nu \Sigma_{f1} = 0.00312$	
$\nu \Sigma_{f2} = 0.149$	
$\nu = 2.42$	
$\chi_1 = 1.0$	
$\chi_2 = 0.$	

Normalize the fluxes to a total power of 2MWT and plot as a function of position. Comment on the results.

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- 6.2** Write your own two-group, one-dimensional computer program in either FORTRAN or BASIC using the methods described in Chapter 6. Using the data given in Problem 6.1, find the value of  $k_{\text{eff}}$  and the two-group flux solution for the UVAR reactor. If possible, compare your solution to that obtained from an available computer code.
- 6.3** Derive the generalized one-dimensional diffusion equation in finite difference form as given by Eq. (6.20).
- 6.4** Using the  $\phi_1$  and  $\phi_2$  solutions from Problem 6.1, obtain equivalent 1-Group constants for each region. Explain your methodology. Now for a certain power level, solve for  $\phi$  in the 1-group problem. Compare the values of  $k_{\text{eff}}$  and the power distributions in the two cases.
- 6.5** Derive the 3-point finite-difference equation for the "mesh-centered" mesh-box formulation, as given by Eq. (6.24).
- 6.6** Derive the 2-point finite-difference equation at a boundary point for the "mesh-centered" formulation, which corresponds to Eq. (6.30) for the "edge-centered" formulation.
- 6.7** The Taylor series expansion of a function  $y(x)$  at a given point gives the corresponding value at another point  $h$  units away according to the expressions

$$y(x \pm h) = y(x) \pm h'y(x) + \frac{h^2 y''(x)}{2!} \pm \frac{h^3 y'''(x)}{3!} + \dots$$

and

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$$y(x \pm 2h) = y(x) \pm 2h'y(x) + \frac{4h^2 y''(x)}{2!} \pm \frac{8h^3 y'''(x)}{3!} + \dots$$

The forward difference operator  $\Delta$  works to the right of the point so that

$$\Delta y(x) = y(x+h) - y(x),$$

and

$$\Delta^2 y(x) = y(x+2h) - 2y(x+h) + y(x).$$

The central difference operator  $\delta$  works about the point, so that

$$\delta^2 y(x) = y(x+h) - 2y(x) + y(x-h).$$

The backward difference operator  $\nabla$  works to the left of the point so that

$$\nabla y(x) = y(x) - y(x-h)$$

and

$$\nabla^2 y(x) = y(x-2h) - 2y(x-h) + y(x).$$

Using the above information, show that the second derivative  $y''(x)$  as approximated by either the forward or backward difference operator is given by the expressions

$$\frac{d^2 y}{dx^2} = \frac{\Delta^2 y(x)}{h^2} + O(h)$$

or

$$\frac{d^2 y}{dx^2} = \frac{\nabla^2 y(x)}{h^2} + O(h).$$

while the second derivative as approximated by the central difference operator is

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$$\frac{d^2 y}{dx^2} = \frac{\delta^2 y(x)}{h^2} + O(h^2).$$

Hence, show that the central difference approximation is more accurate for a given mesh spacing than either the forward or backward difference approximations.

**6.8** You are given the three vectors

$$\underline{x}_1 = \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}, \quad \underline{x}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \underline{x}_3 = \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix}.$$

- a) Do these vectors span the three-dimensional space, that is, are they linearly independent?
- b) Describe the concept of linear independence and its consequences, and demonstrate graphically using the above vectors.
- c) Three orthogonal vectors in three-dimensional space are the vectors

$$\underline{r} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}, \quad \underline{s} = \begin{bmatrix} 0 \\ \sqrt{2} \\ \sqrt{2} \end{bmatrix}, \quad \text{and} \quad \underline{t} = \begin{bmatrix} 0 \\ -\sqrt{2} \\ \sqrt{2} \end{bmatrix}$$

Show that these vectors are orthogonal, and find the corresponding unit vectors.

- d) If  $\underline{x}_1$  is expanded as  $\underline{x}_1 = a\underline{r} + b\underline{s} + c\underline{t}$ , find the coefficients  $a$ ,  $b$ , and  $c$ .

**6.9** You are given the source problem  $\underline{\underline{A}} \underline{x} = \underline{s}$ , where

$$\underline{\underline{A}} = \begin{bmatrix} 2/3 & -1 \\ 0 & 1/2 \end{bmatrix} \quad \text{and} \quad \underline{s} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}.$$

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- a) Find the exact solution  $\underline{x}$  for this problem.

We set up an iterative procedure to solve the problem. Let the  $\underline{\underline{A}}$  matrix be partitioned into the form

$$\underline{\underline{A}} = \underline{\underline{I}} - \underline{\underline{T}},$$

so that the iteration scheme for the  $i$ th iterate is written as

$$\underline{x}^{(i)} = \underline{\underline{T}}\underline{x}^{(i-1)} + \underline{s}.$$

- b) Will the iteration converge? Why? Estimate the number of iterations,  $n$ , needed to reduce the relative error,

$$\varepsilon = \frac{\|\underline{x}^{(n)} - \underline{x}\|}{\|\underline{x}\|},$$

to less than 1%.

- c) Using the initial guess  $\underline{x}^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ , do the first  $n$  iterations to three-place accuracy and compare the relative error obtained to the estimated relative error.
- d) Find an iteration scheme that converges more rapidly.

**6.10** Consider the ordinary eigenvalue problem

$$\underline{\underline{A}}\underline{x} = \lambda\underline{x}, \quad \text{where } \underline{\underline{A}} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix}.$$

- a) Using hand calculations, find the largest eigenvalue and the corresponding eigenvector



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iteratively. Normalize the equations so that the solution vector is a unit vector. Solve at least up to  $\underline{x}^{(4)}$ .

- b) If we multiply through by  $\underline{\underline{A}}^{-1}$ , we obtain the equation

$$\underline{\underline{A}}^{-1} \underline{x} = \frac{1}{\lambda} \underline{x}.$$

Repeat the process done in part a. What does the resulting solution correspond to? (You may have numerical accuracy problems here).

- c) Check your results against those obtained from an available computer root-finding program.

## References

- E.L. Wachspress**, *Iterative Solutions of Elliptic Equations*, (Prentice Hall Publishing Company, Englewood Cliffs, NJ, 1966) Chapters 1, 2 and 3.
- F.B. Hildebrand**, *Methods of Applied Mathematics*, (Prentice Hall Publishing Company, Englewood Cliffs, NJ, 1952) Chapter 1.
- D.R. Vondy, T.B. Fowler and G.W. Cunningham** "VENTURE: A Code Block for Solving Multigroup Neutronics Problems Applying the Finite-Difference Diffusion-Theory Approximation to Neutron Transport, Version II," ORNL-5062/R1, (November 1977).

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## PERTURBATION THEORY

In Chapters 5 and 6 we discussed the static behavior of a reactor system that is describable by the diffusion theory approximation to the neutron transport equation. Here we consider a reactor system that is disturbed in some manner from its critical state. As a result of this disturbance, it exhibits a transient response. We first examine the characteristics of the perturbation to find the driving force for the transient. In Chapter 8, we examine the resulting transient behavior.

A perturbation is defined as a local change in the material properties of the reactor system, for example, the insertion of a control rod or the addition of a soluble absorber into the reactor coolant. Probably the most important thing to realize is that the *effect* of a given perturbation depends upon *where* it is placed in the reactor. This Chapter deals with the subject of perturbation theory, which is a formal way of calculating perturbation effects.

There is another form of perturbation theory, applicable to *inhomogeneous* problems, which has a different interpretation. This form is useful for radiation shielding applications. However, it can also be used for the analysis of fuel pin cells.

Various types of *feedback* mechanisms produce additional perturbations in reactor properties. Using the same formalism, the topics of thermal feedback, fission product poisons and reactor depletion are covered in Chapter 9.

### 7.1 Adjoint Equations

The reactor balance equation, written out as a function of

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both space and energy, is in the form of a generalized eigenvalue problem of the type

$$L\phi_i(\vec{r}, E) = \frac{M\phi_i(\vec{r}, E)}{\lambda_i}, \quad i = 0, 1, 2, \dots \quad (7.1)$$

where

$\phi_i(\vec{r}, E)$  is the flux in the  $i$ th harmonic mode;

$$L = [-\nabla \cdot D \nabla + \Sigma_a + \Sigma_s - \int \Sigma_s(E' \rightarrow E) \phi(E') dE']$$

is the destruction operator;

$$M = [\chi(E) \int \nu \Sigma_f(E') \phi(E') dE']$$

is the production operator; and

$\lambda_i$  is the criticality (eigenvalue) of the  $i$ th harmonic mode.

Mathematically, each eigenvalue problem possesses a dual or adjoint formulation of the type

$$L^* \phi_j^*(\vec{r}, E) = \frac{M^* \phi_j^*(\vec{r}, E)}{\lambda_j}, \quad (7.2)$$

which has the following properties:

1. the eigenvalues are identical to those of the flux problem;
2. the operators  $L^*$  and  $M^*$  can be derived from the corresponding operators  $L$  and  $M$ ;
3. The boundary conditions on  $\phi$  and  $\phi^*$  are identical;
4. the eigenfunction solutions of  $\phi$  and  $\phi^*$  for different characteristic numbers (eigenvalues) are orthogonal in

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a weighted integral sense.

The function  $\phi^*$  is known as the adjoint flux or the importance function, which will be given a physical significance shortly.

We use the "kets" notation, which implies integration over space and energy, to define the adjoint operators. For the production operator, let

$$\iint \phi_j^*(\vec{r}, E) M \phi_i(\vec{r}, E) dE d\vec{r} \equiv \langle \phi_j^*, M \phi_i \rangle. \quad (7.3)$$

The definition of  $M^*$  is then written as

$$\langle \phi_j^*, M \phi_i \rangle \equiv \langle \phi_i, M^* \phi_j^* \rangle = a \text{ number} \quad (7.4)$$

To actually obtain the operator form of  $M^*$ , one must substitute the operator  $M$  into the left-hand side of the definition and change the order of integration by integrating by parts to put the result into the form given in the right-hand side of the expression. A matching of corresponding terms leads to the form of the operator  $M^*$ . The operator  $L^*$  is obtained in a similar manner from the expression

$$\langle \phi_j^*, L \phi_i \rangle \equiv \langle \phi_i, L^* \phi_j^* \rangle = a \text{ number} \quad (7.5)$$

The treatment of the destruction operator is somewhat more complicated than the treatment of the production operator because of the presence of the leakage term. We must integrate this term by parts twice in order to put the left-hand side of the defining equation into the form appearing on the right-hand side. When this operation is done, terms that must be evaluated on the outer boundary of the reactor are obtained. These boundary terms serve to define the boundary conditions on the adjoint flux, and in fact lead to the conclusion that the boundary conditions on the flux and the adjoint are identical. This result might have been

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expected intuitively because of the similar form of the flux and adjoint equations.

**Adjoint Operators  $M^*$  and  $L^*$ .** By definition, the adjoint operator  $M^*$  is obtained from the expression

$$\langle \phi^*, M\phi \rangle \equiv \langle \phi, M^* \phi^* \rangle,$$

where

$$M = \chi(E) \int_0^{E_{\max}} \nu \Sigma_f(E') \{ \} dE.$$

We perform the left-hand integral over space and energy, and then rearrange the resulting product of two integrals and redefine the dummy variables. We obtain the expression:

$$\begin{aligned} & \int \left[ \int_0^{E_{\max}} \phi^*(E) \chi(E) dE \int_0^{E_{\max}} \phi(E') \nu \Sigma_f(E') dE' \right] dr \\ &= \int \left[ \int_0^{E_{\max}} \phi(E') \nu \Sigma_f(E') dE' \int_0^{E_{\max}} \phi^*(E) \chi(E) dE \right] dr \\ &= \int \left[ \int_0^{E_{\max}} \phi(E) \nu \Sigma_f(E) dE \int_0^{E_{\max}} \phi^*(E') \chi(E') dE' \right] dr. \end{aligned} \tag{7.6}$$

Hence, by comparison to the right-hand integral, the adjoint operator is obtained as

$$M^* = \nu \Sigma_f(E) \int_0^{E_{\max}} \chi(E') \{ \} dE'. \tag{7.7}$$

By definition, the adjoint operator  $L^*$  is obtained from the equation

$$\langle \phi^*, L\phi \rangle \equiv \langle \phi, L^* \phi^* \rangle,$$

where,

$$L = -\nabla \cdot D \nabla + \Sigma_a + \Sigma_s - \int_0^{E_{\max}} \Sigma_s(E' \rightarrow E) \{ \} dE'.$$

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We treat the resulting terms separately.

1st term (leakage) - In effect we integrate over space by parts twice (This is one form of Green's Theorem - see **Hildebrand**, *Advanced Calculus for Engineers*). The result is the equation

$$\begin{aligned} & - \int_0^{E_{\max}} \left[ \int \phi^* \nabla \cdot D \nabla \phi \, dr \right] dE \\ & = \int_0^{E_{\max}} \left[ - \oint_{\text{surface}} \phi^* D \nabla \phi \cdot \vec{n} \, dS + \int \nabla \phi^* \cdot D \nabla \phi \, dr \right] dE \end{aligned} \quad (7.8)$$

$$= \int_0^{E_{\max}} \left[ - \oint \phi^* D \nabla \phi \cdot \vec{n} \, dS + \oint \phi D \nabla \phi^* \cdot \vec{n} \, dS - \int \phi \nabla \cdot D \nabla \phi^* \, dr \right] dE.$$

The boundary conditions are either;  $\phi$  and  $\phi^*$  are zero at the surface of the reactor; or  $\nabla \phi$  and  $\nabla \phi^*$  are zero. Thus, both surface integrals vanish.

2nd term (absorption and out-scatter) - This term is simply rearranged to give

$$\int_0^{E_{\max}} \left[ \int \phi^* (\Sigma_a + \Sigma_s) \phi \, dr \right] dE = \int_0^{E_{\max}} \left[ \int \phi (\Sigma_a + \Sigma_s) \phi^* \, dr \right] dE. \quad (7.9)$$

3rd term (in-scatter) - Reverse the order of integration and redefine the dummy variables. One obtains the expression

$$\begin{aligned} & \int \left[ \int_0^{E_{\max}} \phi^*(E) \int_0^{E_{\max}} \Sigma_s(E' \rightarrow E) \phi(E') \, dE' \, dE \right] dr \\ & = \int \left[ \int_0^{E_{\max}} \phi(E') \int_0^{E_{\max}} \Sigma_s(E' \rightarrow E) \phi^*(E) \, dE \, dE' \right] dr \\ & = \int \left[ \int_0^{E_{\max}} \phi(E) \int_0^{E_{\max}} \Sigma_s(E \rightarrow E') \phi^*(E') \, dE' \, dE \right] dr. \end{aligned} \quad (7.10)$$

Hence, by comparison to the right-hand integral, the adjoint operator is defined as

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$$L^* = -\nabla \cdot D \nabla + \Sigma_a + \Sigma_s - \int_0^{E_{\max}} \Sigma_s(E \rightarrow E') \{ \} dE. \quad (7.11)$$

Note the exchange of roles between  $\chi$  and  $\nu \Sigma_f$  in  $M^*$  and the change (reversal) of energy scattering direction in  $L^*$ , which implies a type of transposition from  $M$  and  $L$ , respectively.

**Proof of Orthogonality of  $\phi$  and  $\phi^*$ .** Having obtained the operators  $M^*$  and  $L^*$  from  $M$  and  $L$ , we are in a position to prove orthogonality between  $\phi_i$  and  $\phi_j^*$ . We have the flux equation

$$L\phi_i = \frac{M\phi_i}{\lambda_i}$$

and the adjoint equation

$$L^*\phi_j^* = \frac{M^*\phi_j^*}{\lambda_j}.$$

Multiply the flux equation by  $\phi_j^*$ , multiply the adjoint equation by  $\phi_i$ , and integrate the resulting expressions over energy and the volume of the core. The results are

$$\langle \phi_j^*, L\phi_i \rangle = \frac{\langle \phi_j^*, M\phi_i \rangle}{\lambda_i}$$

and

$$\langle \phi_i, L^*\phi_j^* \rangle = \frac{\langle \phi_i, M^*\phi_j^* \rangle}{\lambda_j}. \quad (7.12)$$

Subtract the second equation from the first, recalling the definitions of the adjoint operators. Since the  $\lambda$ 's are distinct, the result is



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$$\left(\frac{1}{\lambda_i} - \frac{1}{\lambda_j}\right) \langle \phi_j^*, M \phi_i \rangle = 0. \quad (7.13)$$

This equation implies that  $\phi_i$  is orthogonal to  $\phi_j^*$  with respect to the weighting function  $M$ . We arbitrarily normalize  $\phi_j^*$  so that

$$\langle \phi_j^*, M \phi_i \rangle = \delta_{ij}, \quad (7.14)$$

where  $\delta_{ij}$  is the Kroniker delta, which has the value 1 when  $i = j$  and has the value 0 when  $i \neq j$ .

We compare the operators  $L$  and  $L^*$  and the operators  $M$  and  $M^*$  more carefully. The only difference between  $L$  and  $L^*$  is the transposition of the energy variables  $E$  and  $E'$  in the scattering transfer integral. Likewise, the only difference between  $M$  and  $M^*$  is the transposition of the roles of the spectrum function  $\chi(E)$  and the fission production term  $\nu \Sigma_f(E)$  with respect to the integral over energy. We therefore conclude that in the case where energy is not treated explicitly, i.e., the one-speed problem, the corresponding operators are identical.

The one-speed diffusion equation is a special case. For this situation,  $\chi \rightarrow 1$ , giving the relationship

$$M = M^* = \nu \Sigma_f.$$

Likewise,

$$\int_0^{E_{\max}} \Sigma_s(E' \rightarrow E) \{ \} dE \rightarrow \Sigma_s,$$

giving

$$L = L^* = -\nabla \bullet D \nabla + \Sigma_a.$$

We say that the one-speed equation is self-adjoint. Obviously, we then have the condition that

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$$\phi_i = \phi_i^*,$$

which means that the various one-speed harmonic fluxes are orthogonal to one another with respect to  $v\Sigma_f$  as a weighting function.

### 7.2 Matrix Form of the Adjoint Equations

If one proceeds to discretize the reactor balance equation over N space intervals and G energy groups one obtains the vector-matrix form of the generalized eigenvalue problem, namely,

$$\underline{\underline{L}}\underline{\psi}_i = \frac{\underline{\underline{M}}\underline{\psi}_i}{\lambda_i}, \quad i = 0, 1, \dots, (N-1), \quad (7.15)$$

where  $\underline{\underline{L}}$  is the discretized destruction matrix (which is block tri-diagonal for a one-dimensional problem);  $\underline{\underline{M}}$  is the discretized production matrix, (which is block diagonal);  $\underline{\psi}_i$  is the flux super-vector for the  $i$ th harmonic mode, (which is G groups by N mesh intervals long);  $\lambda_i$  is the corresponding criticality of the  $i$ th harmonic mode, where the total number of modes is N.

By standard mathematical techniques, it can be shown that the dual or adjoint to the above problem is the problem

$$\underline{\underline{L}}^T \underline{\psi}_j^* = \frac{\underline{\underline{M}}^T \underline{\psi}_j^*}{\lambda_j}, \quad (7.16)$$

which is sometimes called the "left" eigenvalue problem because it can also be written in the form

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$$\underline{\psi}_j^{*T} \underline{L} = \frac{\underline{\psi}_j^{*T} \underline{M}}{\lambda_j}. \quad (7.17)$$

We make use of the fact that the transpose of a product is the product of the transposes in reverse order to obtain the latter form of the equation.

The proof of orthogonality proceeds as follows: Multiply the flux equation on the left by  $\underline{\psi}_j^{*T}$  and multiply the adjoint equation on the right by  $\underline{\psi}_i$ . Subtraction of the two results gives the equation

$$\underline{\psi}_j^{*T} \underline{L} \underline{\psi}_i - \underline{\psi}_j^{*T} \underline{L} \underline{\psi}_i = \frac{\underline{\psi}_j^{*T} \underline{M} \underline{\psi}_i}{\lambda_i} - \frac{\underline{\psi}_j^{*T} \underline{M} \underline{\psi}_i}{\lambda_j}, \quad (7.18)$$

or, using vector inner-product notation,

$$\left( \frac{1}{\lambda_i} - \frac{1}{\lambda_j} \right) (\underline{\psi}_j^*, \underline{M} \underline{\psi}_i) = 0. \quad (7.19)$$

Hence, the orthogonality relationship is

$$(\underline{\psi}_j^*, \underline{M} \underline{\psi}_i) = \delta_{ij}, \quad (7.20)$$

which is identical in form to the result obtained for the differential equations. One should note that in the vector-matrix case,  $\underline{M}^* = \underline{M}^T$  and  $\underline{L}^* = \underline{L}^T$ , which is a result that could have been anticipated from the original operator definitions.

A diffusion theory computer code such as RAUMZEIT can be used to calculate the fundamental mode solution to the adjoint problem if we simply transpose our input data for each region. The  $\underline{D}$  matrix of diffusion coefficients is diagonal, so it remains the same as before. The  $\underline{H}$  matrix of absorption and group scattering transfer cross sections is not diagonal so we transpose the numbers directly. The balance of the transposition

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can be made by inserting the  $\nu\Sigma_f$  numbers where the input for  $\chi$  is located and vice-versa. The value obtained iteratively for the adjoint  $k_{eff}^*$  turns out to be the same value as is obtained for the regular flux solution, thus proving empirically that the two problems are mathematically related to one another. However, the solution as a function of position will differ considerably from the corresponding flux solution, and it remains for us to find the physical significance of the adjoint.

Some computer codes, such as EXTERMINATOR, which solves the 2D problem, will make the matrix transposition internally when the adjoint option is selected; these codes will save both the flux solution and the adjoint solution for subsequent use in a perturbation calculation. Given some additional data, the code will calculate such core-averaged quantities as the reactivity, lifetime and effective delayed neutron fractions. These topics will be discussed later.

The physical significance of the adjoint is as follows: The adjoint is *proportional* to how *important* a neutron located at position  $\vec{r}$  and having energy  $E$  (or lying in group  $g$ ) is in sustaining the chain reaction. This is tantamount to determining the likelihood that a given neutron will cause a fission reaction to take place. Naturally, we cannot speak of a single neutron but only of the statistical properties of a large number of neutrons similarly situated. A neutron located near the edge of the reactor has a good chance to leak out, so that it is not as important as a neutron in the center of the reactor. A neutron located in a water region is not as important as one located in a fuel region (even if the flux is the same) because there is no uranium to cause fission. A fast neutron in the fuel is not as important as a thermal neutron in the fuel because the cross section for fission is smaller. And so on.

There is another way to explain the physical significance of

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the adjoint. Imagine that we have a critical reactor that has essentially no neutrons in it (after all, the critical state is just a balance between production and loss rates and is independent of the power level). If we now insert a neutron at position  $\vec{r}$  in group  $g$ , neutron multiplication will take place and a new flux distribution will be established. One can think of the adjoint as being proportional to the eventual asymptotic power level reached by the reactor due to this neutron. Putting the neutron near the edge will cause less multiplication than putting it in the center of the reactor, and hence the final power will be lower. The argument proceeds exactly the same as given in the preceding paragraph.

We are led to a very significant concept: the loss of a neutron has an *importance* to the chain reaction that varies with position and is independent of the neutron flux at the position. Hence, if we want to know the *effect* of a material change on the reactor we should really weight the corresponding reaction rate by its importance. In other words, if  $\delta \underline{\underline{H}}$  is a perturbed cross section matrix, then the local effect of adding  $\delta \underline{\underline{H}}$  varies as the product  $\underline{\psi}^{*T}(\vec{r}) \delta \underline{\underline{H}} \underline{\psi}(\vec{r})$ , and the total effect over the reactor varies as  $\int \underline{\psi}^{*T}(\vec{r}) \delta \underline{\underline{H}} \underline{\psi}(\vec{r}) d\mathbf{r} = \text{a number.}$

### 7.3 First-Order Perturbation Theory

Consider the fundamental mode flux and adjoint equations in few-group operator form,

$$\underline{\underline{L}} \underline{\phi}_0 = \frac{1}{\lambda_0} \underline{\underline{M}} \underline{\phi}_0 \quad \text{and} \quad \underline{\underline{L}}^T \underline{\phi}_0^* = \frac{1}{\lambda_0} \underline{\underline{M}}^T \underline{\phi}_0^*, \quad (7.21)$$

together with the appropriate boundary conditions. We now make a slight change in the reactor by, for example, dropping a coin

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into the core. The resulting neutron balance will correspond to a new eigenvalue problem having slightly different properties and a slightly different eigenvalue, namely,

$$\underline{\underline{L}}'\underline{\underline{\phi}}' = \frac{1}{\lambda_{0'}}\underline{\underline{M}}'\underline{\underline{\phi}}'. \quad (7.22)$$

We could solve this problem directly by using a computer code such as RAUMZEIT, but we might not obtain a very accurate value for the reactivity effect because we would have to subtract two values of  $\lambda_0$  that are close together and the numerical error would be large. Instead we use perturbation theory.

Let each of the terms in the perturbed balance be expanded as a small variation about the unperturbed term, i.e., let

$$\begin{aligned} \underline{\underline{L}}' &= \underline{\underline{L}} + \delta\underline{\underline{L}}, \\ \underline{\underline{M}}' &= \underline{\underline{M}} + \delta\underline{\underline{M}}, \\ \underline{\underline{\phi}}' &= \underline{\underline{\phi}} + \delta\underline{\underline{\phi}}, \end{aligned}$$

and

$$\lambda_{0'} = \lambda_0 + \delta\lambda. \quad (7.23)$$

Insert these values into the perturbed balance equation, multiply out the terms, and neglect the second-order terms that are products of the small variations. The perturbed equation becomes (preserving matrix order),

$$(\underline{\underline{L}} + \delta\underline{\underline{L}})(\underline{\underline{\phi}}_0 + \delta\underline{\underline{\phi}})(\lambda_0 + \delta\lambda) = (\underline{\underline{M}} + \delta\underline{\underline{M}})(\underline{\underline{\phi}}_0 + \delta\underline{\underline{\phi}}). \quad (7.24)$$

Expanding out and canceling second-order terms, we obtain

$$\begin{aligned} \lambda_0 \underline{\underline{L}} \underline{\underline{\phi}}_0 + \lambda_0 \delta\underline{\underline{L}} \underline{\underline{\phi}}_0 + \lambda_0 \underline{\underline{L}} \delta\underline{\underline{\phi}} + \lambda_0 \delta\underline{\underline{L}} \delta\underline{\underline{\phi}} + \delta\lambda \underline{\underline{L}} \underline{\underline{\phi}}_0 + \delta\lambda \delta\underline{\underline{L}} \underline{\underline{\phi}}_0 + \delta\lambda \underline{\underline{L}} \delta\underline{\underline{\phi}} + \delta\lambda \delta\underline{\underline{L}} \delta\underline{\underline{\phi}} \\ = \underline{\underline{M}} \underline{\underline{\phi}}_0 + \underline{\underline{M}} \delta\underline{\underline{\phi}} + \delta\underline{\underline{M}} \underline{\underline{\phi}}_0 + \delta\underline{\underline{M}} \delta\underline{\underline{\phi}}. \end{aligned} \quad (7.25)$$

The terms that are underlined can be neglected.

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To get the integrated effect on the core, multiply through by  $\phi_0^{*T}$  and integrate over volume. Using the modified inner-product notation, the result is

$$\begin{aligned} & \lambda_0(\underline{\phi}_0^*, \underline{\underline{L}}\underline{\phi}_0) + \lambda_0(\underline{\phi}_0^*, \delta\underline{\underline{L}}\underline{\phi}_0) + \lambda_0(\underline{\phi}_0^*, \underline{\underline{L}}\delta\phi) + \delta\lambda(\underline{\phi}_0^*, \underline{\underline{L}}\underline{\phi}_0) \\ & = (\underline{\phi}_0^*, \underline{\underline{M}}\underline{\phi}_0) + (\underline{\phi}_0^*, \delta\underline{\underline{M}}\underline{\phi}_0) + (\underline{\phi}_0^*, \underline{\underline{M}}\delta\phi). \end{aligned} \quad (7.26)$$

One pair of terms with underbars drops out because of the weighted flux balance, while a second pair drops out because of the weighted adjoint balance. These terms are of the form,

$$(\underline{\phi}_0^*, \{ \underline{\underline{L}}\underline{\phi}_0 - \frac{\underline{\underline{M}}^T \underline{\phi}_0^*}{\lambda_0} \}) = 0, \quad (7.27)$$

and

$$(\delta\phi, \{ \underline{\underline{L}}^T \underline{\phi}_0^* - \frac{\underline{\underline{M}}^T \underline{\phi}_0^*}{\lambda_0} \}) = 0, \quad (7.28)$$

Note: If the adjoint had not been used as the importance weighing function, then the latter terms would have remained in the equation making the perturbed  $\delta\lambda$  result depend upon the flux variation  $\delta\phi$  itself. When the adjoint is used, the perturbed  $\delta\lambda$  depends to first-order only upon the change in material properties,  $\underline{\underline{\delta L}}$  and  $\underline{\underline{\delta M}}$ . This is significant, because it means that we do not have to calculate the perturbed flux to find the effect of the perturbation on the reactor.

Gathering the remaining three terms, we have an expression for the global effect known as reactivity  $\rho$  (or in this case the change in reactivity,  $\Delta\rho$ ). Reactivity is defined as  $\rho \equiv (k - 1)/k$  and refers to the deviation in  $k$  from a just critical reactor with a multiplication factor of unity. Hence,

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$$\lambda_0 \Delta \rho_0 \approx \frac{\delta \lambda}{\lambda_0} = \frac{(\phi_0^*, \{ \frac{\delta \underline{\underline{M}}}{\lambda_0} - \delta \underline{\underline{L}} \} \phi_0)}{(\phi_0^*, \underline{\underline{L}} \phi_0)} = \frac{(\phi_0^*, \{ \frac{\delta \underline{\underline{M}}}{\lambda_0} - \delta \underline{\underline{L}} \} \phi_0)}{(\phi_0^*, \frac{\underline{\underline{M}}}{\lambda_0} \phi_0)}. \quad (7.29)$$

Note that  $\delta \lambda / \lambda_0 \rightarrow \rho$  as  $\lambda_0 \rightarrow 1$ .

This is the kind of expression that is evaluated in few-group diffusion theory codes such as EXTERMINATOR, where the computed flux and adjoint distributions are saved so that they can be used to perform the integrals for given values of  $\delta \underline{\underline{L}}$  and  $\delta \underline{\underline{M}}$ . In words, the reactivity effect can be stated as

$$\text{Reactivity} = \frac{\left[ \frac{\text{Weighted integral production rate change}}{\text{Total weighted integral production rate}} \right] - \left[ \frac{\text{Weighted integral destruction rate change}}{\text{Total weighted integral production rate}} \right]}{\left[ \frac{\text{Total weighted integral production rate}}{\text{Total weighted integral production rate}} \right]} \quad (7.30)$$

Now that we have derived the general form of the expression for reactivity we must examine each individual term to see how it contributes. We have two types of expressions to consider. The first type appears when we consider fission, absorption, or scattering; the second type appears when we consider leakage.

As an example of the first expression, we have the form

$$\text{Scattering or absorption term} = -(\phi_0^*, \underline{\underline{H}} \phi_0). \quad (7.31)$$

The second type of term, corresponding to leakage, is treated differently. We first use the "first form" of Green's Theorem to obtain a symmetric term that is easier to compute numerically,



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$$\begin{aligned}
 \text{Leakage term} &= (\underline{\phi}_0^*, \nabla \bullet \delta \underline{D} \nabla \underline{\phi}_0) \\
 &= -(\nabla \underline{\phi}_0^*, \bullet \delta \underline{D} \nabla \underline{\phi}_0) + \iint \underline{\phi}_0^{*T} \delta \underline{D} \nabla \underline{\phi}_0 \bullet \vec{n} dS.
 \end{aligned} \tag{7.32}$$

The surface integral is zero because the boundary conditions are either

$$\underline{\phi}_0(\vec{R}) = \underline{\phi}_0^*(\vec{R}) = 0 \quad \text{or} \quad \nabla \underline{\phi}_0(\vec{R}) = \nabla \underline{\phi}_0^*(\vec{R}) = 0.$$

Looking at the individual group-wise contributions, one can make the following general word statement:

$$\left[ \begin{array}{l} \text{Contribution to} \\ \text{reactivity of a} \\ \text{property change} \\ \text{in region} \end{array} \right] = \frac{\int_{\text{Region Volume}} \left[ \begin{array}{l} \text{Importance of} \\ \text{neutrons in the} \\ \text{affected group} \end{array} \right] \times \left[ \begin{array}{l} \text{Group material} \\ \text{property} \\ \text{change} \end{array} \right] \times \left[ \begin{array}{l} \text{Flux of neutrons} \\ \text{in the interacting} \\ \text{group} \end{array} \right] dr}{\left[ \begin{array}{l} \text{Total weighted} \\ \text{production rate} \end{array} \right]} \tag{7.33}$$

Typical terms are as follows (numerator only):

*Absorption and Out-scatter-diagonal matrix elements, only one group affected.*

$$\left[ \begin{array}{l} \text{Typical term for} \\ \text{absorption in group } g \end{array} \right] = - \int_{\text{Region}} \phi_g^* \delta \Sigma_{ag} \phi_g dr.$$

Absorption leads to a decrease in  $\rho$

*In-scatter-off-diagonal matrix elements, two groups affected.*

$$\left[ \begin{array}{l} \text{Typical term for scatter} \\ \text{from group } g' \text{ to } g \end{array} \right] = + \int_{\text{Region}} \phi_g^* \delta \Sigma_{sg' \rightarrow g} \phi_{g'} dr.$$

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In-scatter leads to an increase in  $\rho$ .

*Fission* - two groups affected.

$$\left[ \begin{array}{l} \text{Typical term for fission} \\ \text{in group } g', \text{ leads to a} \\ \text{neutron appearing in } g \end{array} \right] = + \int_{\text{Region}} \phi_g^* \chi_g \frac{\delta \nu \Sigma_{fg'}}{\lambda_0} \phi_{g'} d\mathbf{r}.$$

Fission leads to an increase in  $\rho$ .

*Leakage*-diagonal matrix elements, only one group affected, uses gradients.

$$\left[ \begin{array}{l} \text{Typical term for} \\ \text{leakage in group } g \end{array} \right] = - \int_{\text{Region}} \nabla \phi_g^* \bullet \delta D_g \nabla \phi_g d\mathbf{r}.$$

Leakage leads to a decrease in  $\rho$ .

In the corresponding one-speed case, where the flux is self-adjoint, we have the special reactivity expression,

$$\lambda_0 \Delta \rho_0 = \frac{\int_{\text{Region}} \left( \frac{\delta \nu \Sigma_f}{\lambda_0} - \delta \Sigma_a \right) \phi^2 d\mathbf{r} - \int_{\text{Region}} \delta D (\nabla \phi)^2 d\mathbf{r}}{\int_{\text{Core}} \frac{\nu \Sigma_f \phi^2 d\mathbf{r}}{\lambda_0}}. \quad (7.34)$$

### 7.4\* Perturbation Effects on Higher Harmonic Modes

In the previous section, we computed the change in criticality of the fundamental mode of a reactor due to the presence of a material perturbation. It should be fairly obvious that the same material change will also produce a change in the criticality of the higher harmonic modes, that is to say, the material change will alter the eigenvalue spectrum of the

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reactor. The derivation that we followed in the case of the fundamental mode is perfectly general and leads to identical expressions for the higher harmonic modes. However, we denote the criticality change by the symbol  $\delta$ , namely,

$$\delta_i = \frac{(\phi_i^*, \{ \frac{\delta M}{\lambda_i} - \delta L \} \phi_i)}{(\phi_i^*, \frac{M}{\lambda_i} \phi_i)}, \quad (7.35)$$

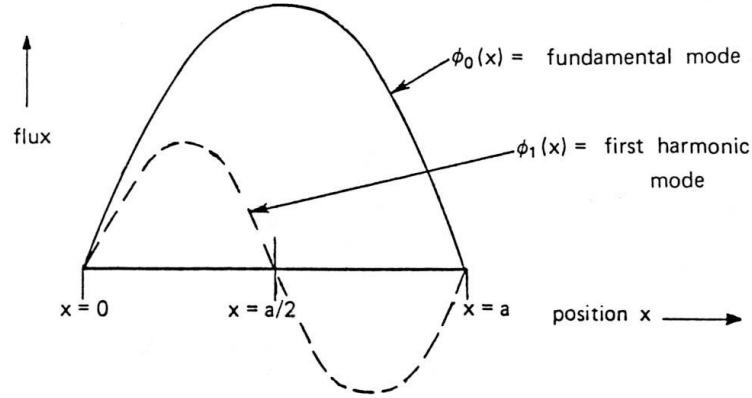
with the understanding that for the fundamental mode, the reactivity  $\rho_0 = \delta_0$ .

Refer for the moment to the one-speed case, which is illustrated in Figure 7.1. The reactor equations are self-adjoint in this instance so that the flux and the importance functions are identical. One can easily see that a perturbation near the *center* of the core will have a *maximum* effect upon the fundamental mode because both the flux and the importance are near their maximum values, while it will have a *minimum* effect on the first harmonic mode because it is near a node point. In fact, a symmetric perturbation, such as the removal of fuel from the center region of the reactor to flatten the power profile and give a more uniform fuel burnup, will cause a much larger decrease in the criticality of the fundamental mode than in the first harmonic mode. The result is a net decrease in the fundamental-to-first-harmonic-mode eigenvalue difference, referred to as the *eigenvalue separation*,

$$ES_i \equiv \frac{\lambda_0 - \lambda_i}{\lambda_0 \lambda_i},$$

which implies that the modified core will be more susceptible to excitation of the harmonic modes during transient situations. The implications of this statement will be examined later.

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**Fig. 7.1** Typical Fundamental and First-Harmonic Flux Modes

We return to the definition of reactivity. If the reactor is critical initially and at steady state, then the reactivity perturbation serves as the driving function for the subsequent transient response of the system. The global behavior of the system, i.e., the total reactor power, varies as a direct function of  $\rho_0$ . The higher harmonic modes contribute to the transient by inducing a change in the flux shape with time. The amount of contribution turns out to be inversely proportional to the amount of sub-criticality of the harmonic mode in question (eigenvalue separation) and directly proportional to the excitation of the harmonic mode. The excitation in turn is a reactivity expression of the type

$$\rho_i = \frac{(\underline{\phi}_i^*, \{ \frac{\delta \mathbf{M}}{\lambda_0} - \delta \mathbf{L} \} \underline{\phi}_0)}{(\underline{\phi}_0^*, \frac{\mathbf{M}}{\lambda_0} \underline{\phi}_0)}, \quad (7.36)$$

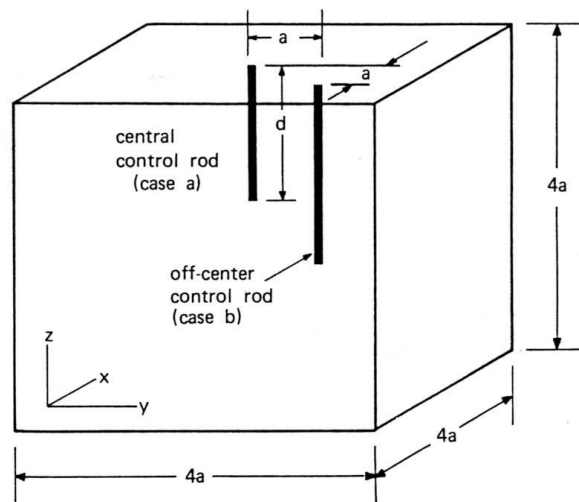
which indicates that the perturbed fundamental-mode-reaction-rate couples to the  $i$ th harmonic mode by virtue of the importance of that particular mode. Excitation of a given mode can be avoided

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by proper placement of the perturbation, e.g., symmetric perturbations will not excite the first harmonic mode of an initially symmetric system.

### 7.5 Control Rod Worth

Although first-order perturbation theory is only accurate when small changes in reactor parameters are considered, it can be used to give qualitative insight into the behavior of a control rod as a function of position in a reactor. Consider, for example, the case of a single control rod of cross sectional area  $A$  and macroscopic cross section  $\Sigma_{ar}$  that is to be inserted into a just critical bare cubical reactor  $4a$  centimeters on a side which includes the extrapolation distance. We assume that one-speed diffusion theory is applicable to this problem, and consider two separate cases: (a) the control rod is located in the center of the  $x$ - $y$  plane; and (b) the control rod is located at a distance  $a$  centimeters from the center in both the  $x$  and  $y$  directions. The situation is pictured in Figure 7.2.



**Fig. 7.2** Control Rod Insertion in a Bare Cubical Reactor

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In order to proceed we require the flux and adjoint solutions for the unrodded core. Assuming spatial separability, the fundamental mode solution can be found by the methods discussed previously to be

$$\phi(x, y, z) = C \cos\left(\frac{\pi x}{4a}\right) \cos\left(\frac{\pi y}{4a}\right) \cos\left(\frac{\pi z}{4a}\right), \quad (7.37)$$

where the origin is taken at the center of the reactor. Since the flux is self-adjoint in the one-speed case,  $\phi^* = \phi$ , and the reactivity worth of any perturbation in the initially critical ( $k_{\text{eff}} = \lambda_0 = 1$ ) core is given by Eq. (7.34).

If one considers that the control rod region has a very small volume, which is initially empty, one can obtain a reasonably accurate analytical approximation for both the numerator and the denominator of the reactivity expression. In the denominator, if one ignores the small empty region, the integral becomes

$$\begin{aligned} (\phi, M\phi) &\approx C^2 \int_{-2a}^{+2a} \int_{-2a}^{+2a} \int_{-2a}^{+2a} v \Sigma_f \cos^2\left(\frac{\pi x}{4a}\right) \cos^2\left(\frac{\pi y}{4a}\right) \cos^2\left(\frac{\pi z}{4a}\right) dx dy dz \\ &= (2a)^3 C^2 v \Sigma_f. \end{aligned} \quad (7.38)$$

In the numerator,  $\delta M = 0$  and the x-y integral simplifies to the product of  $\delta L$  and the flux at the x and y positions times the cross sectional area A. For the fully inserted central control rod (case a), we obtain the expression

$$\begin{aligned} (\phi, -\delta L\phi) &\approx -C^2 \Sigma_{ar} A \int_{-2a}^{+2a} \cos^2\left(\frac{\pi z}{4a}\right) dz \cos^2(0) \cos^2(0) \\ &= -2a C^2 \Sigma_{ar} A. \end{aligned} \quad (7.39)$$

For the fully inserted rod located at  $x = a$ ;  $y = a$  (case b), we have

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$$\begin{aligned}
 (\phi, -\delta L \phi) &\approx -C^2 \sum_{ar} A \int_{-2a}^{+2a} \cos^2\left(\frac{\pi z}{4a}\right) dz \cos^2\left(\frac{\pi}{4}\right) \cos^2\left(\frac{\pi}{4}\right) \\
 &= -\frac{a}{2} C^2 \sum_{ar} A.
 \end{aligned} \tag{7.40}$$

The control rod in case (b) is only worth 1/4 as much as the central control rod. In other words, it would take four control rods in the outer positions to equal one control rod in the center of the core. The total reactivity worth of the central control rod is

$$\rho(0,0,p=4a) \approx \frac{-2aC^2 \sum_{ar} A}{(2a)^3 C^2 \nu \sum_f} = \frac{-\sum_{ar} A}{4a^2 \nu \sum_f}. \tag{7.41}$$

The relative integral control rod worth as a function of control rod depth  $p$  in either case is given by the expression

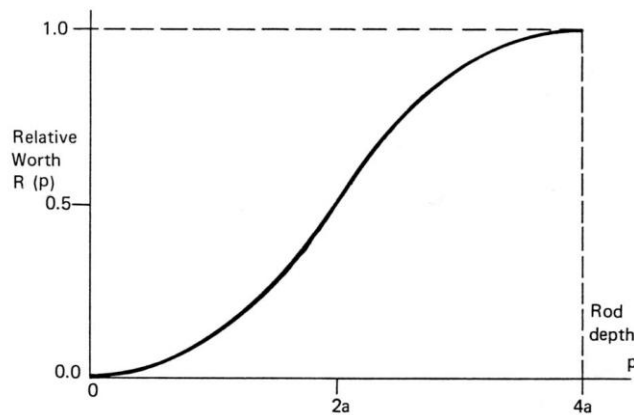
$$\begin{aligned}
 R(p) &\equiv \frac{\rho(x,y,p)}{\rho(x,y,p=4a)} = \frac{\int_{2a-p}^{2a} \cos^2\left(\frac{\pi z}{4a}\right) dz}{\int_{-2a}^{2a} \cos^2\left(\frac{\pi z}{4a}\right) dz} \\
 &= \frac{p}{4a} - \frac{\sin \pi \left(1 - \frac{p}{2a}\right)}{2\pi} = \frac{p}{4a} - \frac{\sin \frac{\pi p}{2a}}{2\pi}.
 \end{aligned} \tag{7.42}$$

The relative integral control rod worth curve is a sigmoid as shown in Figure 7.3. The control rod has its maximum worth per centimeter of insertion at the center of the core, as seen by taking the derivative of the above expression to obtain

$$\frac{dR}{dp} = \frac{1}{4a} \left(1 - \cos \frac{\pi p}{2a}\right), \tag{7.43}$$

which has its maximum at  $p = 2a$ .

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**Fig 7.3** Relative Control Rod Worth vs. Depth

Although the above results are qualitatively correct, they are inaccurate for at least two different reasons. First, the change in cross sections, represented by  $\delta L$ , is not small; neither are the variations in the flux,  $\delta \phi$ , and the adjoint,  $\delta \phi^*$ . Hence, perturbation theory is not accurate to first order. As a matter of fact, diffusion theory itself is not accurate in the vicinity of the control rods. Second, the flux in a real reactor is generally not separable; the repositioning of a control rod usually leads to a flux tilt whose magnitude depends upon the relative excitations of the harmonic flux modes, i.e., the eigenvalue separations. This leads to what is known as a control-rod-interaction effect, where the worth of a given control rod depends upon the position of the other control rods. Nevertheless, actual control rod worth curves look remarkably similar to the curve pictured in Figure 7.3.

Perhaps the most practical way to obtain the relative control rod worth curves for a given reactor model is to perform a series of three-dimensional few-group diffusion theory calculations, using a code such as VENTURE or 3DB. We use "effective" control rod cross sections, and place the control rods in varying positions. The flux tilt is automatically



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included and the reactivity worths can be obtained by subtraction of the  $k_{\text{eff}}$  values according to the equation

$$\Delta\rho = \frac{k_{\text{eff}} - k_{\text{eff}0}}{k_{\text{eff}} k_{\text{eff}0}}. \quad (7.44)$$

where  $k_{\text{eff}0}$  is for the unrodded core.

### 7.6\* Inhomogeneous Case

The inhomogeneous problem has a slightly different formulation than the homogeneous eigenvalue problem, but has a *significantly* different physical interpretation. In its simplest form, usually applied where there is no fission contribution, the flux problem is of the operator form,

$$L\phi(\vec{r}, E) = S(\vec{r}, E). \quad (7.45)$$

The flux  $\phi$  at any position in space  $\vec{r}$  at any energy  $E$  is driven by the source distribution  $S$ , and is affected by the loss operator  $L$ . Usually the source is a point source located somewhere in space, or is uniform over a small localized spatial region.

We can write a corresponding inhomogeneous adjoint equation of the form

$$L^*\phi^*(\vec{r}, E) = R(\vec{r}, E), \quad (7.46)$$

where  $L^*$  is derived from  $L$  as in Eq. (7.11). The adjoint source  $R$  is usually taken equal to a detector activation cross section or to a radiation dose conversion factor. The detector is also usually localized in space at some considerable distance away from the source. We can interpret  $\phi^*$  as being proportional to the *contribution* to the detection or dose rate in the detector of

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neutrons of any energy  $E$  located at any local position  $\vec{r}$  in space. It is a detection "importance".

First, multiply Eq. (7.45) by  $\phi^*$ , multiply Eq. (7.46) by  $\phi$ , and integrate over *all* space. Assume that the external boundary conditions on both  $\phi$  and  $\phi^*$  are either zero flux or symmetry. In "kets" notation, the results are

$$\langle \phi^*, L\phi \rangle = \langle \phi^*, S \rangle, \quad (7.47)$$

and

$$\langle \phi, L^* \phi^* \rangle = \langle R, \phi \rangle. \quad (7.48)$$

If we subtract Eq. (7.48) from Eq. (7.47), and use the definition of  $L^*$ , we obtain

$$\langle \phi^*, S \rangle_{\text{source volume}} = \langle R, \phi \rangle_{\text{detector volume}} = \text{Dose Rate}. \quad (7.49)$$

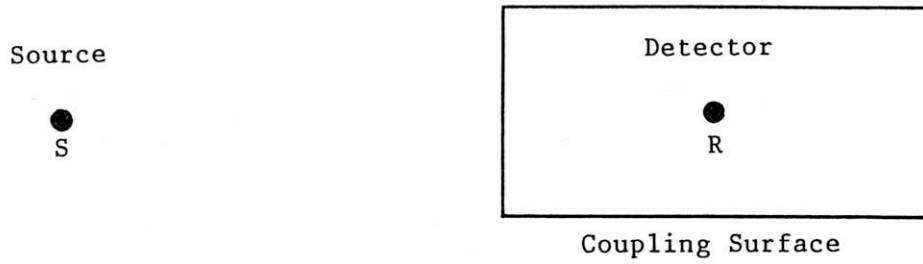
This result states that we can determine the dose or detection rate *either* by knowing the flux at the detector or by knowing the importance at the source! In many cases, it is difficult to determine either of these quantities accurately at the position of the other because of computational and geometrical limitations. However, this mathematical result gives rise to a possible *hybrid* method where both problems are solved separately by appropriate means over a portion of the phase space where they *can be computed accurately*; then the results are coupled together at a suitable interface.

Consider the schematic situation shown in Figure 7.4. As before, weight Eq. (7.45) by  $\phi^*$  and Eq. (7.46) by  $\phi$ . This time, however, integrate over *only* a portion of the space up to the coupling surface, *including* the detector but *excluding* the source. When the resulting equations are subtracted there will be no direct contribution from the source, but there will be a surface integral representing its effect. The result comes from

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a direct application of the second form of Green's theorem, where  $\vec{n}$  is the unit outward normal to the surface:

$$\begin{aligned}
 \text{Dose Rate} &= \underset{\text{volume}}{\langle R, \phi \rangle_{\text{detector}}} \\
 &= \int_0^{E_{\max}} \left[ \oint \{ \phi D \nabla \phi^* - \phi^* D \nabla \phi \} \cdot \vec{n} \, dS \right] dE.
 \end{aligned} \tag{7.50}$$



**Figure 7.4** Idealized Point Source and Detector

In words, Eq. (7.50) states that the dose rate is equal to the sum of the flux weighted adjoint current *leaving* the volume across the surface and the adjoint weighted neutron current *entering* the volume across the surface. Both of these terms may be rather accurately computed at the coupling surface, and therefore the dose rate is accurately determined. Application of the chain rule provides a computationally more convenient form,

$$\text{Dose rate} = \int_0^{E_{\max}} \left[ \oint_{\text{outward}} D \nabla \phi^* \phi \cdot \vec{n} \, dS \right] dE. \tag{7.51}$$

The hybrid method in its transport theory form has been successfully used in complex radiation shielding calculations, where the forward solution of the source problem has been obtained from the deterministic  $S_n$  code DORT, and the adjoint

## NUCLEAR REACTOR THEORY AND DESIGN

solution has been obtained from the stochastic Monte Carlo code MORSE. The resulting combination is known as the MASH code. The basic ideas, however, are applicable to any problem where geometrical difficulties preclude the full solution of the problem by a forward flux solution alone.

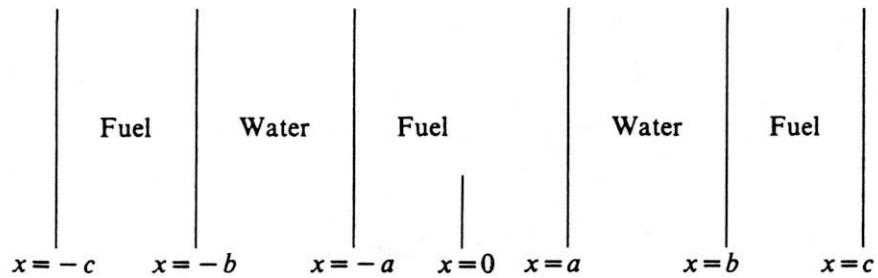
### Problems

**7.1** Refer to Problem 6.1 and its numerical solution. Do the following additional steps:

- a) Transpose the given  $\underline{\underline{L}}$  and  $\underline{\underline{M}}$  matrices as described in Section 7.2, and calculate the adjoint group fluxes for the cylindrical UVAR reactor model using an available one-dimensional computer program;
- b) Compare the  $k_{\text{eff}}$  values obtained in the two cases;
- c) Plot the relative adjoint group fluxes as a function of position, and compare them to the regular fluxes;
- d) Plot the product  $\phi_g \phi_g^*$  for both the fast and thermal groups as a function of position in the core;
- e) Comment on where you think a given control rod should be placed to be most effective.

**7.2** You are given a critical symmetric slab reactor that has a water region between the fuel regions, as shown below.

## NUCLEAR REACTOR THEORY AND DESIGN



If the flux goes to zero at  $x = \pm c$  and is describable using two groups, do the following:

- Sketch the fast and thermal flux distributions that you might expect to find in this reactor and explain the physical reasons for the magnitudes observed if the water is 10 cm thick.
- Sketch the corresponding fast and thermal adjoint distributions and explain the physical reasons for the magnitudes observed.
- How would the results change if the water region were 20 centimeters thick?

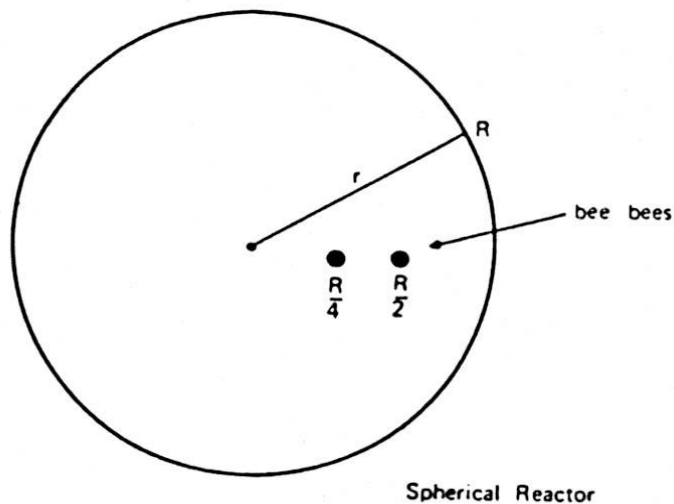
**7.3\*** This problem concerns the lambda-mode eigenvalues and corresponding few-group eigenvectors. Do the following:

- Write down the general balance equation for the  $i$ th harmonic *flux mode* together with the appropriate boundary conditions; explain the terms.
- Write down the corresponding general balance equation for the  $i$ th harmonic *adjoint mode* together with the appropriate boundary conditions; explain the terms.
- Discuss the properties of the above equations.

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d) List as many instances as you can think of where the harmonic modes come into play and discuss each one fully.

- 7.4 You are given a bare, spherical, homogeneous reactor describable by one-group diffusion theory. The boundary conditions are the following: (1) the flux is zero at the outer radius,  $r = R$ ; and (2) the flux is finite and symmetric at the center,  $r = 0$ . What is the relative reactivity worth of a small perturbation, for example a boron-filled bee-bee placed at  $r = R/2$  compared to the same bee-bee placed at  $r = R/4$ ?

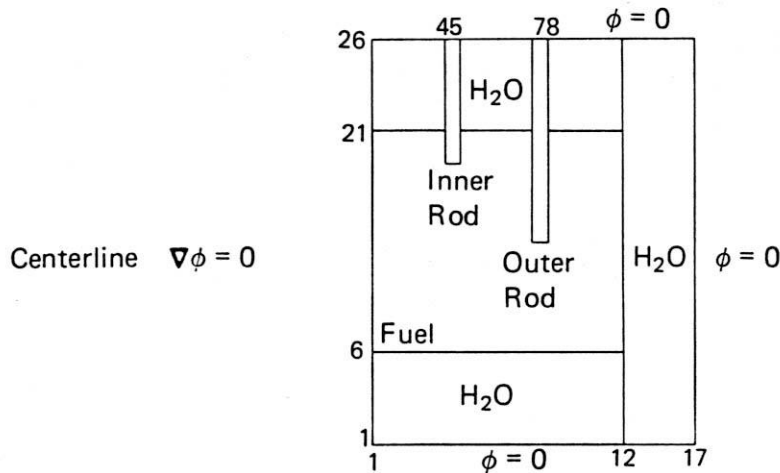


- 7.5 The UVAR is a 2MW swimming pool reactor. If a visitor dropped a nickel into the pool and it slowly fell through the water and thence into the center of the critical core, what would be the approximate reactivity worth of the nickel (in cents) as a function of position?  $1\$ = 0.007$  for UVAR. Assume that a nickel weighs 5 g and is made entirely of nickel which has a macroscopic absorption cross section of  $\Sigma_{an} = 0.42 \text{ cm}^{-1}$ . Assume that the UVAR can be adequately

## NUCLEAR REACTOR THEORY AND DESIGN

described by one-group diffusion theory as a homogeneous spherical reactor with a radius of  $R = 26$  cm surrounded by an infinite water reflector. Take the macroscopic absorption cross section of the core to be  $\Sigma_{ac} = 0.091 \text{ cm}^{-1}$ , and the diffusion coefficient to be  $D_c = 0.192 \text{ cm}$ . Use an effective  $L_c^2 = 52 \text{ cm}^2$ . Take the macroscopic absorption cross section of the water to be  $\Sigma_{aw} = 0.0196 \text{ cm}^{-1}$ , and the diffusion coefficient to be  $D_w = 0.146 \text{ cm}$ .

- 7.6\*** This is a control rod interaction study. You are given the following 2D reactor model in RZ geometry, which can be solved using a computer code such as EXTERMINATOR.



The control rods are one mesh space wide. Take 2" mesh spacing in the  $r$  direction in the fuel and 1" in the outer reflector. Take 4" mesh spacing in the  $z$  direction in the fuel and 1" in the end reflectors. If you have the possibility, use more but smaller mesh spaces to obtain more accurate results. Note that most codes accept the mesh spacing in centimeters. Use  $\epsilon = 10^{-3}$  for the point-wise flux convergence or  $10^{-5}$  for the  $k_{eff}$  convergence. Since this is effectively a 3D problem use the 2 group cross sections given below with  $B^2 = 0$ :

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- a) Find the control rod worth of the central control rod given that the outer rod is at 1/2 depth. Plot the integral rod worth curve. Also, calculate the total worth of the central rod without the outer rod, and the corresponding adjoint flux. Plot the flux traverse above and below the rod tip (three or four inches).
- b) Find the control rod worth of the outer control rod given that the central rod is at 1/2 depth. Plot the integral rod worth curve. Also, calculate the total worth of the outer rod without the central rod, and the corresponding adjoint flux. Plot the flux traverse above and below the rod tip (three or four inches)
- c) Comment on the differences between the results of parts a) and b).

#### Material Properties

Fuel	Water	Control Rod
$D_1 = 1.2$	$D_1 = 1.4$	$D_1 = 4.0$
$D_2 = 0.225$	$D_2 = 0.16$	$D_2 = 0.10$
$\Sigma_{s1 \rightarrow 2} = 0.05$	$\Sigma_{s1 \rightarrow 2} = 0.06$	$\Sigma_{s1 \rightarrow 2} = 0.10$
$\Sigma_{a1} = 0.005$	$\Sigma_{a1} = 0.0002$	$\Sigma_{a1} = 0$
$\Sigma_{a2} = 0.10$	$\Sigma_{a2} = 0.02$	$\Sigma_{a2} = 2.0$
$\nu \Sigma_{f1} = 0.005$	-	-
$\nu \Sigma_{f2} = 0.115$	-	-
$\chi_1 = 1.$		
$\chi_2 = 0.$		



## NUCLEAR REACTOR THEORY AND DESIGN

### Reference

**J. Lewins**, *Importance. The Adjoint Function*, (Pergamon Press, London, 1965), Chapters 1 and 2.



## REACTOR KINETICS

When we speak of reactor kinetics, we usually refer to the short-time scale (seconds) behavior of a reactor in the absence of feedback other than delayed neutrons. This type of behavior would be typical of a reactor initially operating at a steady low power level that is perturbed by the movement of a control rod. Reactor dynamics, on the other hand, refers to the general case where feedback mechanisms such as temperature and pressure changes come into play. We treat reactor dynamics in Chapter 9.

As a first step, we derive the time-dependent neutron balance equations in few-group diffusion theory form. We see that these equations can, in principle, be solved numerically to obtain the complete transient solution as a function of space and time. While this approach is computationally feasible, the general nature of the transient response is not easily seen.

To make the problem more understandable, we must reduce the neutron balance equations to a form that is essentially independent of space. We accomplish this by weighting the balance equations by a suitable (adjoint) function and integrating over space. The resulting equations are known as the point kinetics equations because they represent an "effective" point reactor in which the time behavior at all positions is identical. In the process, we lose the direct physical meanings of the parameters; they become "effective" as well. But we gain the ability to solve the resulting time-dependent equations analytically using integrating factors, Laplace transforms or matrix techniques. The solutions thus obtained tell us a great deal about the kinetic behavior of reactors.

We conclude the Chapter with a perturbation theory derivation of the point kinetics equations. This derivation

## NUCLEAR REACTOR THEORY AND DESIGN

gives us insight into the conditions under which point kinetics are valid, and shows us the proper way to calculate the various effective parameters needed in the model.

### 8.1 Multigroup Reactor Kinetics Equations

When we consider the dynamic behavior of a low-power reactor in the absence of feedback effects, we must remember that the steady state neutron balance includes both the prompt neutrons given off at the moment of fission and the delayed neutrons given off during the decay of the delayed neutron precursor atoms. Therefore, it is not sufficient to just add a time derivative term to the neutron balance equation; the time-dependent precursor balances must also be considered. The equations, in fact, are coupled together and must be solved simultaneously.

Recall that there are numerous ( $> 100$ ) fission products that can lead to delayed neutron emission, and that the exact mixture for a given fissionable isotope is a function of the fission product yield curve for that particular isotope. Fortunately, the net effect of all precursors can be adequately represented by six effective "groups" of precursors whose half-lives vary from approximately 55 s down to about 0.25 s. These are given in Table 8.1 for the thermal neutron fission of  $^{233}\text{U}$ ,  $^{235}\text{U}$  and  $^{239}\text{Pu}$ . The relative yields and half-lives were obtained by "least squares" fits of experimental data.

The delayed neutrons are also born at a lower energy than the prompt neutrons. As discussed previously, each delayed neutron is emitted at a discrete energy, but because a delayed neutron group is made up of several different contributions, each group has an effective neutron emission spectrum. The average energies for the delayed neutron groups of  $^{235}\text{U}$  are given in Table 8.2.

For uranium-235, the delayed neutron fraction is  $\beta = \sum_{i=1}^6 \beta_i = 0.0065$ . This means that the fraction  $(1 - \beta)$  of the total

# NUCLEAR REACTOR THEORY AND DESIGN

fission neutron production is prompt, and that the fraction  $\beta_i$  of the total fission neutron production is delayed in the  $i$ th precursor group.

**Table 8.1**

Delayed Neutron Data for Thermal Fission of  $^{233}\text{U}$ ,  $^{235}\text{U}$ , and  $^{239}\text{Pu}$

$^{233}\text{U}$				
Group	Half-life (sec)	Decay constant $\lambda_i$ (sec $^{-1}$ )	Yield (neutrons per fission)	Fraction $\beta_i$
1	55.00	0.0126	0.00057	0.000224
2	20.57	0.0337	0.00197	0.000777
3	5.00	0.139	0.00166	0.000655
4	2.13	0.325	0.00184	0.000723
5	0.615	1.13	0.00034	0.000133
6	0.277	2.50	0.00022	0.000088
Total yield:			0.0066	
Total delayed fraction ( $\beta$ ):				0.0026
$^{235}\text{U}$				
Group	Half-life (sec)	Decay constant $\lambda_i$ (sec $^{-1}$ )	Yield (neutrons per fission)	Fraction $\beta_i$
1	55.72	0.0124	0.00052	0.000215
2	22.72	0.0305	0.00346	0.001424
3	6.22	0.111	0.00310	0.001274
4	2.30	0.301	0.00624	0.002568
5	0.610	1.14	0.00182	0.000748
6	0.230	3.01	0.00066	0.000273
Total yield:			0.0158	
Total delayed fraction ( $\beta$ ):				0.0065
$^{239}\text{Pu}$				
Group	Half-life (sec)	Decay constant $\lambda_i$ (sec $^{-1}$ )	Yield (neutrons per fission)	Fraction $\beta_i$
1	54.28	0.0128	0.00021	0.000073
2	23.04	0.0301	0.00182	0.000626
3	5.60	0.124	0.00129	0.000443
4	2.13	0.325	0.00199	0.000685
5	0.618	1.12	0.00052	0.000181
6	0.257	2.69	0.00027	0.000092
Total yield:			0.0061	
Total delayed fraction ( $\beta$ ):				0.0021

\*Reproduced from G. R. Keepin, *Physics of Nuclear Kinetics*, 1965, with permission of the publishers, Addison-Wesley/W. A. Benjamin, Inc., Advanced Book Program, Reading, Mass., USA.

# NUCLEAR REACTOR THEORY AND DESIGN

**Table 8.2**

Mean Energies of the Delayed Neutron Groups for  $^{235}\text{U}$  Fission

Group	$\bar{E}$ (keV)
1	$399 \pm 7$
2	$428 \pm 9$
3	$439 \pm 9$
4	$516 \pm 9$
5	$502 \pm 9$
6	$454 \pm 10$

M.F. Villani et al., **NSE 111**, p422 - 432 (1992)

We shall write the precursor balance equations for the six precursor groups at position  $\vec{r}$  in the reactor. These are simply

*rate of change*                      fission  
*of precursors*                      production rate              decay

$$\frac{\partial C_i(\vec{r}, t)}{\partial t} = \int_0^\infty \beta_i \nu \Sigma_f(\vec{r}, E', t) \phi(\vec{r}, E', t) dE' - \lambda_i C_i(\vec{r}, t); \quad (8.1)$$

for  $i = 1, 6$ .

In this equation,  $\Sigma_f(\vec{r}, E', t) \phi(\vec{r}, E', t)$  is the fission rate at position  $\vec{r}$  for neutrons of energy  $E'$ , and  $\beta_i \nu$  is the fractional production of precursor atoms which emit a single delayed neutron per decay. We must integrate over all energies to obtain the total precursor production rate at time  $t$  at point  $\vec{r}$ . This equation is only valid if the precursors stay at the position where they are born (no circulating fuel solutions or slurries).

The neutron balance now contains both prompt-contributions from fission and delayed-contributions from the decay of precursor atoms. For the purpose of this treatment we will use diffusion theory although the transport equation will lead to the same form of the "point" reactor kinetics equations. The neutron balance is

# NUCLEAR REACTOR THEORY AND DESIGN

$$\left[ \begin{array}{c} \text{Rate of change of} \\ \text{neutron density} \end{array} \right] = \left[ \begin{array}{c} \text{Production rate due to} \\ \text{fission, delayed neutrons} \\ \text{and sources} \end{array} \right] - \left[ \begin{array}{c} \text{Loss rate due to} \\ \text{leakage, absorption,} \\ \text{and scattering} \end{array} \right],$$

or the equation:

$$\begin{aligned} \text{rate of change} \quad \text{prompt fission} \\ \frac{1}{v(E)} \frac{\partial \phi(\vec{r}, E, t)}{\partial t} = \chi_p(E) \int_0^\infty (1 - \beta) v \Sigma_f(\vec{r}, E') \phi(\vec{r}, E', t) dE' \\ \text{in scatter} \quad \text{delayed production} \quad \text{source} \\ + \int_0^\infty \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', t) dE' + \sum_{i=1}^6 \chi_{di}(E) \lambda_i C_i(\vec{r}, t) + Q(\vec{r}, E) \\ \text{absorption and} \quad \text{leakage} \\ \text{out scatter} \\ - \Sigma_T(\vec{r}, E, t) \phi(\vec{r}, E, t) + \nabla \cdot D(\vec{r}, E) \nabla \phi(\vec{r}, E, t). \end{aligned} \quad (8.2)$$

The terms are defined as follows:

$(1 - \beta) v \Sigma_f(\vec{r}, E') \phi(\vec{r}, E')$  is the production of prompt neutrons alone, since the fraction  $\beta$  are delayed and must be subtracted out. We integrate over all energies to obtain the total prompt production;

$\chi_p(E)$  is the prompt neutron spectrum, usually taken to be the fission spectrum, which differs somewhat for different fissionable isotopes;

## NUCLEAR REACTOR THEORY AND DESIGN

$\chi_{di}(E)$  is the delayed neutron spectrum for the  $i$ th group, which is lower in average energy than the prompt spectrum. For lower emission energies, the probability of leakage before the neutron thermalizes is smaller than for fission neutrons, thus giving the delayed neutrons a relatively higher survival probability.

**Multigroup Equations.** We next usually discretize the energy range into energy groups. As we have seen previously, the scattering integral leads to group transfer cross sections. A typical group flux equation (for single-group down-scatter only) is the equation

$$\begin{array}{ccccc} & & & \text{delayed} & \\ & & & \text{production} & \\ \text{rate of change} & \text{prompt fission} & & & \\ \frac{1}{v_g} \frac{\partial \phi_g(\vec{r}, t)}{\partial t} = (1 - \beta) \chi_{pg} \left[ \sum_{g'=1}^G v \Sigma_{fg'} \phi_{g'} \right] + \sum_{i=1}^6 \lambda_i \chi_{dig} C_i \end{array}$$

(8.3)

in scatter
source
absorption and
leakage  


out scatter

$$+ \Sigma_{sg-1 \rightarrow g} \phi_{g-1} + Q_g - (\Sigma_{ag} + \Sigma_{sg \rightarrow g+1}) \phi_g + \nabla \cdot D_g \nabla \phi_g;$$

for  $g = 1, G$ .

The precursor equations, in turn, are

$$\begin{array}{ccccc} \text{rate of change} & \text{production} & \text{decay} & & \\ \frac{\partial C_i(\vec{r}, t)}{\partial t} = \beta_i \left[ \sum_{g'=1}^G v \Sigma_{fg'} \phi_{g'} \right] - \lambda_i C_i; & \text{for } i = 1, 6. \end{array}$$

(8.4)



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We also have appropriate boundary and initial conditions.

As before, we now write all of the multi-group equations in a single vector-matrix equation. First we define the following vectors and matrices:

$$\underline{\phi} \equiv \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \vdots \\ \phi_G \end{bmatrix}; \quad \underline{F} \equiv \begin{bmatrix} \nu \Sigma_{f1} \\ \nu \Sigma_{f2} \\ \vdots \\ \vdots \\ \nu \Sigma_{fG} \end{bmatrix}; \quad \underline{Q} \equiv \begin{bmatrix} Q_1 \\ Q_2 \\ \vdots \\ \vdots \\ Q_G \end{bmatrix};$$

$$\underline{\chi}_p \equiv \begin{bmatrix} \chi_{p1} \\ \chi_{p2} \\ \vdots \\ \vdots \\ \chi_{pG} \end{bmatrix}; \quad \underline{\chi}_{di} \equiv \begin{bmatrix} \chi_{di1} \\ \chi_{di2} \\ \vdots \\ \vdots \\ \chi_{diG} \end{bmatrix}; \quad \underline{D} \equiv \begin{bmatrix} D_1 & & & & \\ 0 & D_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & D_G \end{bmatrix}.$$

$$\underline{T} \equiv \begin{bmatrix} 1/v_1 & & & & 0 \\ & 1/v_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 1/v_G \end{bmatrix}; \quad \underline{H} \equiv \begin{bmatrix} (\Sigma_{a1} + \Sigma_{s1 \rightarrow 2}) & 0 & & & 0 \\ -\Sigma_{s1 \rightarrow 2} & (\Sigma_{a2} + \Sigma_{s2 \rightarrow 3}) & & & \\ & & \ddots & & \\ & & & \ddots & 0 \\ & & & & -\Sigma_{sG-1 \rightarrow G} \quad \Sigma_{aG} \end{bmatrix}.$$

The matrices  $\underline{D}$  and  $\underline{T}$  are diagonal, while the matrix  $\underline{H}$  has elements on the diagonal and contains at least a row of terms just below the diagonal when there is down-scatter only. This is the same DEAF $\chi$ -type notation that we have encountered previously for the static multi-group case, with the addition of the prompt and delayed spectrum vectors and the inverse neutron velocity matrix.

## NUCLEAR REACTOR THEORY AND DESIGN

With the above definitions, the multi-group kinetics equations can be written as follows:

$$\begin{aligned} \frac{\partial}{\partial t} \underline{\phi}(\vec{r}, t) = & (1 - \beta) \underline{\chi}_p \underline{F}^T \underline{\phi}(\vec{r}, t) + \sum_{i=1}^6 \underline{\chi}_{di} \lambda_i C_i(\vec{r}, t) \\ & + \underline{Q}(\vec{r}, t) - \underline{H} \underline{\phi}(\vec{r}, t) + \nabla \bullet \underline{D} \nabla \underline{\phi}(\vec{r}, t) \end{aligned} \quad (8.5)$$

and

$$\begin{aligned} \frac{\partial C_i(\vec{r}, t)}{\partial t} = & \beta_i \underline{F}^T \underline{\phi}(\vec{r}, t) - \lambda_i C_i(\vec{r}, t), \\ & \text{for } i = 1, 6. \end{aligned} \quad (8.6)$$

Of course, in order to solve these equations we need boundary conditions and initial conditions. The boundary conditions are usually

$$\underline{\phi}(\vec{R}, t) = 0 \quad \text{or} \quad \nabla \underline{\phi}(\vec{R}, t) = 0,$$

while initial conditions are usually

$$\underline{\phi}(\vec{r}, 0) = \underline{\phi}_0(\vec{r})$$

and

$$C_i(\vec{r}, 0) = C_{i0}(\vec{r}), \quad \text{for } i = 1, 6.$$

Note that we have obtained a coupled set of six precursor and G flux equations that must be solved simultaneously. By making a finite difference approximation in one or more space dimensions and time, these equations can be solved numerically, e.g., by the RAUMZEIT code.

### 8.2 Interpretation of Spatial Kinetics Results

Using the multi-group reactor kinetics equations we can

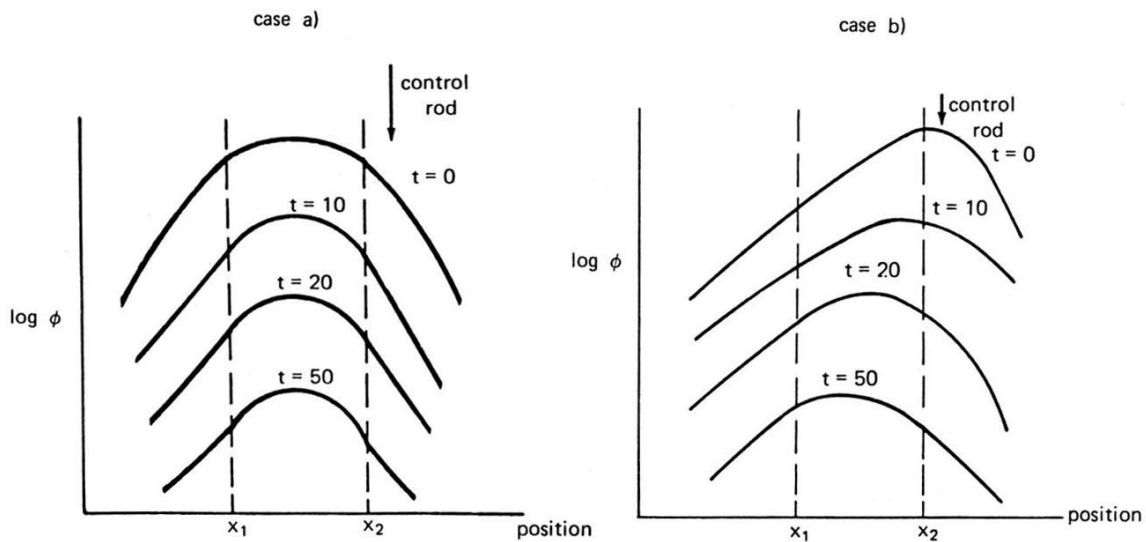
## NUCLEAR REACTOR THEORY AND DESIGN

calculate the time-dependent behavior of a reactor during a transient situation. Several few-group diffusion theory codes exist which can be used for this purpose such as WIGLE, RAUMZEIT, TWIGLE, HEXNODYN, etc. As an example, we consider a control rod insertion transient. The overall space-time behavior is a superposition of an overall magnitude change and a spatial flux change or "tilt." Two such computational results are qualitatively plotted in Figure 8.1 for a one-dimensional model where the control rod is being inserted on the right-hand side of the core. The positions  $x_1$  and  $x_2$  represent the locations of neutron flux monitors such as ionization chambers.

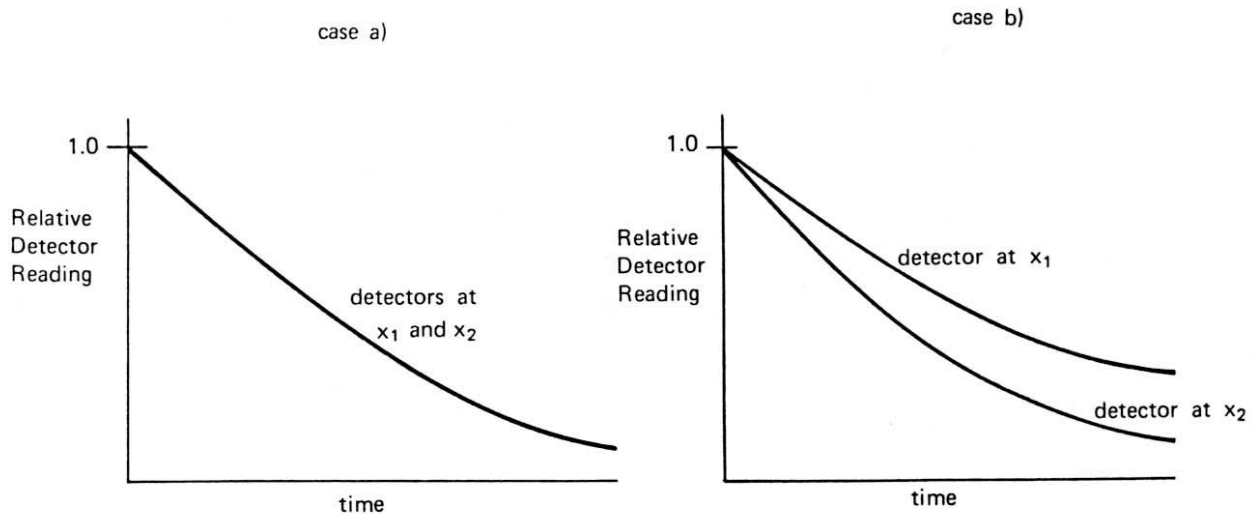
In case (a), the flux shape remains relatively unchanged but the magnitude decreases greatly. In case (b), both the flux shape and the magnitude change. In order to interpret these results more fully we plot the time-dependent readings of the two detectors, normalized to their respective initial readings. These are shown in Figure 8.2. For the reactor model described by case (a), the flux shape does not vary appreciably with time. Space and time are essentially *separable* and the reactor behaves as a single unit. We call this behavior "point kinetics." On the other hand, in case (b) the flux shape tilts appreciably to the left in a direction away from the neutron absorbing control rod. Space and time are clearly not separable and the behavior must be described by "spatial kinetics."

In the latter case, the most useful method of presentation of the results is in the form of a global amplitude function vs. time and a normalized shape function vs. position at several different times. The amplitude function is taken to be the total power normalized to unit total power, i.e., the area under the curve is constant.

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**Fig. 8.1** Time-Dependent Thermal Flux vs. Position



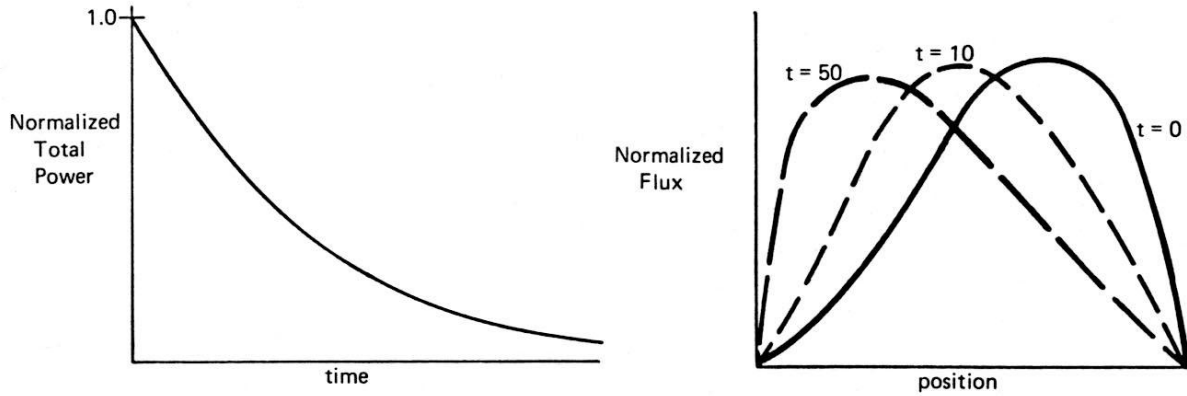
**Fig. 8.2** Normalized Detector Reading vs. Time

These are shown in Figure 8.3. The time-dependent amplitude function can be related to the reactivity inserted into the reactor through the Inhour Equation that will be discussed later. The extent of the shape change is a measure of the susceptibility of the reactor to excitation of the harmonic flux modes.

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We visualize the transient behavior of the reactor qualitatively as being a linear combination of harmonic mode solutions of the form

$$\phi(\underline{r}, t) = a_0(t)\phi_0(\underline{r}) + a_1(t)\phi_1(\underline{r}) + a_2(t)\phi_2(\underline{r}) + \dots \quad (8.7)$$



**Fig. 8.3** Transient Amplitude and Shape Functions

Without going through an actual derivation, we can state that the coefficients of the higher harmonic modes,  $a_1(t)$ ,  $a_2(t)$ , etc., consist of two main factors:

1. the *susceptibility* of the reactor to a flux tilt, which varies as the reciprocal of the difference in the eigenvalues, i.e.,  $1/(\lambda_0 - \lambda_i)$ , for  $i = 1, 2, \dots$ ;
2. the *reactivity excitation* of the harmonic mode,  $\rho_i$ , which depends upon where the perturbation is inserted. The excitation is minimal if the perturbation is inserted at a spatial node, or zero crossing, of the harmonic mode in question.

As a reactor core becomes larger, all else being equal, the

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harmonic modes become less and less sub-critical and the eigenvalue differences become smaller; the susceptibility of the reactor to a flux tilt increases. On the other hand, in order to strongly excite the first harmonic mode, we must make an off-center perturbation. In this regard symmetrically placed perturbations will lead to minimum flux tilts by virtue of balancing effects. Control rods are always operated in symmetric banks in commercial power reactors for just this reason.

### 8.3 Point Kinetics Equations

Consider the various terms present in Eqs. (8.3) and (8.4). The important dynamically varying terms are the flux and the precursor concentrations. Their analogs in the point kinetics equations are the effective neutron density,  $n$ , and the effective precursor concentrations,  $c_i$ . The inhomogeneous source term is replaced with an effective source,  $q$ . The delayed neutron fractions,  $\beta_i$ , enter as effective delayed fractions,  $\bar{\beta}_i$ . All of the production and loss terms combine to become an effective reactivity,  $\rho$ . And finally, the  $1/v$  term combines with the fission production term to give the effective time to generate a new neutron,  $\Lambda$ . As a matter of fact, the only quantities that retain their physical meanings are the decay constants,  $\lambda_i$ . The point kinetics equations are written as

$$\frac{dn}{dt} = \frac{\rho - \bar{\beta}}{\Lambda} n + \sum_{i=1}^6 \lambda_i c_i + q, \quad (8.8)$$

and

$$\frac{dc_i}{dt} = \frac{\bar{\beta}_i n}{\Lambda} - \lambda_i c_i, \quad \text{for } i = 1, 6. \quad (8.9)$$

In this form, to complete the problem statement we need only the

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initial conditions

$$n(0) = n_0 \quad \text{and} \quad c_i(0) = c_{i0}, \quad \text{for } i = 1, 6.$$

We have obtained a coupled set of seven time dependent equations. We can write the set in vector-matrix form. Let the following terms be defined:

$$\underline{\underline{N}} \equiv \begin{bmatrix} n \\ c_1 \\ c_2 \\ \cdot \\ \cdot \\ \cdot \\ c_6 \end{bmatrix}; \quad \underline{\underline{B}} \equiv \begin{bmatrix} \frac{\rho - \bar{\beta}}{\Lambda} & \lambda_1 & \lambda_2 & \lambda_3 & \cdot & \cdot & \lambda_6 \\ \frac{\bar{\beta}_1}{\Lambda} & -\lambda_1 & 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{\bar{\beta}_6}{\Lambda} & \cdot & \cdot & \cdot & \cdot & \cdot & -\lambda_6 \end{bmatrix};$$

$$\underline{\underline{S}} = \begin{bmatrix} q \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}; \quad \underline{\underline{N}}_0 = \begin{bmatrix} n_0 \\ c_{10} \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ c_{60} \end{bmatrix}.$$

With these definitions, the entire set of equations becomes the inhomogeneous first-order vector-matrix ordinary differential equation

$$\dot{\underline{\underline{N}}} = \underline{\underline{B}}\underline{\underline{N}} + \underline{\underline{S}}, \tag{8.10}$$

with the initial condition  $\underline{\underline{N}}_0$ . If the matrix  $\underline{\underline{B}}$  is not a

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function of time, then this equation has constant coefficients and its solution is given as a sum of exponentials. The constants in the exponentials are the eigenvalues of the  $\underline{\underline{B}}$  matrix, which are the roots of the characteristic equation. On the other hand when the matrix  $\underline{\underline{B}}$  is time dependent, the differential equation has time varying coefficients and the solutions are not exponentials. Looking at the  $\underline{\underline{B}}$  matrix we see that the only factor present that is sensibly time dependent is the reactivity  $\rho$ . Hence simple analytic solutions are only obtainable for step changes in reactivity, that is to say, for the case of an instantaneous change in reactivity from  $\rho = 0$  to  $\rho = \text{constant}$ .

The general solution of the point kinetics equations for a constant step reactivity insertion is given in terms of the eigenvalues of the  $\underline{\underline{B}}$  matrix, which are obtained by setting the determinant  $|\underline{\underline{B}} - \omega \underline{\underline{I}}| = 0$ . The result is called the characteristic equation of the matrix; in this particular case it is a seventh-order algebraic equation in the parameter  $\omega$  that can be solved for  $\omega_0, \omega_1, \dots, \omega_6$ . The equation is normally written in the form

$$\rho = \omega\Lambda + \sum_{i=1}^6 \frac{\bar{\beta}_i \omega}{\omega + \lambda_i}. \quad (8.11)$$

In this form it is called the Inhour equation.

An identical result is obtained if exponential solutions are assumed of the form

$$n(t) = \tilde{n} e^{\omega t} \quad \text{and} \quad c_i(t) = \tilde{c}_i e^{\omega t}.$$

Upon substitution into the original set of ordinary differential equations and cancellation of the common exponential factor, the resulting algebraic equations can be combined into the Inhour equation. Similar results are obtained using Laplace transforms.



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The resulting neutron density solution is a sum over the homogeneous solutions plus the particular solution, and takes the form

$$n(t) = \sum_{j=0}^6 A_j e^{\omega_j t} + n_{\text{particular}}. \quad (8.12)$$

The corresponding precursor solutions are of the form

$$c_i(t) = \sum_{j=0}^6 A_{ij} e^{\omega_j t} + c_{i \text{ particular}}, \quad \text{for } i = 1, 6. \quad (8.13)$$

However, the coefficients  $A_{ij}$  are not independent of the coefficients  $A_j$  because they are related by the initial balance or equilibrium situation. The particular solutions arise as a result of the inhomogeneous source term in the balance equations.

A much more elegant solution form can be obtained by applying an integrating factor directly to the inhomogeneous vector-matrix differential equation. For  $\rho = \text{constant}$ , the complete solution can be written in the form

$$\underline{N}(t) = \exp(\underline{B}t) \underline{N}_0 + \int_0^t \exp(\underline{B}(t-\tau)) \underline{S}(\tau) d\tau. \quad (8.14)$$

The factor  $\exp(\underline{B}t)$  is itself a matrix that can be expressed directly in terms of the eigenvalues ( $\omega_j$ ) of the  $\underline{B}$  matrix. One uses Sylvester's theorem, which in this particular case gives

$$\exp(\underline{B}t) = \sum_{j=0}^6 \exp(\omega_j t) \frac{\prod_{k \neq j}^6 (\underline{B} - \omega_k \underline{I})}{\prod_{k \neq j}^6 (\omega_j - \omega_k)}. \quad (8.15)$$

Hence, one can solve the entire problem in a straightforward mechanistic manner.

We return now to the characteristic roots of the Inhour

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equation. For positive  $\rho$ , one of the roots will be positive and the other six negative; for negative  $\rho$ , all of the roots are negative. In fact, it can be shown that the values of  $\omega$  form the sequence

$$\omega_0 > \omega_1 > \omega_2 > \omega_3 > \omega_4 > \omega_5 > \omega_6 ,$$

and are bounded by the decay constants of the delayed neutron groups according to the following inequalities:

$$\omega_0 > -\lambda_1 ,$$

$$-\lambda_1 > \omega_1 > -\lambda_2 ,$$

$$-\lambda_2 > \omega_2 > -\lambda_3 ,$$

$$-\lambda_3 > \omega_3 > -\lambda_4 ,$$

$$-\lambda_4 > \omega_4 > -\lambda_5 ,$$

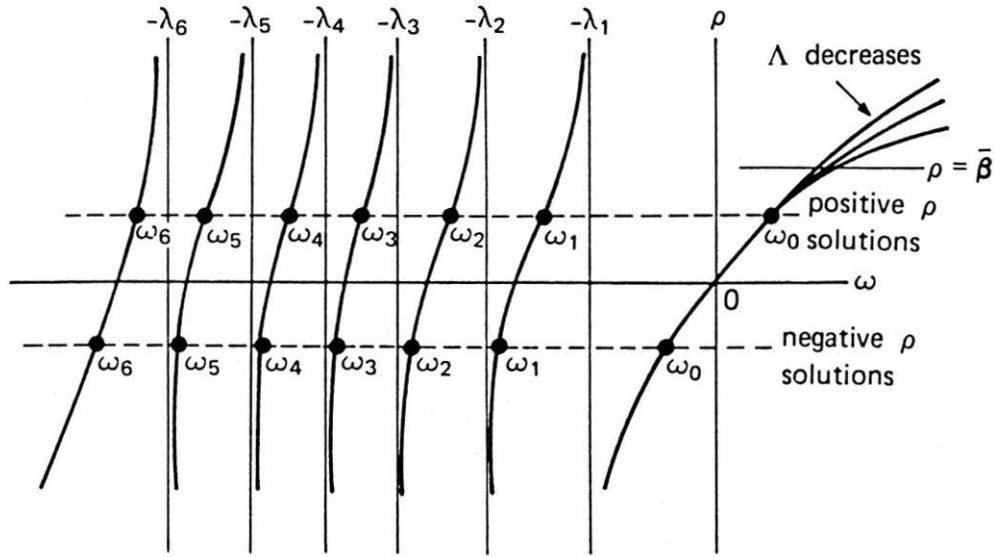
$$-\lambda_5 > \omega_5 > -\lambda_6 ,$$

$$-\lambda_6 > \omega_6 > -\Lambda^{-1} .$$

A qualitative (not to scale) plot of the Inhour equation appears in Figure 8.4.

For either positive or negative reactivity, after sufficient time has passed, the solutions corresponding to  $\omega_1, \dots, \omega_6$  will have decayed away leaving a persisting asymptotic solution that is proportional to  $e^{\omega_0 t}$ . This asymptotic solution can be measured easily, for example, by plotting the reactor flux vs. time on semi-logarithmic paper and taking the slope of the curve at large values of  $t$ .

## NUCLEAR REACTOR THEORY AND DESIGN



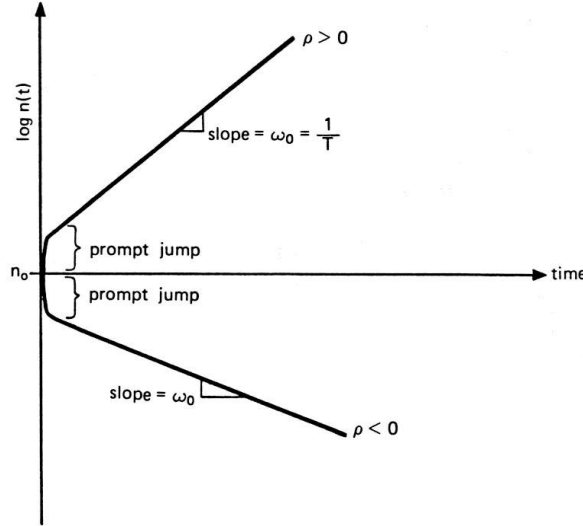
**Fig. 8.4** General plot of  $\omega$  vs.  $\rho$

The reciprocal of the slope is known as the reactor period and is given by the expression

$$T = \frac{1}{\omega_0}. \quad (8.16)$$

A qualitative plot of the neutron density vs. time for the same amount of positive and negative reactivity insertion for  $|\rho| < \bar{\beta}$  is given in Figure 8.5. Two observations can be made. First, the solutions for  $\omega_1, \dots, \omega_6$  die out rather quickly giving rise to what appears to be an initial jump in the neutron density. Second, the period for a given positive reactivity insertion, i.e., for the removal of a control rod, is invariably shorter than the period obtained for an equal but opposite action. In other words, it is easier to increase reactor power as a function of time than it is to decrease it.

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**Fig. 8.5** Neutron Density vs. Time for  $|\rho| < \bar{\beta}$

There are several special cases of interest. For example, when  $\rho$  is very small, the asymptotic period is very large and  $\omega_0 \ll |\lambda_1|$ . In addition, since  $\Lambda$  is usually of the order of  $10^{-3}$  to  $10^{-6}$  s,  $\Lambda \ll \sum_{i=1}^6 (\bar{\beta}_i / \lambda_i)$ . Hence,

$$\omega_0 \approx \frac{\rho}{\sum_{i=1}^6 \frac{\bar{\beta}_i}{\lambda_i}} \quad \text{for } |\rho| \ll \bar{\beta}. \quad (8.17)$$

The response in this case is governed entirely by the precursors. On the other hand, when  $\rho$  is large and positive, the period is very short and  $\omega_0 \gg \lambda_1$ . In this case

$$\omega_0 \approx \frac{\rho - \bar{\beta}}{\Lambda} \quad \text{for } \rho > \bar{\beta}. \quad (8.18)$$

The response in this case is governed entirely by the prompt neutrons. Finally, when  $\rho$  is negative and very large algebraically, the value of  $\omega_0 \rightarrow -\lambda_1$ , which is the decay constant of the longest-lived precursor group. The corresponding maximum negative asymptotic period is  $T \approx 80$  s.

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The value of  $\rho = \bar{\beta}$  is the transition point between a kinetic behavior dominated by delayed neutrons and one dominated by prompt neutrons. When  $\rho < \bar{\beta}$ , but positive, the reactor is said to be "delayed critical," while when  $\rho \geq \bar{\beta}$  the reactor is said to be "prompt critical," which is usually considered to be a hazardous situation, sometimes called an excursion.

### 8.4 Results for One Group of Delayed Neutrons

Since the transient behavior of a perturbed reactor system depends upon both the prompt neutrons and the delayed neutrons, the simplest approximation to the point kinetics equations that still retains the correct qualitative behavior consists of using one average group of delayed neutrons. In this case, the equations become tractable without the use of the powerful vector-matrix methods.

We write the source-free point kinetics equations with one equivalent group of delayed neutrons as

$$\frac{dn}{dt} = \frac{\rho - \bar{\beta}}{\Lambda} n + \lambda c \quad (8.19)$$

and

$$\frac{dc}{dt} = \frac{\bar{\beta} n}{\Lambda} - \lambda c, \quad (8.20)$$

where  $n(0) = n_0$  and  $c(0) = c_0$ . We apply the method of Laplace transforms to solve these coupled ordinary differential equations. Specifically, taking transforms we obtain the equivalent representation in terms of the transform variable  $s$ , namely,

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$$s\bar{n}(s) - n_0 = \frac{\rho - \bar{\beta}}{\Lambda}\bar{n}(s) + \lambda\bar{c}(s) \quad (8.21)$$

and

$$s\bar{c}(s) - c_0 = \frac{\bar{\beta}}{\Lambda}\bar{n}(s) - \lambda\bar{c}(s). \quad (8.22)$$

These are two coupled algebraic equations in the transformed variables that explicitly contain the initial conditions. Solving the latter equation for  $\bar{c}(s)$  in terms of  $\bar{n}(s)$ , and substituting this value into the former, leads to the expression

$$\bar{n}(s) = \frac{n_0(s + \lambda) + \lambda c_0}{\left[ (s + \lambda) \left( s - \frac{\rho - \bar{\beta}}{\Lambda} \right) - \frac{\lambda \bar{\beta}}{\Lambda} \right]}. \quad (8.23)$$

In order to find the inverse Laplace transform of this expression, i.e., the solution as a function of time, we must set the denominator equal to zero to find the poles of the equation. This characteristic equation can be manipulated into the following form,

$$\rho = s\Lambda + \frac{\bar{\beta}s}{s + \lambda}, \quad (8.24)$$

which is recognized to be the Inhour equation for one group of delayed neutrons. Further manipulation gives a quadratic form for the two roots of the equation, namely,

$$s = -\frac{\bar{\beta} - \rho + \lambda\Lambda}{2\Lambda} \left[ 1 \pm \sqrt{1 + \frac{4\lambda\rho\Lambda}{(\bar{\beta} - \rho + \lambda\Lambda)^2}} \right]. \quad (8.25)$$

In the usual situation, where  $|\rho| < \bar{\beta}$ , the following inequality is valid, namely,

$$\Lambda\lambda \ll (\bar{\beta} - \rho) \ll 1.$$

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Under these conditions, we can use the approximation  $\sqrt{1 + \varepsilon} \approx 1 + \varepsilon/2$ , for  $\varepsilon \ll 1$ . The two roots are approximately

$$\omega_0 \approx \frac{\lambda \rho}{\bar{\beta} - \rho} \quad \text{and} \quad \omega_1 \approx -\frac{\bar{\beta} - \rho}{\Lambda}, \quad (8.26)$$

and the transform takes the form

$$\bar{n}(s) = \frac{n_0(s + \lambda) + \lambda c_0}{(s - \omega_0)(s - \omega_1)}. \quad (8.27)$$

**Positive Step Change in Reactivity from Steady State.** To proceed further, one needs to specify the initial conditions more fully. One possible situation is the addition of a positive step of reactivity,  $\rho < \bar{\beta}$ , to a system that is initially at steady state with a neutron density  $n_0$ . In this case, the precursors are in equilibrium initially with the neutron density so that, setting  $dc/dt|_{t=0} = 0$ , we obtain the relationship

$$c_0 = \frac{\bar{\beta}}{\Lambda \lambda} n_0.$$

Hence, the transform takes the form

$$\bar{n}(s) = \frac{n_0 \left( s + \lambda + \frac{\bar{\beta}}{\Lambda} \right)}{(s - \omega_0)(s - \omega_1)} \approx \frac{n_0 \left[ \frac{\bar{\beta}}{\bar{\beta} - \rho} \right]}{s - \omega_0} - \frac{n_0 \left[ \frac{\rho}{\bar{\beta} - \rho} \right]}{s - \omega_1}, \quad (8.28)$$

to the same approximation given above.

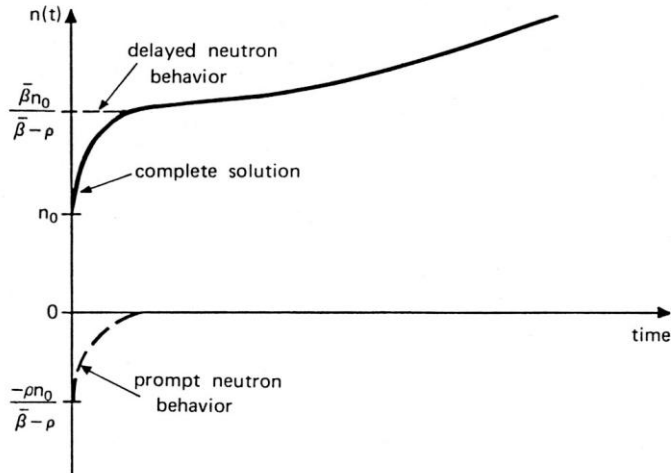
The corresponding time-dependent solution is therefore simply

$$n(t) = n_0 \left\{ \left[ \frac{\bar{\beta}}{\bar{\beta} - \rho} \right] \exp \left( \frac{\lambda \rho}{\bar{\beta} - \rho} t \right) - \left[ \frac{\rho}{\bar{\beta} - \rho} \right] \exp \left( \frac{\bar{\beta} - \rho}{\Lambda} t \right) \right\}. \quad (8.29)$$

This solution is plotted in Figure 8.6. The prompt neutron

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behavior, which varies as  $\exp -[(\bar{\beta} - \rho)/\Lambda]t$ , is seen to give rise to a short, decaying transient. This is reasonable on physical grounds because the reactor is sub-critical with respect to prompt neutrons alone.



**Fig. 8.6** Transient Neutron Density After a Step Change in Reactivity

After the prompt transient has died out, the solution behaves as though only the slow positive component was present. The apparent initial fractional change in the neutron density,  $\bar{\beta} / (\bar{\beta} - \rho)$ , is known as the "prompt jump." Since a positive reactivity worth of  $\rho = \bar{\beta}$  represents the transition from a behavior dependent upon delayed neutrons to a behavior dependent upon prompt neutrons, the reactivity unit commonly used is called dollars, defined as

$$1\$ \equiv \frac{\rho}{\bar{\beta}}.$$

In this regard the prompt jump can also be written in the form



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$1/(1 - \beta)$ . Note that the dollar unit is a function of reactor type and reactor fuel through the quantity  $\beta$ . Reactors having different fuels behave similarly for the same reactivity insertions in dollars. Operating reactivity insertions are usually kept in the range of cents, where a cent is one-hundredth of a dollar. There is of course, no prompt jump at all if  $\rho \geq \beta$  because the reactor is then critical or supercritical on prompt neutrons alone; the neutron density would increase very rapidly with time, governed by the time scale of the neutron generation time.

**The Prompt-Jump Approximation.** The complete set of point reactor kinetics equations is somewhat cumbersome to solve numerically because these equations contain widely differing time constants. Equations of this type are said to be "stiff," and accuracy can usually be obtained only by using time steps that are comparable to the shortest time constant in the system. As we have seen, six of the equations have large time constants corresponding to the delayed neutron half-lives while the seventh has a short time constant which corresponds to the generation time  $\Lambda$ . This latter equation gives rise to the short-time-scale transient behavior and the prompt jump.

If we are primarily interested in the long-term solution of the reactor kinetics equations for slow variations of reactivity and for  $\rho < \beta$ , we can eliminate the stiffness in the equations by neglecting the prompt solution. Formally, we neglect the term  $\Lambda (dn/dt)$  in the set of equations, which reduces the order of the system by one and gives an algebraic equation coupling  $n(t)$  and the  $c_i(t)$ . This is called the "prompt-jump approximation." This approximation can also be made in the space-dependent kinetics formulation if desired.

For the example given in the previous section, neglecting

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$\Lambda (dn/dt)$  gives a first-order differential equation whose solution is

$$n(t) \approx n_0 \frac{\bar{\beta}}{\bar{\beta} - \rho} \exp \left[ \frac{\lambda \rho}{\bar{\beta} - \rho} t \right]. \quad (8.30)$$

This is seen to be identical to the first term in the complete solution. Information on the initial transient is completely lost. However, the solution as given is accurate over the long term.

When numerical solutions are to be calculated, say for a slowly varying  $\rho(t)$ , the time steps used in this case could be rather large. This is quite an economical situation when the reactor kinetics equations are to be solved simultaneously with fluid flow and heat transfer equations, for example in a pump flow-coast-down transient calculation. Such calculations are often done in the safety analysis of a large PWR or BWR to ensure that the design is adequate to withstand normally expected transient situations such as a pump circuit-breaker trip.

**Constant Source Problem.** We now consider the case of a sub-critical reactor that contains a steady source of neutrons, e.g., a Pu-Be source. The point kinetics equations for one delayed neutron precursor group are

$$\frac{dn}{dt} = \frac{\rho - \bar{\beta}}{\Lambda} n + \lambda c + q \quad (8.31)$$

and

$$\frac{dc}{dt} = \frac{\bar{\beta}}{\Lambda} n - \lambda c. \quad (8.32)$$

Since these equations are inhomogeneous, they admit particular solutions. Furthermore, since the system is sub-critical, all of the homogeneous solutions have negative exponentials, which means

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that they die out with time. Hence, in the steady state, only the particular solutions are important.

In this particular case, we guess that the particular solutions will be constants, which correspond to the situation where the neutrons supplied by the source and any subsequent neutron multiplication just equal the total neutron destruction rate. Substitution of constants into the differential equations gives the solutions

$$n_p(t) = -\frac{q\Lambda}{\rho} \quad \text{and} \quad c_p(t) = -\frac{\bar{\beta}q}{\lambda\rho}, \quad (8.33)$$

which are both positive because the reactivity is negative.

### 8.5 Experimental Measurement of Control Rod Worth

There are a number of ways to experimentally measure the worth of control rods in a reactor, all of which are based upon the ideas presented in this chapter. Detailed descriptions of these methods are beyond the scope of this treatment; only a brief outline of the basic principles will be given. The commonly used methods are:

1. *Rod Bump.* The reactor is initially critical. A control rod is withdrawn a small amount and the asymptotic reactor period is measured by taking the slope of the measured  $n(t)$  vs.  $t$  curve, as plotted on semi-logarithmic paper. The corresponding reactivity is computed from the Inhour equation. The reactor is returned to critical by addition of a compensatory reactivity, e.g., boric acid is added to the coolant, and the process is repeated. This method is commonly used to calibrate control rods in a reactor.

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2. *Sub-critical Multiplication.* The reactor is initially sub-critical with a source present, and the neutron density at any position in the reactor is inversely proportional to the reactivity. The relative reactivity worth of a control rod at any position in the core is related to the reactivity worth of the initial configuration by the ratio of the count rates obtained by a given neutron detector in the two cases. Specifically, if CR represents count rate,

$$\frac{\rho_{rod}}{\rho_{initial}} = \frac{CR_{initial}}{CR_{rod}}. \quad (8.34)$$

Of course, the initial reactivity,  $\rho_{initial}$ , must be measured by an auxiliary means.

3. *Source Jerk.* The reactor is initially sub-critical with a neutron source present, and a steady state neutron density is attained. The neutron density magnitude is measured using a neutron detector. At  $t = 0$ , the source is jerked out of the core, initiating a transient downward neutron flux variation. The reactivity worth of the system is measured from the ratio of the count rates before and after the source removal using the prompt-jump expression, i.e.,

$$\frac{CR_{0+}}{CR_0} = \frac{\bar{\beta}}{\beta - \rho}. \quad (8.35)$$

4. *Rod Drop.* The reactor is initially critical. At  $t = 0$ , the control rod is allowed to fall by gravity to its fully inserted position. As in the source-jerk experiment the reactivity is implied from a ratio of detector count rates using the prompt-jump expression.

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5. *Pulsed Neutron Source.* The reactor is either critical or sub-critical. Neutrons are injected into the system by a pulsed neutron generator such as a Cockcroft-Walton accelerator, which uses a deuterium or tritium target and an accelerated deuteron beam. Since the reactor is prompt sub-critical, the neutron flux as measured by a detector will decay on a short-time scale as  $\exp[-(\bar{\beta} - \rho)t/\Lambda]$ . Measurement of the slope of the decay curve vs. time plotted on semi-logarithmic paper, allows calculation of the reactivity. Similar results can be obtained from "noise" correlation measurements.

In any event,  $\bar{\rho}$  reactivity is not measured directly but only as the ratio of  $\rho/\bar{\beta}$ , i.e., in  $\$$ . This is not at all surprising since each of the parameters in the point kinetics equations is a defined quantity. It does imply, however, that there is a certain ambiguity in all measurements of reactor kinetics parameters and that certain quantities must be calculated in order to obtain reactivity worth.

**Additional Comments.** All of the above equations and solutions have been predicated on the assumption that the reactor system has a sufficient neutron population so that it is deterministic in nature. However, a treatment also exists for the situation where this condition is not true. The reactor must then be described by stochastic kinetics. Examples of the latter case are the initial startup of a new reactor in the absence of a neutron source. The Godiva experiments are a case in point.

The mathematics of stochastic kinetics will not be treated here. Suffice it to say that the ordinary kinetics equations describe the mean behavior of the stochastic model, but that the stochastic equations also predict the statistical chance that the

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mean behavior will be obtained.

### 8.6\* "Point" Kinetics Equations Derivation

The multi-group formulation given previously can be used to solve the non-separable space-time kinetics problem. When the reactor is sufficiently small so that it is spatially well-coupled and the space and time variables are essentially separable, we can consider that the spatial flux shape changes negligibly during a transient. In this case, we can treat the entire reactor dynamically as a "point" having certain weighted average properties. Here we derive the point reactor kinetics equations in a proper fashion.

Starting with the multi-group reactor kinetics equations, we obtain the point kinetics equations by performing the following operations:

1. Multiply the vector flux equation by the spatial fundamental mode adjoint vector taken at the initial time,  $\underline{\phi}^*(\vec{r})$ , and integrate over the volume of the reactor;
2. Multiply each precursor equation by  $\underline{\phi}^* \chi_{di}$  and integrate over the volume of the reactor;
3. Simplify the resulting equations by defining various global terms such as reactivity, lifetime, generation time, effective delayed neutron fractions, etc.

The adjoint is used as a weighting function to ensure that all neutrons are given the proper importance in the integral neutron balance. The weighting factor  $\chi_{di}$  is included in the precursor equations to produce integral terms that are similar to those found in the neutron balance equation.

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The flux equations give, after weighting and integration, an equation of the form:

$$\begin{aligned}
 & \text{rate of change} \quad \text{leakage} \\
 & \frac{d}{dt}(\phi_0^*(\vec{r}), \underline{\underline{T}}\phi(\vec{r}, t)) = (\phi_0^*, \nabla \bullet \underline{\underline{D}} \nabla \phi) \\
 & \text{absorption and scattering} \quad \text{prompt neutron production} \\
 & - (\phi_0^*, \underline{\underline{H}}\phi) + (1 - \beta)(\phi_0^*, \underline{\underline{\chi}}_p \underline{\underline{F}}^T \phi) \\
 & \text{delayed neutron production} \quad \text{source} \\
 & + \sum_{i=1}^6 \lambda_i (\phi_0^*, \underline{\underline{\chi}}_{di} C_i) + (\phi_0^*, \underline{\underline{Q}}).
 \end{aligned} \tag{8.36}$$

The precursor equations give, after weighting and integration, an equation of the form:

$$\begin{aligned}
 & \text{rate of change} \quad \text{precursor production} \\
 & \frac{d}{dt}(\phi_0^*, \underline{\underline{\chi}}_{di} C_i) = \beta_i (\phi_0^*, \underline{\underline{\chi}}_{di} \underline{\underline{F}}^T \phi) \\
 & \text{decay} \\
 & - \lambda_i (\phi_0^*, \underline{\underline{\chi}}_{di} C_i) \quad \text{for } i=1, 6.
 \end{aligned} \tag{8.37}$$

Obviously, we would like to simplify these equations by defining an "effective neutron density" and also an "effective precursor concentration." Define the effective neutron density as

$$n(t) \equiv (\phi_0^*, \underline{\underline{T}}\phi(\vec{r}, t)) = \left[ \begin{array}{c} \text{Weighted neutron popu-} \\ \text{lation in the core} \end{array} \right]. \tag{8.38}$$

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Furthermore, factorize the time-dependent flux into an amplitude factor that has a strong dependence on time and a shape factor that has a weak dependence on time. We can compute the shape function using static codes such as EXTERMINATOR. Specifically, let

$$\underline{\phi}(\vec{r}, t) \equiv n(t) \underline{\psi}(\vec{r}, t). \quad (8.39)$$

Conceptually, this substitution allows us to work with the known shape function  $\underline{\psi}(\vec{r})$  rather than with the unknown flux function  $\underline{\phi}(\vec{r}, t)$ . Point kinetics is really valid only when the shape function is in fact a constant proportional to the initial fundamental mode flux, i.e.,

$$\left[ \begin{array}{l} \text{Strict point kinetics} \\ \text{validity condition} \end{array} \right] \text{ is } \underline{\psi}(\vec{r}, t) \propto \underline{\phi}_0(\vec{r}).$$

When this condition is not valid, it is still possible to use a form of point kinetics by periodically updating all of the definitions. One such method is called the quasi-static method. Note that, with the above factorization, the shape function is normalized to unity, as can be shown by substitution, i.e.,

$$(\underline{\phi}_0^*, \underline{T} \underline{\psi}) = 1. \quad (8.40)$$

The weighted and integrated balance equations are, in fact, the point kinetics equations when certain definitions are made. Let the total weighted production rate be defined as the integral containing both the prompt and delayed neutron production, i.e.,

$$\mathbf{M}(t) \equiv \left( \underline{\phi}_0^*, \left[ (1 - \beta) \underline{\chi}_p \underline{F}^T + \sum_{i=1}^6 \beta_i \underline{\chi}_{di} \underline{F}^T \right] \underline{\psi} \right). \quad (8.41)$$

Then we can obtain an expression for the generation time,  $\Lambda$ , of the entire reactor as



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$$\Lambda(t) \equiv \frac{(\underline{\phi}_0^*, \underline{T}\underline{\psi})}{M(t)} = \left[ \frac{\text{Weighted total neutron density}}{\text{Weighted total production rate}} \right]. \quad (8.42)$$

In the same manner, the effective delayed neutron fraction,  $\bar{\beta}_i$  is defined as

$$\bar{\beta}_i = \beta_{ieff}(t) \equiv \frac{(\underline{\phi}_0^*, \beta_i \underline{\chi}_{di} \underline{F}^T \underline{\psi})}{M(t)} = \left[ \frac{\text{Weighted production rate of group } i \text{ delayed neutrons}}{\text{Weighted total production rate}} \right]. \quad (8.43)$$

Obviously

$$\bar{\beta} = \sum_{i=1}^6 \bar{\beta}_i.$$

For a thermal reactor,  $\bar{\beta}_i > \beta_i$  because delayed neutrons are more important than fast neutrons since they have a smaller leakage probability.

We insert the shape function in Eq. (8.6), add and then subtract a term containing  $\beta_i$ , and divide by  $(\underline{\phi}_0^*, \underline{T}\underline{\psi})$ . The result can be written as the following equation:

$$\begin{aligned} \frac{dn}{dt} = & \frac{\left( \underline{\phi}_0^*, \left\{ \nabla \bullet \underline{D}\nabla - \underline{H} + \left[ (1 - \beta) \underline{\chi}_p \underline{F}^T + \sum_{i=1}^6 \beta_i \underline{\chi}_{di} \underline{F}^T \right] \right\} \underline{\psi} \right)}{(\underline{\phi}_0^*, \underline{T}\underline{\psi})} n(t) \\ & - \frac{\sum_{i=1}^6 (\underline{\phi}_0^*, \beta_i \underline{\chi}_{di} \underline{F}^T \underline{\psi})}{(\underline{\phi}_0^*, \underline{T}\underline{\psi})} n(t) + \frac{\sum_{i=1}^6 \lambda_i (\underline{\phi}_0^*, \underline{\chi}_{di} C_i)}{(\underline{\phi}_0^*, \underline{T}\underline{\psi})} + \frac{(\underline{\phi}_0^*, Q)}{(\underline{\phi}_0^*, \underline{T}\underline{\psi})}. \end{aligned} \quad (8.44)$$

The precursor equations can be treated similarly to obtain the

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expression

$$\begin{aligned} & \frac{d(\underline{\phi}_0^*, \underline{\chi}_{di} C_i)}{dt(\underline{\phi}_0^*, \underline{T}\psi)} \\ &= \frac{(\underline{\phi}_0^*, \underline{\beta}_i \underline{\chi}_{di} \underline{F}^T \underline{\psi})}{(\underline{\phi}_0^*, \underline{T}\psi)} n(t) - \lambda_i \frac{(\underline{\phi}_0^*, \underline{\chi}_{di} C_i)}{(\underline{\phi}_0^*, \underline{T}\psi)}, \quad \text{for } i = 1, 6. \end{aligned} \quad (8.45)$$

We make the following additional definitions: The dynamic reactivity is defined as

$$\begin{aligned} \rho(t) &\equiv \frac{M(t) - (\underline{\phi}_0^*, [\underline{H} - \nabla \bullet \underline{D}\nabla] \underline{\psi})}{M(t)} \\ &= \frac{\left[ \frac{\text{Weighted total production}}{\text{rate}} \right] - \left[ \frac{\text{Weighted total loss}}{\text{rate}} \right]}{\left[ \frac{\text{Weighted total production}}{\text{rate}} \right]}. \end{aligned} \quad (8.46)$$

The weighted precursor concentrations are

$$c_i(t) \equiv \frac{(\underline{\phi}_0^*, \underline{\chi}_{di} C_i)}{(\underline{\phi}_0^*, \underline{T}\psi)}, \quad \text{for } i = 1, 6. \quad (8.47)$$

The weighted source is

$$q(t) \equiv \frac{(\underline{\phi}_0^*, \underline{Q})}{(\underline{\phi}_0^*, \underline{T}\psi)}. \quad (8.48)$$

The quantities  $\rho$ ,  $\bar{\beta}$ , and  $\Lambda$  have at best a weak dependence on time while the major dependence is contained in the factors  $n(t)$  and  $c_i(t)$ .

Using the above definitions the point kinetics equations are

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obtained in the familiar form given by Eqs. (8.8) and (8.9).

### 8.7 Method of Obtaining $\rho$ , $\Lambda$ , $\ell$ , and $\bar{\beta}$

The EXTERMINATOR code numerically solves the static eigenvalue problem to give the flux vector  $\underline{\phi}_0$  and the fundamental mode eigenvalue  $\lambda_0 = k_{\text{eff}}$ . By repeating the problem using  $\underline{\underline{L}}^T$  and  $\underline{\underline{M}}^T$ , the code also produces the adjoint flux  $\underline{\phi}_0^*$ . These are used to make static estimates of the dynamic values of  $\rho$ ,  $\Lambda$ ,  $\ell$ , and  $\bar{\beta}$ .

The primary difference between the static and dynamic calculations is the form of the production operator. In addition, the static problem contains  $\lambda_0$  while the dynamic problem does not. For all of the static definitions, the approximation used is the following,

$$\begin{aligned} \mathbf{M} &= \left( \underline{\phi}_0^*, \left[ (1 - \beta) \underline{\chi}_p \underline{\mathbf{F}}^T + \sum_{i=1}^6 \beta_i \underline{\chi}_{di} \underline{\mathbf{F}}^T \right] \underline{\psi} \right) \\ &\approx \left( \underline{\phi}_0^*, \frac{\underline{\chi}_p \underline{\mathbf{F}}^T}{\lambda_0} \underline{\phi}_0 \right) = \left( \underline{\phi}_0^*, \frac{\underline{\mathbf{M}}}{\lambda_0} \underline{\phi}_0 \right). \end{aligned} \tag{8.49}$$

This is to say that the slightly different importance of the delayed neutrons due to their lower energy spectrum is ignored, and a correction is made for  $k_{\text{eff}} \neq 1.0$ . We shall use this approximation to redefine our quantities of interest.

**Lifetime.** The lifetime,  $\ell$ , is the weighted integral time that the average neutron lives before being captured or being leaked from the core.

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In words, it is

$$[Lifetime] = \left[ \frac{\text{Mean free path for loss}}{\text{Average velocity of neutron}} \right],$$

or in the one-speed, bare core approximation,

$$\ell = \frac{l}{v(\Sigma_a + DB^2)}.$$

The perturbation theory equivalent is to weight the  $1/v$  factors in the numerator and the losses  $\underline{\underline{L}}$  in the denominator to obtain

$$\ell \equiv \frac{(\underline{\phi}_0^*, \underline{\underline{T}} \underline{\phi}_0)}{(\underline{\phi}_0^*, \underline{\underline{L}} \underline{\phi}_0)} = \frac{(\underline{\phi}_0^*, \underline{\underline{T}} \underline{\phi}_0)}{\left( \underline{\phi}_0^*, \frac{\underline{\underline{M}}}{\lambda_0} \underline{\phi}_0 \right)}. \quad (8.50)$$

One must input the inverse velocities for  $\underline{\underline{T}}$  to the EXTERMINATOR code.

**Generation Time.** The generation time,  $\Lambda$ , is the weighted integral time until a neutron is produced. In words, it is

$$[Generation\ time] = \left[ \frac{\text{Mean free path for production}}{\text{Average velocity of neutron}} \right],$$

or in the one-speed bare core approximation,

$$\Lambda = \frac{l}{v \Sigma_f}.$$

The perturbation theory equivalent is

$$\Lambda \equiv \frac{(\underline{\phi}_0^*, \underline{\underline{T}} \underline{\phi}_0)}{(\underline{\phi}_0^*, \underline{\underline{M}} \underline{\phi}_0)} \quad (8.51)$$

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By comparing the equations for  $\ell$  and  $\Lambda$ , we find a simple relationship between them, namely,

$$\ell = \lambda_0 \Lambda = k_{\text{eff}} \Lambda. \quad (8.52)$$

**Effective Delayed Neutron Fraction.** Delayed neutrons are born as a physical fraction  $\beta$  of the total fission neutron production, but they are more important than fission neutrons because they are born at a lower energy. One might ask the question: If the delayed neutrons were all born with a fission spectrum, what effective fraction would be needed to give them the same importance as they have in the actual situation? In words, this equation is

$$\beta_i [\text{Actual importance}] = \bar{\beta}_i \left[ \frac{\text{Importance if emitted with a fission spectrum}}{\text{Importance of fission spectrum}} \right].$$

The expression evaluated by EXTERMINATOR is

$$\bar{\beta}_i \equiv \beta_i \frac{(\underline{\phi}_0^*, \underline{\chi}_{di} \underline{F}^T \underline{\phi}_0)}{(\underline{\phi}_0^*, \underline{\chi}_p \underline{F}^T \underline{\phi}_0)} = \beta_i \frac{(\underline{\phi}_0^*, \underline{\chi}_{di} \underline{F}^T \underline{\phi}_0)}{(\underline{\phi}_0^*, \underline{M} \underline{\phi}_0)}. \quad (8.53)$$

One must input the values of  $\beta_i$  and the  $\underline{\chi}_{di}$  vectors that describe the delayed neutron spectra.

**Reactivity.** There is a conceptual difference between the static and dynamic definitions of the reactivity,  $\rho$ . In the dynamic case, we take the weighted integral difference between total production and loss to determine the  $\Delta k$  difference from a critical state of  $k_{\text{eff}} = 1.0$ . In the static case we assume that the reactor is effectively critical at  $k_{\text{eff}} = \lambda_0$  and hence we compute the  $\Delta \rho$  for a change in the production and loss terms of an amount  $\delta \underline{M}$  and  $\delta \underline{L}$ . Also, in the static case we ignore the slight difference in importance between the prompt and delayed neutrons in the  $\underline{M}$  and  $\delta \underline{M}$  terms.

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The reactivity expressed in static terms is

$$[Reactivity] = \frac{\left[ \frac{\text{Weighted total production}}{\text{rate change}} \right] - \left[ \frac{\text{Weighted total loss}}{\text{rate change}} \right]}{\left[ \frac{\text{Weighted total production}}{\text{rate}} \right]}$$

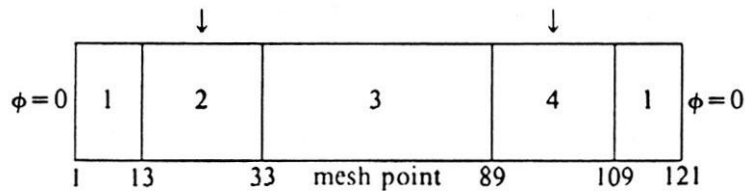
or

$$\lambda_0 \Delta \rho_0 = \frac{\left( \phi_0^*, \left\{ \frac{\delta \mathbf{M}}{\lambda_0} - \delta \mathbf{L} \right\} \phi_0 \right)}{\left( \phi_0^*, \frac{\mathbf{M}}{\lambda_0} \phi_0 \right)}. \quad (8.54)$$

One sees that the fission terms are divided by  $\lambda_0$  to correct to  $k_{\text{eff}} = 1$ .

### Problems

**8.1\*** Few-group computer codes such as RAUMZEIT or WIGLE can be used to compute a one-dimensional spatial transient. The geometry is shown below.



The transient is caused by changes in thermal absorption,  $\Sigma_{a2}$  in region 2 or 4. Material 1 is a reflector material, and the others are fuels. The material properties of the four different region types are the following:

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Region	Material Properties $\begin{pmatrix} \text{group 1} \\ \text{group 2} \end{pmatrix}$					Delayed Neutron Data		
	$D$	$\Sigma_a$	$\Sigma_{s1 \rightarrow 2}$	$\nu\Sigma_f$	$\chi_p$	Delayed Neutron Group	$\bar{\beta}_i$	$\lambda_i \text{ sec}^{-1}$
1	1.64	0.0003	0.0384	0.	—	1	0.00021	0.0124
	0.268	0.118	—	0.	—	2	0.00143	0.0305
2	1.47	0.0056	0.0132	0.00517	1.0	3	0.00127	0.111
	0.527	0.129	—	0.135	0.	4	0.00257	0.301
3	1.47	0.0056	0.0132	0.00516	1.0	5	0.00075	1.14
	0.528	0.130	—	0.134	0.	6	0.00027	3.01
4	1.47	0.0054	0.0134	0.00518	1.0		0.00650	
	0.530	0.124	—	0.137	0.			

Use two neutron groups, six precursor groups, and a total of 121 mesh points. Use slab geometry with a zero flux boundary condition on each outer surface. The transverse buckling can be taken to be  $B^2 = 0.001 \text{ cm}^{-2}$ . The mesh spacings are uniform and will be one of the four values: 2.0 cm; 2.25 cm; 2.5 cm; 2.75 cm.

a) Long-time-scale Down-transients (four problems)

Double the thermal group  $\Sigma_a$  in region 4 and hold it fixed at that value. Use the prompt jump option. Take 1 s time steps for 30 s. Also do a static flux calculation with the new  $\Sigma_a$  value.

Plot: (a) Initial thermal flux shape normalized to unit power.

(b) Final thermal flux shape normalized to unit power,

(c) Flux shape at 5 seconds;

(d) Flux shape at 30 seconds;

(e) Power vs. time on semi-log paper.

Compare results using different sized mesh spaces.

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### b) Short-time-scale Down-transients (four problems)

Double the thermal group  $\Sigma_a$  in region 4 and hold it fixed at that value. Use  $1/v_1 = 10^{-8}$  and  $1/v_2 = 5 \times 10^{-6}$  s/cm. Take ten steps at  $\Delta t = 10^{-5}$  s and the rest of the steps at  $\Delta t = 10^{-4}$  s. Also do a static flux calculation using the new  $\Sigma_a$  value. Watch for numerical instability.

Plot: (a) Initial thermal flux shape normalized to unit power;

(b) Final thermal flux shape normalized to unit power;

(c) Flux shape at  $10^{-3}$  seconds;

(d) Power vs. time on semi-log paper.

Compare your results to those for another mesh spacing.

### c) Short-time-scale Up-transients (four problems)

Decrease the thermal group  $\Sigma_a$  in region 2 by 20% of its original value and hold it fixed. Use  $1/v_1 = 10^{-8}$  and  $1/v_2 = 5 \times 10^{-6}$  s/cm. Take ten steps at  $\Delta t = 10^{-5}$  s, and the rest of the steps at  $\Delta t = 10^{-4}$  s. Also do a static flux calculation using the new  $\Sigma_a$  value. Watch for numerical instability.

Plot: (a) Initial thermal flux shape normalized to unit power;

(b) Final thermal flux shape normalized to unit power;

(c) Flux shape at  $10^{-3}$  s;

(d) Power vs. time on semi-log paper. Note that the transient is not initially exponential although the change in



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material properties is constant with time. Explain.

Compare your results to those for another mesh spacing.

- 8.2\*** You are given the time-dependent few-group neutron balance equation (ignoring delayed neutrons)

$$\underline{\underline{T}} \dot{\underline{\phi}}(r,t) = (\underline{\underline{M}} - \underline{\underline{L}}) \underline{\phi}(r,t),$$

where  $\underline{\underline{T}}$  is a matrix of inverse group velocities and  $\underline{\underline{M}}$  and  $\underline{\underline{L}}$  are the production and loss operators, respectively.

Assume that the time behavior is asymptotic and of the form

$$\underline{\phi}(r,t) = \underline{\Phi}(r) e^{\alpha t}.$$

Obtain the  $\omega$ -mode eigenvalue problem by substituting the asymptotic form into the balance equation. Derive the corresponding  $\omega$ -mode adjoint problem and demonstrate the biorthogonality property of the  $\omega$ -modes.

- 8.3** Consider the point reactor kinetics equations with two delayed precursor groups. Derive the inhour equation for a step change in  $\rho$  by finding the characteristic equation for the vector-matrix formulation of this problem.
- 8.4** A reactor has been operating at a steady state neutron density of  $n_0$ . At time  $t = 0$ , a neutron vacuum cleaner instantaneously removes all of the neutrons in the system, leaving only the precursors. If the vacuum cleaner is turned off immediately, write expressions for the resulting neutron density and precursor concentration as a function of time after this action. Assume that the system is adequately described by one effective group of delayed

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neutron precursors.

- 8.5** You are given a reactor that is initially critical with a neutron density of  $n_0$  neutrons/cm<sup>3</sup>. Assume point kinetics is valid with one group of precursors. At time  $t = 0$ , an additional  $c_0$  precursors/cm<sup>3</sup> are instantaneously injected into the system. Calculate  $n(t)$  and  $c(t)$  after the injection in terms of  $n_0$ ,  $c_0$ , and  $\Lambda$ . Does  $\rho$  enter into your equations?
- 8.6** Assume that the reactivity insertion upon control rod withdrawal is given by  $\rho(t) = at$  where  $a = 10^{-5}$  and  $t$  is in seconds. Assume that throughout the time that  $\rho(t)$  is changing,  $dc_i(t)/dt = 0$  in the point reactor kinetic equations, i.e., there is an exact balance between production and loss by radioactive decay of the precursor concentrations.
- Determine the response of the reactor to this change in reactivity.
  - Compute the time needed to double the neutron density if  $\Lambda = 5 \times 10^{-4}$  s.
  - How many cents worth of reactivity will be introduced in 80 s assuming  $\beta = .008$  (UVAR core)?
- 8.7** A point reactor with one group of delayed neutron precursors operates at equilibrium in the sub-critical state ( $\rho$  is negative) when a source of strength  $Q$  is present.
- If the source is extracted suddenly at time  $t = 0$ , find the time-dependent neutron density. List any assumptions you make.
  - If  $\rho = -10\beta$ , find the value of the neutron density at  $t = 0+$  after the source is removed.

## NUCLEAR REACTOR THEORY AND DESIGN

### References

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- A. Radkowsky, ed.,** *Naval Reactors Physics Handbook, 1*, (United States Atomic Energy Commission, Washington, D.C., 1964) Chapter 5.
- G.R. Keepin,** *Physics of Nuclear Kinetics*, (Addison-Wesley Publishing Company, Reading, MA, 1965).



## POISONING, TEMPERATURE EFFECTS AND DEPLETION IN REACTORS

When any nuclear reactor operates at an appreciable power level for a period of time ranging from hours to months, a significant number of atoms in the reactor undergo nuclear transmutation. Most of the atomic species in the reactor absorb neutrons to some extent, usually becoming radioactive isotopes that then decay to other isotopes or capture neutrons and transmute again. Fertile isotopes, such as  $^{238}\text{U}$ , cannot only capture neutrons, transmute and then decay to higher  $Z$  materials such as  $^{239}\text{Pu}$ , but they can also split into pairs of light isotopes in a myriad of ways leading to a variety of fission products.

The equations governing the total number of atoms of a given type at any physical location in the reactor are generally first-order, coupled, ordinary differential equations. Unfortunately, in all too many cases, the equations do not have constant coefficients. Quite often, some of the equations are nonlinear. Hence, while the formulation of the problem is relatively easy, analytic solutions are often hard to obtain. One is usually forced to solve poisoning and depletion problems numerically, in conjunction with the solution of the space-dependent reactor problem, often with temperature effects included insofar as the temperature modifies the atom densities through expansion and affects local neutron spectra.

The reasons for the above situation are not difficult to understand. Whenever the atom density or cross section of a nuclide changes, or other atom species appear, one obtains a

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reactivity effect. Nuclear reactors must be kept in a critical state during normal operation, and therefore some type of control action must be taken to compensate for these reactivity variations. The two effects combine to shift the spatial flux distribution as a function of time. Furthermore, reactors are usually operated at constant power, so that when the fuel begins to deplete, the average flux level must rise to compensate.

Fortunately, the various possible dynamic effects have significantly different *time constants* so that we can usually isolate the treatment into essentially non-over-lapping categories. The usual categories are:

1. Seconds to minutes - reactor kinetics and dynamics including prompt thermal feedback effects;
2. Hours to days - fission product poisons such as xenon and samarium, including power feedback effects;
3. Weeks to years - fuel depletion, breeding, and burnable poisons.

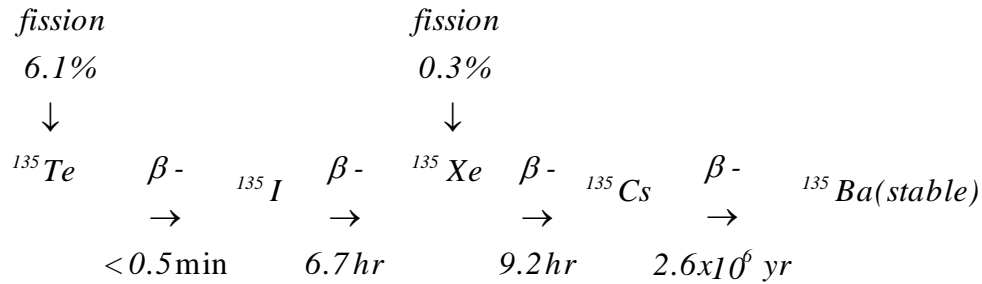
### 9.1 The Fission Product Xenon-135

Xenon-135 is a very important fission product for three different reasons. First, because the mass number 135 lies near the peak of the "double hump" fission product yield curve, it has a very high chain yield, over 6% for  $^{235}\text{U}$  fission. Second, xenon has a very high cross section,  $\sigma_a = \sim 3 \times 10^6$  barns, because it has a giant resonance at thermal neutron energies that fosters the maximum cross section predicted theoretically using the optical model of the nucleus. Third, the associated half-lives of the important members in the 135 chain are of the order of several hours, causing the effects to appear rapidly during normal reactor operation.

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The above factors lead to two separate problems involving xenon: (1) the poisoning problem, which occurs during startup, load changes, and shutdown of the reactor; and (2) the xenon oscillation problem, which involves damped or growing spatial power shifts that can occur during normal operation of the reactor at a constant total power level. We shall examine both problems in some detail.

The 135 chain for  $^{235}\text{U}$  fission is



The tellurium decays so rapidly that the iodine is produced almost immediately; the iodine can therefore be considered to be the direct product of fission. We must write a balance equation for both the iodine and the xenon at each spatial position in the reactor. The iodine equation is

$$\text{change} \quad \text{fission yield} \quad \text{decay} \tag{9.1}$$

$$\frac{dI(\vec{r},t)}{dt} = \gamma_1 \Sigma_f(\vec{r})\phi(\vec{r},t) - \lambda_1 I(\vec{r},t).$$

For simplicity, we use one-group theory, but the fission cross section and the flux could be written as multi-group vectors if desired. The corresponding xenon equation is

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$$\begin{array}{ccccc}
 & \textit{iodine} & \textit{fission} & \textit{xenon} & \\
 \textit{change} & & & & \\
 & \textit{decay} & \textit{yield} & \textit{decay} & \textit{burnup}
 \end{array}$$

(9.2)

$$\frac{dX(\vec{r},t)}{dt} = \lambda_I I(\vec{r},t) + \gamma_x \sum_f(\vec{r})\phi(\vec{r},t) - \lambda_x X(\vec{r},t) - \sigma_{ax}\phi(\vec{r},t)X(\vec{r},t).$$

We ignore burnup of the iodine because the absorption cross section is small and  $\sigma_{aI}\phi \ll \lambda_I$ . In addition, we have the spatial flux equation

$$L\phi(\vec{r},t) = \frac{1}{\lambda_0}M\phi(\vec{r},t). \tag{9.3}$$

The reactor balance equation has *purposely* been written as a static balance equation instead of a time-dependent equation. On the time scale involved in xenon poisoning effects, one can ignore the delayed neutrons and the time rate of change of the flux. However, to the extent that the xenon exerts a reactivity effect, some external control action must be taken to maintain the criticality at the value of  $k_{\text{eff}} = \lambda_0 = 1$ . The control action for a commercial reactor is invariably a *symmetric* movement of a *bank* of control rods, designed to produce a minimum local perturbation and avoid excitation of harmonic flux modes.

### 9.2 Xenon Poisoning

Xenon poisoning is significant only in a thermal reactor because only the thermal cross section of xenon is large. If one makes the approximation that the *flux is constant and does not vary* during the transient xenon behavior, then the xenon and iodine equations are linear with constant coefficients and can be solved analytically. To be rigorous, one should use the multi-group formulation, but it is a reasonably good approximation to



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treat the equations as a one-group problem if one remembers that almost all fission occurs in the thermal group and the xenon absorption occurs there too.

Reactor design calculations are usually done to check three separate xenon conditions: (1) no xenon; (2) equilibrium xenon; and (3) peak xenon. We have already discussed how to calculate the "no xenon" case numerically in Chapter 6. This gives a flux shape  $\phi(\vec{r})$  that can be used to calculate the equilibrium xenon. Equilibrium means no change with time; this condition may be obtained by setting  $dI/dt$  and  $dX/dt$  equal to zero. The result at any spatial position is

$$I_{\infty}(\vec{r}) = \frac{\gamma_I \Sigma_f(\vec{r}) \phi(\vec{r})}{\lambda_I}, \quad (9.4)$$

and

$$X_{\infty}(\vec{r}) = \frac{\lambda_I I_{\infty}(\vec{r}) + \gamma_x \Sigma_f(\vec{r}) \phi(\vec{r})}{\lambda_x + \sigma_{ax}(\vec{r}) \phi(\vec{r})} \quad (9.5)$$

$$= \frac{(\gamma_I + \gamma_x) \Sigma_f(\vec{r}) \phi(\vec{r})}{\lambda_x + \sigma_{ax}(\vec{r}) \phi(\vec{r})}.$$

We keep  $\sigma_{ax}$  as a function of position because the local neutron spectrum determines the average microscopic cross section used in the equation.

We recall that the neutron flux varies over at least an order of magnitude from the center to the outside of a reactor. In the high flux limit where burnup of xenon is much more important than decay, i.e., when  $\sigma_{ax}\phi \gg \lambda_x$ , we can ignore  $\lambda_x$  in the denominator of Eq. (9.5) to obtain the effective equilibrium xenon macroscopic cross section,

$$\Sigma_{ax}^{\infty}(\vec{r}) = \sigma_{ax}(\vec{r}) X_{\infty}(\vec{r}) \approx (\gamma_I + \gamma_x) \Sigma_f(\vec{r}). \quad (9.6)$$

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The resultant reactivity worth is approximately

$$\rho_{ax}^{\infty} = \frac{\left( \phi^*(\vec{r}), -\sum_{ax}^{\infty}(\vec{r})\phi(\vec{r}) \right)}{\left( \phi^*(\vec{r}), \nu \sum_f(\vec{r})\phi(\vec{r}) \right)} \approx -\frac{(\gamma_I + \gamma_x)}{\nu} = -0.0262 \quad (9.7)$$

Hence, the  $k_{eff}$  of the core with all control rods out must be at least 1.0262 in order to allow the reactor to operate with xenon present, and the control rods must be able to compensate for this reactivity, which is greater than  $4\beta$ , when there is no xenon. In the general case, when  $\sigma_{ax}\phi$  is not much greater than  $\lambda_x$ , the reactivity effect is less than that given above because of the extra term in the denominator. It is

$$\rho_{ax}^{\infty} = \frac{\left( \phi^*(\vec{r}), \frac{(\gamma_I + \gamma_x)\sigma_{ax}(\vec{r})\sum_f(\vec{r})\phi(\vec{r})}{\lambda_x + \sigma_{ax}(\vec{r})\phi(\vec{r})} \phi(\vec{r}) \right)}{\left( \phi^*(\vec{r}), \nu \sum_f(\vec{r})\phi(\vec{r}) \right)}, \quad (9.8)$$

We note the rather curious appearance of  $\phi^2(\vec{r})$  terms in the numerator of the above expression. When combined with the adjoint flux shape, which tends to peak in the same spatial position in the reactor, the xenon in the highest flux position in the reactor is very strongly weighted in computing the reactivity effect in the core. Hence, *three-dimensional* solutions are usually required if an accurate representation of the effect of xenon is to be obtained.

### 9.3 General Transient Solution for Buildup of Xenon and Iodine

The general solution to the xenon poisoning problem, when the flux is constant during the transient, is easily obtained using Laplace transforms. The iodine equation becomes

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$$s\bar{I}(s) - I_0 = \frac{\gamma_I \Sigma_f \phi}{s} - \lambda_I \bar{I}(s),$$

or

$$\bar{I}(s) = \frac{I_0}{(s + \lambda_I)} + \frac{\gamma_I \Sigma_f \phi}{s(s + \lambda_I)}. \quad (9.9)$$

The solution is obtained by taking the inverse transform of each term, yielding

$$I(t) = I_0 e^{-\lambda_I t} + \frac{\gamma_I \Sigma_f \phi}{\lambda_I} (1 - e^{-\lambda_I t}). \quad (9.10)$$

This is the sum of a term representing decay of any iodine initially present plus buildup of iodine due to operation at the flux  $\phi$ .

The xenon equation is transformed similarly and becomes

$$s\bar{X}(s) - X_0 = \lambda_I \bar{I}(s) + \frac{\gamma_x \Sigma_f \phi}{s} - \lambda_x \bar{X}(s) - \sigma_{ax} \phi \bar{X}(s),$$

or

$$\begin{aligned} \bar{X}(s) = & \frac{\gamma_x \Sigma_f \phi}{s(s + \lambda_x + \sigma_{ax} \phi)} + \frac{X_0}{(s + \lambda_x + \sigma_{ax} \phi)} + \frac{\lambda_I I_0}{(s + \lambda_I)(s + \lambda_x + \sigma_{ax} \phi)} \\ & + \frac{\gamma_I \lambda_I \Sigma_f \phi}{s(s + \lambda_I)(s + \lambda_x + \sigma_{ax} \phi)}. \end{aligned} \quad (9.11)$$

The solution is obtained by inverting each term, giving

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$$\begin{aligned}
 X(t) = & \frac{\gamma_x \Sigma_f \phi}{\lambda_x + \sigma_{ax} \phi} (1 - e^{-(\lambda_x + \sigma_{ax} \phi)t}) + X_0 e^{-(\lambda_x + \sigma_{ax} \phi)t} \\
 & + \frac{\lambda_I I_0}{(\lambda_x + \sigma_{ax} \phi - \lambda_I)} \{ e^{-\lambda_I t} - e^{-(\lambda_x + \sigma_{ax} \phi)t} \} \\
 & + \frac{\gamma_I \Sigma_f \phi}{\lambda_x + \sigma_{ax} \phi} - \frac{\gamma_I \Sigma_f \phi}{(\lambda_x + \sigma_{ax} \phi - \lambda_I)} e^{-\lambda_I t} + \frac{\lambda_I \gamma_I \Sigma_f \phi e^{-(\lambda_x + \sigma_{ax} \phi)t}}{(\lambda_x + \sigma_{ax} \phi)(\lambda_x + \sigma_{ax} \phi - \lambda_I)}.
 \end{aligned} \tag{9.12}$$

To check the generality of the equations, try the following cases:

- (a) *Initial value.* Let  $t = 0$  so that  $e^{-at} = 1$ . Then  $I(0) = I_0$  and  $X(0) = X_0$  as expected.
- (b) *Equilibrium value.* Let  $t = \infty$  so that  $e^{-at} = 0$ . Then

$$I_{\infty} = \frac{\gamma_I \Sigma_f \phi}{\lambda_I},$$

and

$$X_{\infty} = \frac{(\gamma_I + \gamma_x) \Sigma_f \phi}{\lambda_x + \sigma_{ax} \phi},$$

as obtained previously

- (c) *Peak xenon at shutdown.* Let  $\phi = 0$ . Then the equations reduce to

$$I(t) = I_0 e^{-\lambda_I t}, \tag{9.13}$$

and

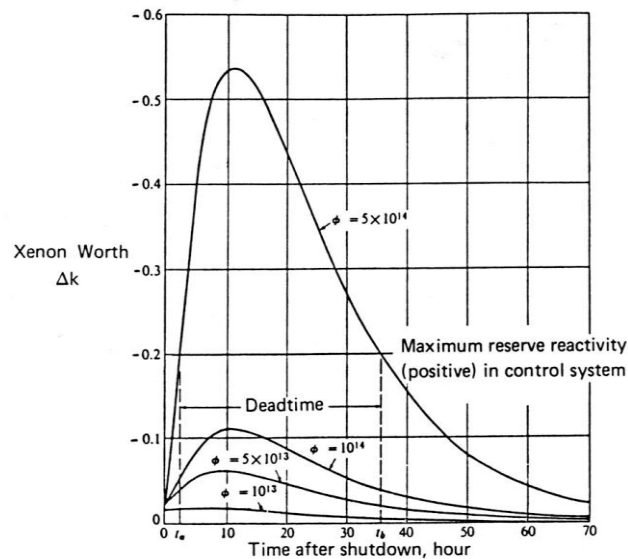
$$X(t) = X_0 e^{-\lambda_x t} + \frac{\lambda_I I_0}{\lambda_x - \lambda_I} \{ e^{-\lambda_I t} - e^{-\lambda_x t} \}. \tag{9.14}$$

We find the time  $t_{\max}$  at which the peak xenon occurs by

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setting  $dX/dt = 0$ . If shutdown begins from equilibrium, we use  $I_\infty$  and  $X_\infty$  for the initial values in Eqs. (9.13) and (9.14). The amount of xenon present at time  $t_{\max}$  is called "peak xenon," which can be many times greater than the equilibrium value depending upon the magnitude of the equilibrium flux *before* shutdown.

The solution to the xenon buildup problem is a curve that peaks at approximately eleven hours after shutdown and then decays with the half-life of xenon. If the flux is less than about  $4.0 \times 10^{11}$  n/cm<sup>2</sup>-s, no peak is observed at all. As the flux is increased above  $10^{13}$  n/cm<sup>2</sup>-s, a considerable amount of xenon may be present, possibly exceeding the reserve reactivity of the control rods. In such a case, there is nothing to do but wait until the xenon decays so that the reactor can be restarted. This waiting period is called the "deadtime." The curves for shutdown from several different flux levels are shown in Figure 9.1.



**Fig. 9.1** Xenon Worth vs. Time After Shutdown

(From *Introduction to Nuclear Reactor Theory* by J.R. Lamarsh, 1966, Addison Wesley)

**Vector-Matrix Formulation.\*** The iodine and xenon differential equations can be put into the form of a first-order matrix differential equation. We define the following

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quantities:

$$\underline{\underline{N}} \equiv \begin{bmatrix} \underline{I} \\ \underline{X} \end{bmatrix}; \quad \underline{N}_0 \equiv \begin{bmatrix} \underline{I}_0 \\ \underline{X}_0 \end{bmatrix}; \quad \underline{S} \equiv \begin{bmatrix} \gamma_I \Sigma_f \phi \\ \gamma_x \Sigma_f \phi \end{bmatrix};$$

and

$$\underline{\underline{B}} \equiv \begin{bmatrix} -\lambda_I & 0 \\ \lambda_I & (\lambda_x + \sigma_{ax}\phi) \end{bmatrix}.$$

With these definitions, the problem reduces to the form

$$\dot{\underline{\underline{N}}} = \underline{\underline{B}}\underline{\underline{N}} + \underline{S}. \quad (9.15)$$

If the flux is constant, then the matrix  $\underline{\underline{B}}$  is constant and the general solution can be written immediately as the equation

$$\underline{\underline{N}} = [\exp \underline{\underline{B}}t] \underline{N}_0 + \int_0^t \exp \underline{\underline{B}}(t - \tau) \underline{S}(\tau) d\tau. \quad (9.16)$$

The matrix  $[\exp \underline{\underline{B}}t]$  can be expressed in terms of the characteristic values or eigenvalues of the  $\underline{\underline{B}}$  matrix using Sylvester's theorem. These eigenvalues are obtained from the expression

$$|\underline{\underline{B}} - \omega \underline{\underline{I}}| = 0, \quad (9.17)$$

or, written out,

$$\begin{bmatrix} (-\lambda_I - \omega) & 0 \\ \lambda_I & -(\lambda_x + \sigma_{ax}\phi) - \omega \end{bmatrix} = 0.$$

The solutions are obviously  $\omega_0 = -\lambda_I$  and  $\omega_1 = -(\lambda_x + \sigma_{ax}\phi)$ , which lead to solutions for the xenon and iodine equations containing linear combinations of the exponentials,

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$$e^{-\lambda_I t} \text{ and } e^{-(\lambda_X + \sigma_{ax}\phi)t}.$$

But these are precisely the factors appearing in the solutions obtained using Laplace transforms.

### 9.4 Spatial Xenon Transients

The analytic solution to the xenon poisoning problem for a constant flux level, obtained in the previous section, is valid at any local point in the reactor. In actual practice the flux does indeed vary with time, but if the time interval is taken to be short with respect to the half-lives of the xenon and iodine, then the flux does not vary greatly. This suggests a quasi-static method of calculating the transient effects of xenon in the system.

We start at  $t = 0$  with a static calculation of the spatial flux distribution in a reactor system plus initial conditions on xenon and iodine. Assuming that the flux at each spatial location is constant over a time step  $\Delta t_1$ , we then compute the xenon and iodine at time  $t' = \Delta t_1$  using Eqs. (9.10) and (9.12). The xenon distribution, thus obtained, is used in a new static flux calculation to obtain the corresponding flux distribution at time  $t'$ . Since xenon primarily affects the destruction operator, the equation to be solved is

$$L(\vec{r}, t')\phi(\vec{r}, t') = \frac{1}{\lambda_0} M(\vec{r})\phi(\vec{r}, t').$$

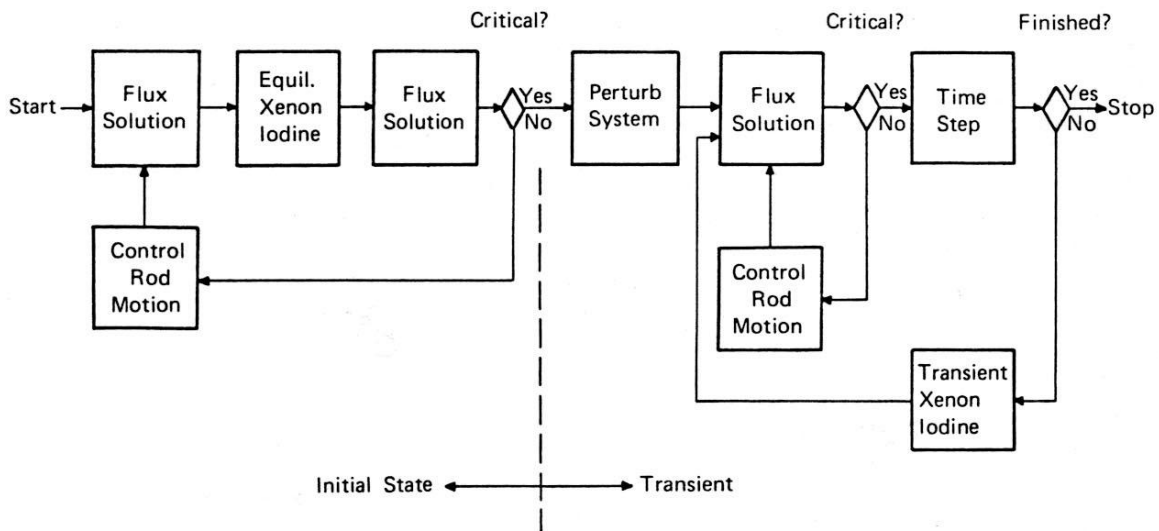
We can now do a control rod search to maintain criticality at the original value of  $k_{\text{eff}} = \lambda_0$ , if desired. Temperature feedback can also be included by simultaneously doing a heat balance and computing the corresponding reactivity effects.

Using the new flux at time  $t'$ , plus the new xenon and iodine

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as initial conditions, another time step  $\Delta t_2$  can be taken to find the xenon and iodine at  $t'' = t' + \Delta t_2$ . Another static flux calculation gives the corresponding spatial flux distribution. The procedure can be repeated for as many time steps as desired, thus tracing out the complete spatial xenon transient. Under certain conditions, the spatial solution is found to oscillate with time, and this is known as a xenon-induced spatial power oscillation.

A block diagram of the quasi-static process of solution is given in Figure 9.2. Naturally, the accuracy attained depends upon the size of the time steps used because the spatial flux is not really constant with time. The numerical solutions tend to predict longer oscillation periods and smaller growth rates than are actually present, if large time steps are taken. However, means exist for estimating the correct values from the data obtained, so this is not a major limitation of the method.



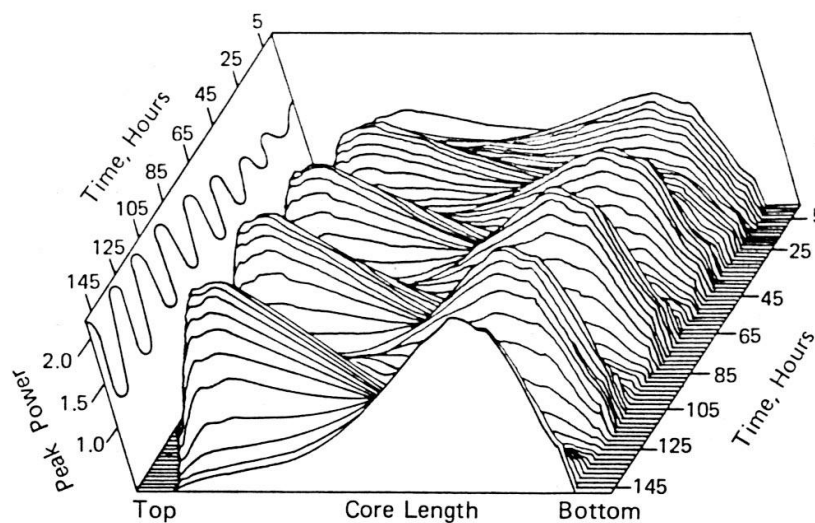
**Fig. 9.2** Block Diagram of Practical Solution Procedure for Spatial Xenon Transients



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### 9.5 Xenon-Induced Spatial Power Oscillations

Xenon oscillations have indeed been observed in large, high power, thermal reactors. A spatial xenon oscillation starts as follows: Suppose that for some reason the flux increases slightly on one side of the reactor and decreases slightly on the other. Where the flux increases, more xenon will burn out, and where it decreases less xenon will burn out than in the initial state. The immediate effect is positive reactivity on the side where the flux increased, and vice-versa, tending to *reinforce* the original unbalance. This trend continues until such a time that the increased iodine production on the high-flux side begins to result in increasing xenon, and the contrary. Then the flux on the high-flux side begins to decrease and vice-versa. Eventually the flux will be peaked on the opposite side of the core as shown in Figure 9.3. Continuation of the process is, in fact, a side-to-side oscillation. The spatial distribution of power shifts from side to side even though the total power remains constant.



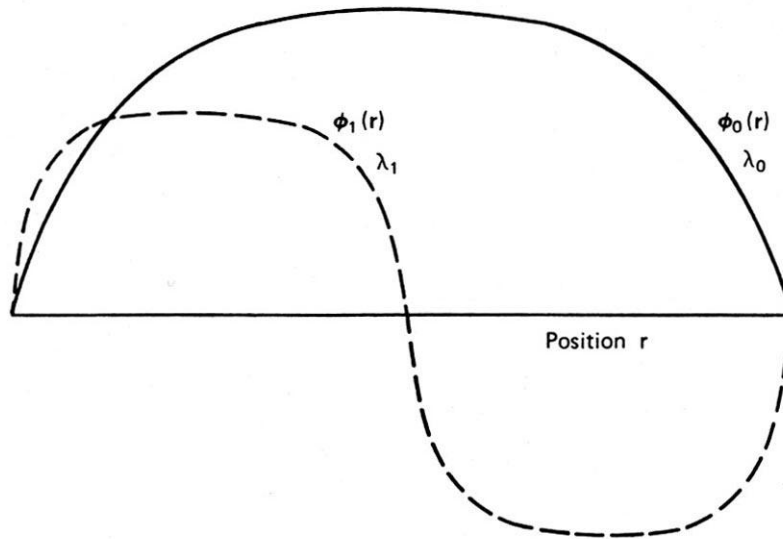
**Fig. 9.3** Schematic of a Spatial Xenon Oscillation

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We can postulate theoretically that the oscillation is composed of an interaction between the fundamental mode and the first-harmonic mode solutions to the neutron balance equations, as shown in Figure 9.4, and is of the form

$$\phi(\vec{r}, t) = \phi_0(\vec{r}) + a(t)\phi_1(\vec{r}), \quad (9.18)$$

where  $a(t)$  is a time-dependent modal combining coefficient. We find that the solution contains three important factors: (1) the difference in criticality between the fundamental and first harmonic modes,  $\lambda_0 - \lambda_1$ ; (2) the "effective" flux level or operating power of the reactor; and (3) the effective thermal feedback and void feedback contributions.



**Fig. 9.4** Harmonic Flux Modes

An important point to realize is the fact that large commercial thermal power reactors of the pressurized water or gas-cooled types can be expected to exhibit xenon spatial oscillations. The eigenvalue difference for these reactors, namely,  $\lambda_0 - \lambda_1$ , may be less than 0.01, while the average

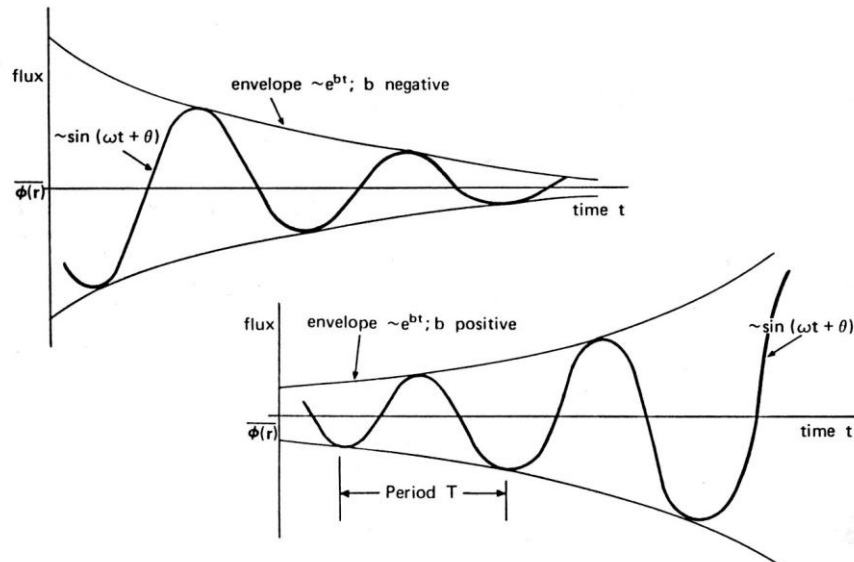
## NUCLEAR REACTOR THEORY AND DESIGN

thermal neutron flux level may exceed  $10^{13}$  n/cm<sup>2</sup>-s. Both factors tend to promote the possibility of oscillations. Negative feedback, on the other hand, tends to act as a stabilizing influence to balance against the tendency to oscillate. In fact, it is the large amount of negative feedback from void formation that makes boiling water reactors *stable* to xenon oscillations.

When oscillations are observed, then to first order at any spatial point, the time behavior is a damped or growing sinusoid about the average flux value, of the form

$$\phi(\vec{r}, t) = \overline{\phi(\vec{r})} + A(\vec{r})e^{bt}\sin(\omega t + \theta). \quad (9.19)$$

$A(\vec{r})$  is an initial value, e.g., induced by control action. The exponent  $b$  is called the damping factor; it can be either positive or negative. The oscillation period is given by  $T = 2\pi/\omega$ ; it is typically 15 hours or greater. This means that the period of an oscillation is longer than the work-shift time of a reactor operator! The quantity  $\theta$  is simply a phase angle. Examples of both damped and growing xenon oscillations are shown in Figure 9.5.



**Fig. 9.5** Schematic of Damped and Growing Xenon Oscillations

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There exist analytically derived correlations that can fairly successfully predict the growth factor  $b$  and period  $T$  of a xenon oscillation. One of these correlations is illustrated in Figures 9.6 and 9.7 for a  $^{235}\text{U}$  fueled reactor. The dimensionless parameters that appear here can be defined approximately as the susceptibility factor,

$$\Omega \approx \nu(\lambda_0 - \lambda_1) + \Omega_{\text{feedback}}, \quad (9.20)$$

and the dimensionless effective flux level,

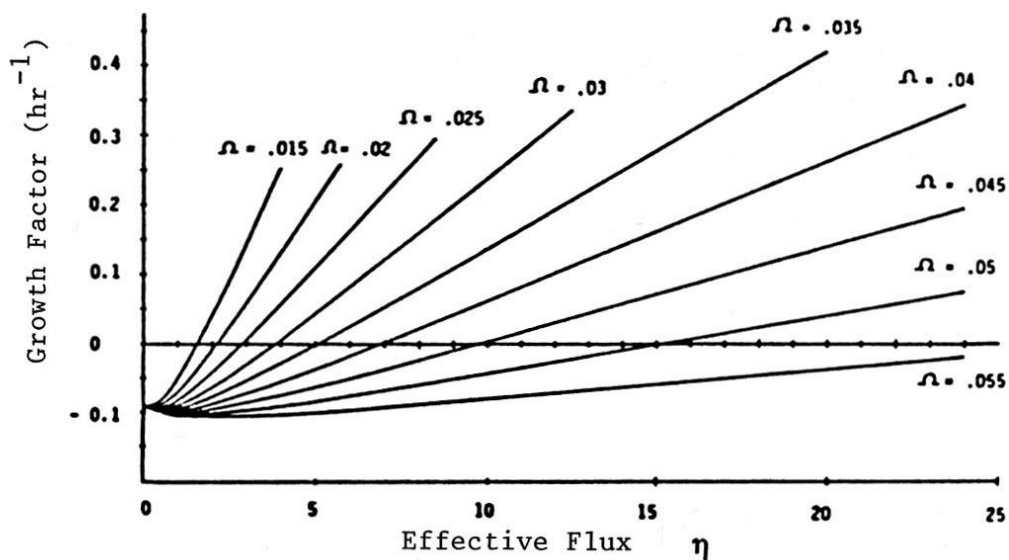
$$\eta = \frac{\sigma_{ax}}{\lambda_x} \frac{\int_{\text{core}} \phi_1^2 \sum_f \phi_0 dr}{\int_{\text{core}} \phi_1^2 \sum_f dr}. \quad (9.21)$$

The first-harmonic flux  $\phi_1$ , used in the calculation of  $\eta$ , is that flux shape corresponding to the *smallest* value of  $\lambda_0 - \lambda_1$ , which happens to be the first axial harmonic for a PWR and the first azimuthal harmonic for an HTR.

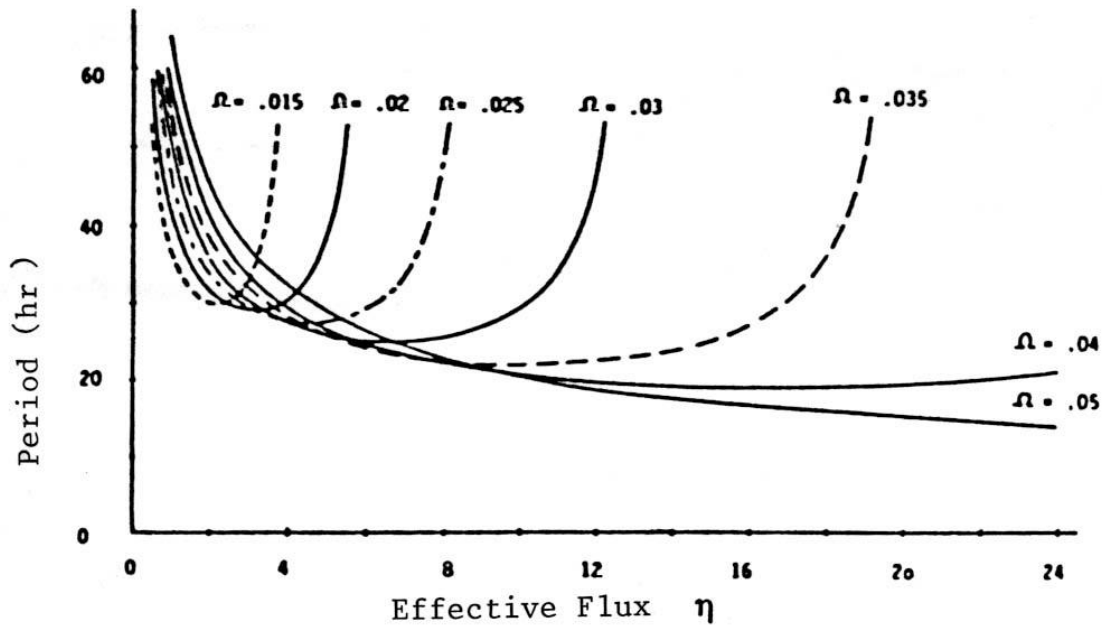
One sees that oscillations are initiated by increasing the effective power level ( $\eta$ ) for a given reactor, or by changing the susceptibility ( $\Omega$ ) by increasing the reactor dimensions and/or flattening the flux. The more peaked the flux distribution happens to be in the direction *perpendicular* to the direction of oscillation, the higher the value of  $\eta$  becomes for a given average power level, thus reducing the stability of the core against oscillations.

For a growing oscillation, the reactor operator *must* take control action at some point to safely stop the transient. From an optimal standpoint, the most effective action is not intuitively obvious because of the time lag built into the xenon and iodine equations. Qualitatively, control action should be taken just before the flux oscillation maximum is reached, and then in the direction of reducing the flux. The action should then be released as the oscillation crosses the null point.

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**Fig. 9.6** True Growth Factor vs.  $\eta, \Omega$  for a Reactor Loaded with Pure <sup>235</sup>U,  $\gamma_i = 0.0617$ ,  $\gamma_x = 0.0024$



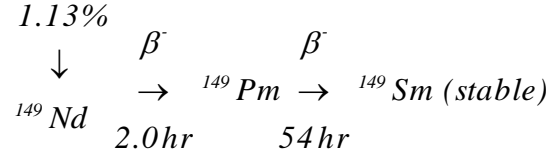
**Fig. 9.7** True Period vs.  $\eta, \Omega$  for a Reactor Loaded with Pure <sup>235</sup>U

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### 9.6 Samarium Poisoning

The fission product  $^{149}\text{Sm}$  is stable and has an average thermal neutron absorption cross section at 20°C of 58,500 barns.

The chain yield is only 1.13%, so that samarium is not as much a problem as xenon, but it is sufficiently important that its behavior must be considered. The Mass 149 chain is



Usually the neodymium is ignored, and promethium is assumed to be the direct product of fission. Using this assumption, the balance equations are

$$\frac{dP}{dt} = \gamma_p \Sigma_f \phi - \lambda_p P, \quad (9.22)$$

and

$$\frac{dS}{dt} = \lambda_p P - \sigma_{as} \phi S. \quad (9.23)$$

These equations are considerably simpler than the xenon equations. The equilibrium values are obtained by setting the derivatives to zero, so that production equals loss. The equilibrium values are

$$P_\infty = \frac{\gamma_p \Sigma_f \phi}{\lambda_p}, \quad (9.24)$$

and

$$S_\infty = \frac{\gamma_p \Sigma_f}{\sigma_{as}}. \quad (9.25)$$

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We immediately see that the maximum reactivity effect for a bare core is

$$\rho_{\text{samarium}}^{\infty} = \frac{(\phi^*, -\gamma_p \Sigma_f \phi)}{(\phi^*, \nu \Sigma_f \phi)} = \frac{-\gamma_p}{\nu} = -0.00463 \quad (9.26)$$

**General Solution for Constant Flux.** Taking Laplace transforms, the promethium equation becomes the following, using the initial condition  $P(0) = P_0$ :

$$s\bar{P}(s) - P_0 = \frac{\gamma_p \Sigma_f}{s} - \lambda_p \bar{P}(s),$$

or

$$\bar{P}(s) = \frac{P_0}{s + \lambda_p} + \frac{\gamma_p \Sigma_f \phi}{s(s + \lambda_p)}. \quad (9.27)$$

Hence, the time-dependent solution is

$$P(t) = P_0 e^{-\lambda_p t} + \frac{\gamma_p \Sigma_f \phi}{\lambda_p} (1 - e^{-\lambda_p t}). \quad (9.28)$$

The samarium equation becomes, using the initial condition  $S(0) = S_0$ ,

$$s\bar{S}(s) - S_0 = \lambda_p \bar{P}(s) - \sigma_{as} \phi \bar{S}(s),$$

or

$$\bar{S}(s) = \frac{S_0}{s + \sigma_{as} \phi} + \frac{\lambda_p P_0}{(s + \sigma_{as} \phi)(s + \lambda_p)} + \frac{\lambda_p \gamma_p \Sigma_f \phi}{s(s + \sigma_{as} \phi)(s + \lambda_p)}. \quad (9.29)$$

The time-dependent solution to this equation is

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$$\begin{aligned}
 S(t) = S_0 e^{-\sigma_{as}\phi t} + \frac{\lambda_p P_0}{(\lambda_p - \sigma_{as}\phi)} \{ e^{-\sigma_{as}\phi t} - e^{-\lambda_p t} \} \\
 + \frac{\gamma_p \Sigma_f}{\sigma_{as}} - \frac{\lambda_p \gamma_p \Sigma_f}{\sigma_{as}(\lambda_p - \sigma_{as}\phi)} e^{-\sigma_{as}\phi t} + \frac{\gamma_p \Sigma_f \phi}{(\lambda_p - \sigma_{as}\phi)} e^{-\lambda_p t}.
 \end{aligned}
 \tag{9.30}$$

As a check: at  $t = 0$ ,

$$S(0) = S_0, \text{ and } P(0) = P_0;$$

and at  $t = \infty$ ,

$$S_\infty = \frac{\gamma_p \Sigma_f}{\sigma_{as}} \text{ and } P_\infty = \frac{\gamma_p \Sigma_f \phi}{\lambda_p}.$$

For the samarium buildup problem after shutdown, let the flux go to zero to obtain the following equations:

$$P(t) = P_0 e^{-\lambda_p t}, \tag{9.31}$$

and

$$S(t) = S_0 + P_0(1 - e^{-\lambda_p t}). \tag{9.32}$$

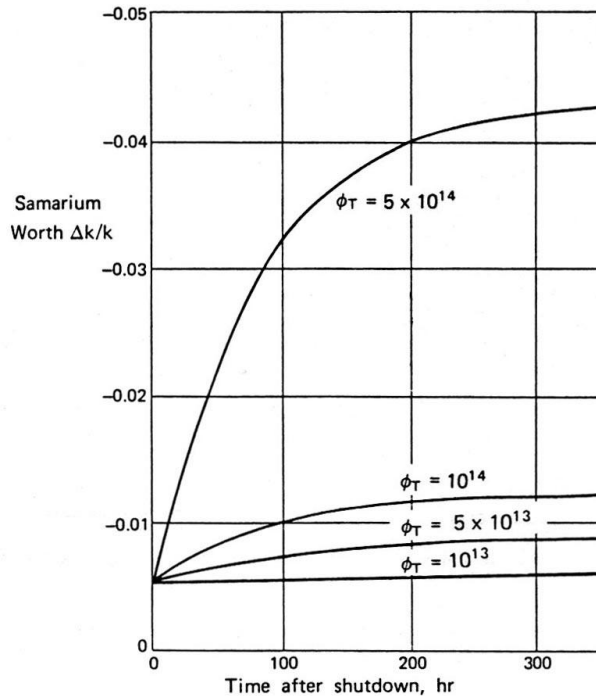
$S_0$  and  $P_0$  are obtained from the general solution just prior to shutdown.

After shutdown, all burnup of samarium ceases so that samarium simply builds up as the existing promethium decays. This means that there must always be sufficient reserve reactivity tied up in the control rods to override the samarium, so that one can restart the reactor and burn the samarium back to equilibrium levels. Fortunately, the reactivity tied up by samarium is not excessive. The approximate shutdown curve is shown in Figure 9.8. Note that the time scale is considerably longer than for xenon.



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As seen in the xenon discussion, the general solution to the samarium equations can also be used over discrete time steps, where the flux remains constant, to compute the samarium at any space point in the reactor. Thus, a spatial samarium transient can also be calculated numerically. Fortunately, the samarium equations do not lead to potential spatial power oscillations.



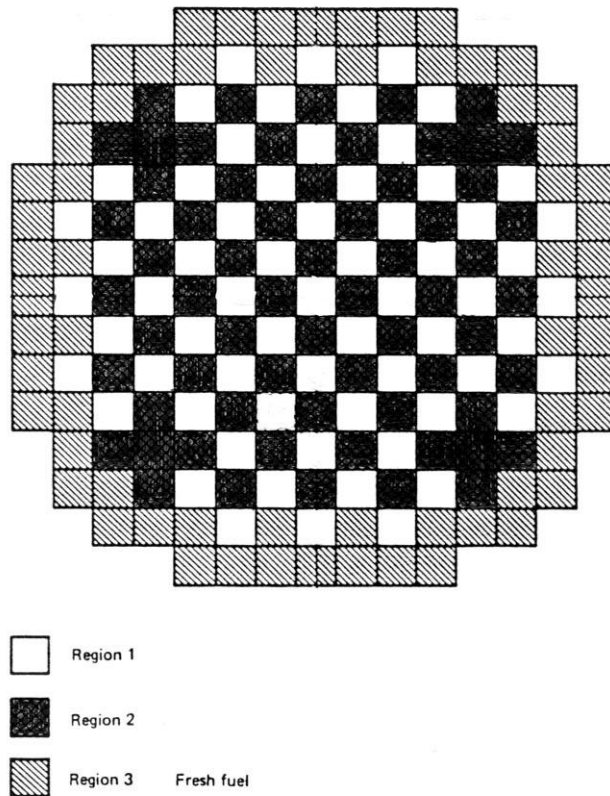
**Fig. 9.8** Samarium Buildup After Reactor Shutdown

### 9.7 Temperature Effects on Reactivity

Because of a desire to obtain a relatively high uniform burnup of the fuel in a nuclear reactor for economic reasons, and at the same time to avoid having "hot spots" where the local power production significantly exceeds the average power production, the fuel loading in power reactors is generally designed to be spatially non-uniform. The core is loaded in

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zones of varying enrichments of  $^{235}\text{U}$ , with the lowest enrichment usually being set in the center of the core where the thermal flux tends to be the highest. Modern fuel management schemes add new fuel on the periphery and scatter-load once- and twice-burned fuel in the center region. In any event, the power distribution is spatially non-uniform at the beginning-of-life of the core (BOL) and varies in a spatially non-uniform manner as the fuel depletes to end-of-life (EOL). A typical fuel-loading pattern is shown in Figure 9.9.



**Fig. 9.9** Scattered Fuel Loading Arrangement for a Three-Cycle Reactor.

The coolant usually enters at the bottom of the core at a temperature dependent upon external power demand, and flows

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upward through the fuel assemblies in separate flow channels, mixing in an upper plenum at the top of the core. There are sometimes even two separate passes through different parts of the core, with mixing in between passes. This implies that the temperature distribution of the coolant is also spatially non-uniform, and furthermore implies that the power distribution and the temperature distribution do not coincide.

If the fuel elements are composed of uranium dioxide rods, the temperature of the fuel rods will significantly exceed the temperature of the coolant because of the low thermal conductivity of the  $\text{UO}_2$ . For a given change in reactor power, the average temperature of the fuel rods could vary by a significantly greater degree than the coolant temperature and also vary much more rapidly because of the difference in specific heats.

We would like to be able to represent the reactivity effects of temperature or power changes in terms of coefficients of reactivity, since these effects are important feedback mechanisms that help determine the stability and dynamic behavior of the operating reactor to variations in power production. We usually speak of the moderator coefficient,  $\alpha_m(\Delta k/k/^\circ\text{F}_m)$ , the fuel or Doppler coefficient,  $\alpha_f(\Delta k/k/^\circ\text{F}_f)$ , and the power coefficient,

$$\alpha_p \equiv \alpha_m \partial T_m / \partial P + \alpha_f \partial T_f / \partial P \quad (\Delta k/k/MWT). \quad (9.33)$$

Although there has been a shift to SI units in some areas, English units are still commonly used in thermal reactor design and will be retained here.

The three most important mechanisms for instituting a reactivity change as a result of a temperature or power change are the following:

1. *Thermal expansion.* This effect is most prominent for the coolant, but also affects other materials to a

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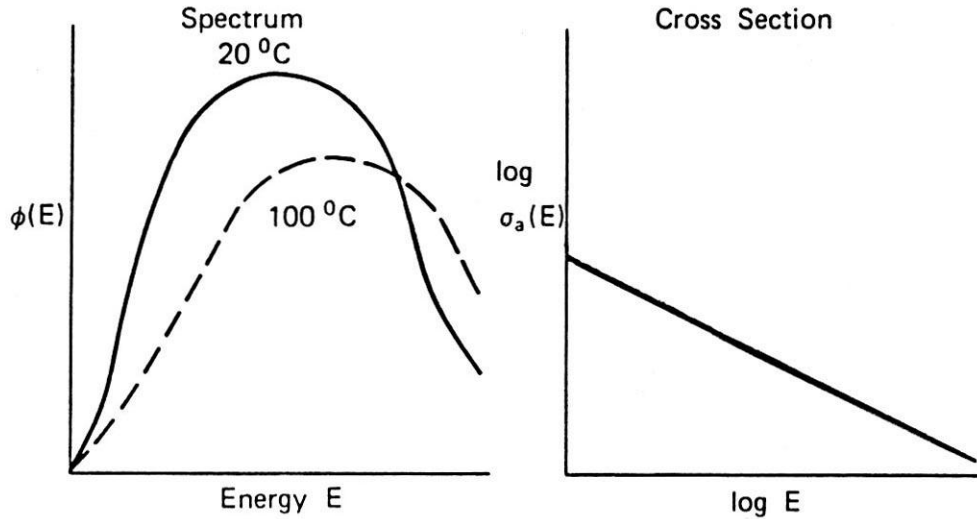
lesser extent. A change in volume density modifies the atom densities of all constituents and hence affects the macroscopic cross sections, i.e.,  $\delta\sigma N(T_m) \rightarrow \delta\Sigma(T_m)$ .

2. *Spectrum shift.* An increase of temperature increases the energy distribution of the vibrating atoms comprising the material. Since the cross sections at thermal energy are generally of the form  $\sigma_a(E) = \sigma_0 v_0/v$ , an upward shift in spectrum leads to a lower average cross section for the thermal group, i.e.,

$$\bar{\sigma}_a = \frac{\int_{\text{thermal}} \sigma_a(E) \phi(E) dE}{\int_{\text{thermal}} \phi(E) dE}.$$

This can be understood by examining Figure 9.10. Hence, we have a macroscopic cross-section variation due to temperature changes, namely,

$$N\delta\sigma(T_m) \rightarrow \delta\Sigma(T_m).$$

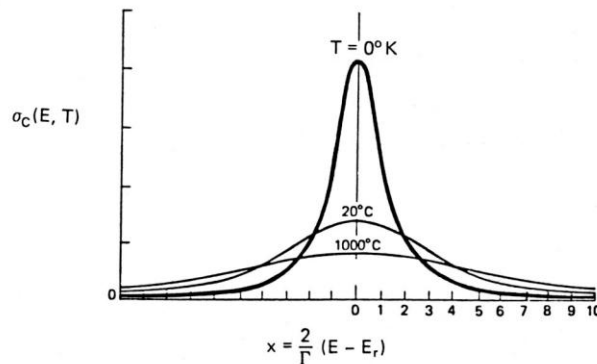


**Fig. 9.10** Thermal Spectra and Thermal Cross Sections

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3. *Doppler broadening of resonances*, with effects due to fuel lumping. Reaction rates are a function of the atom density, neutron density, cross section, and the relative velocity between the atom and the neutron, i.e.,  $v_r = |\vec{V} - \vec{v}|$ . When the reaction rate is averaged over the distribution function of atom velocities, in order to find the effective cross section that corresponds to the actual neutron flux, one finds that the effective cross section curve is broadened as temperature increases. This is shown in Figure 9.11.

In certain situations where the fuel is lumped, the net absorption rate can increase significantly with temperature. Note that this refers to the fuel temperature, which may be significantly different from the moderator temperature; even the rate of change of fuel temperature with time after a power change may be greater than that for the moderator. Hence, temperature coefficients have associated time constants, and may have to be treated as separate entities in reactor dynamics situations.



**Fig. 9.11** Illustration of Doppler Broadening with Temperature

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Since each of the three mechanisms leads to spatial changes in macroscopic cross sections in each energy group, we can in fact use our perturbation theory approach to properly average the spatial changes over the core to obtain a reactivity effect. This is one valid way to evaluate temperature coefficients, given the known temperature change in each part of the core and the corresponding cross section change. Another possible approach is to simply calculate the value of  $k_{\text{eff}}$  numerically for two separate reactors whose cross sections correspond to operation at two different temperatures (averaged over the core) or two different power levels. The appropriate temperature or power coefficient is then equal to the difference in  $k_{\text{eff}}$  values divided by the difference in average temperature or power values. The perturbation theory approach, when it can be implemented with existing computer codes, is the more accurate approach to use because the reactivity changes are generally small.

For a large commercial pressurized water reactor (PWR), typical values of the moderator coefficient,  $\alpha_m$ , are in the range of  $\alpha_m = \pm 3 \times 10^{-5} \Delta k/k/^\circ\text{F}_m$ . This is primarily a coolant density effect. The coefficient is usually positive at BOL because the water contains soluble poison such as boric acid, and thermal expansion leads to less absorber being present in the core. At EOL, when the poison concentration is low, the coefficient is negative because the primary effect is a variation in neutron moderation properties. The average temperature of the coolant is approximately 580°F, and the temperature rise across the core is typically 50°F. Therefore, a 10% change in reactor power corresponds to a reactivity insertion of about 2¢.

The fuel coefficient,  $\alpha_f$ , is typically in the range of  $\alpha_f = -1 \times 10^{-5} \Delta k/k/^\circ\text{F}_f$ . The actual amount of reactivity feedback depends upon how much the average fuel temperature changes, since this effect is related to Doppler broadening of resonances. The fuel temperature rise, in turn, depends upon the

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diameter of the  $\text{UO}_2$  pellets, so this is a design consideration. Needless to say, the power coefficient,  $\alpha_p$ , must always be negative in order to have a stable reactor system. Hence, the magnitude of the negative fuel feedback effect must be large enough to be able to overcome the possible positive moderator coefficient at BOL. It should also be noted that Doppler broadening of fission resonances will occur. In a reactor that contains highly-enriched uranium, this can potentially lead to a very small Doppler coefficient. This is an important design consideration.

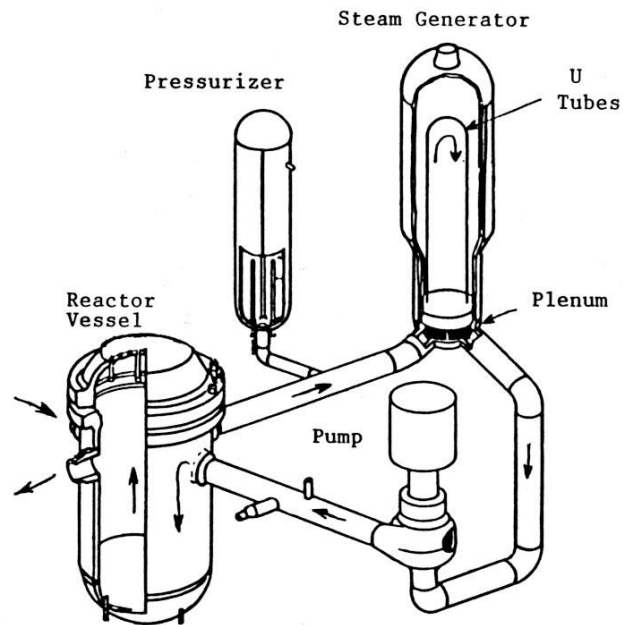
### 9.8 Effect of Thermal Feedback on Reactor Kinetics

When a reactor operates at a high power level, both Doppler and moderator temperature feedback come into play. The total reactivity driving the combined system becomes the sum of the externally applied control such as control rod motion and boron "shim" plus the thermal feedback. The important thing to notice is that the reactor kinetics equations become augmented by the heat balance equations. Furthermore, the external heat transfer in the steam generator must also be included, and possibly even the turbine equations. Hence, the order of the system of differential equations can become fairly large, especially if the reactor flux distribution is calculated using a spatially-dependent or nodal model.

A single loop of a typical PWR reactor system is shown in Figure 9.12. To fully model the system dynamically we need to write separate equations for the core, plenums, piping, pressurizer, steam generator tubes, etc., for each loop in the system, plus as much spatial detail in the core as desired. This is a formidable job. In earlier times, a very large analog computer would have been completely dedicated to this task for

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periods of months to years. Present practice involves the direct integration of coupled systems of perhaps hundreds of ordinary differential equations on a digital computer. A typical dynamics code of this type is the RETRAN code, which was developed for the Electric Power Research Institute (EPRI).



**Fig. 9.12** Pressurized water reactor coolant system

To illustrate the ideas involved, we consider a simplified reactor system where the reactor is described by the point kinetics equations with one group of delayed neutrons. We lump the fuel and calculate a single average fuel temperature. We lump the steam generator and let the secondary side be a simple power demand. The block diagram of this system is shown in Figure 9.13. The differential equations governing the system are the following:

- a. *Reactor Kinetics* (point kinetics, one group of precursors). Since the reactor power is proportional to the flux times the macroscopic fission cross



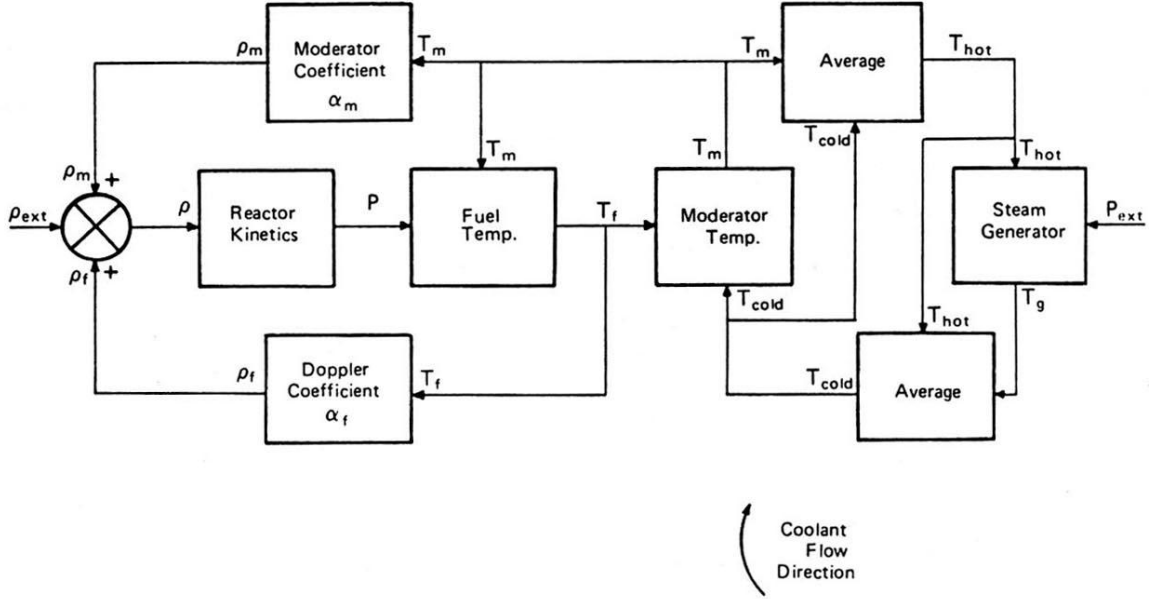
## NUCLEAR REACTOR THEORY AND DESIGN

section, we can write the point kinetics equations using the power  $P$  in place of the neutron density  $n$ . Hence, we have the kinetics equations

$$\frac{dP}{dt} = \frac{\rho - \bar{\beta}}{\Lambda} P + \lambda c, \quad (9.34)$$

and

$$\frac{dc}{dt} = \frac{\bar{\beta} P}{\Lambda} - \lambda c. \quad (9.35)$$



**Fig. 9.13** Block Diagram of a Simplified Reactor System with Thermal Feedback

- b. *Fuel Temperature,  $T_f$ .* Assume that the power is released only in the fuel and that we can characterize the fuel by an average fuel temperature. The balance equation then becomes

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$$\begin{array}{ccccc} \text{rate of} & \text{power} & \text{conduction} & & \\ \text{heat up} & \text{in} & \text{heat transfer} & & \end{array}$$

(9.36)

$$m_f c_f \frac{dT_f}{dt} = P - hA(T_f - T_m),$$

where  $m_f$  is the mass of fuel (lb),  $c_f$  is the specific heat of fuel (Btu/lb-°F), and  $A$  is the heat transfer area (ft<sup>2</sup>).

- c. *Moderator Temperature,  $T_m$ .* Assume that the heat is transferred from the fuel to the coolant, which is then moved by convection out of the core. We lump all of the coolant in the core and give it an average temperature  $T_m$ , and consider separately the inlet temperature,  $T_{cold}$ , and the outlet temperature,  $T_{hot}$ . The balance equation is

$$\begin{array}{ccccc} \text{rate of} & \text{conduction} & \text{convection} & & \\ \text{heat up} & & \text{out} & & \end{array}$$

(9.37)

$$m_m c_m \frac{dT_m}{dt} = hA(T_f - T_m) - W c_m (T_{hot} - T_{cold}).$$

where  $m_m$  is the mass of moderator in the reactor and  $c_m$  is the specific heat. The quantity  $W$  is the coolant mass flow rate in lb/hr. We also need the definition of the average temperature, which is

$$T_m = \frac{T_{hot} + T_{cold}}{2}. \quad (9.38)$$

- d. *Steam Generator,  $T_g$ .* Assume a simplified steam generator, where the steam side simply acts as an external load demand,  $P_{ext}$ . In this case the balance equation is

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$$\begin{array}{ccc} \text{rate of} & \text{convection} & \text{external} \\ \text{heatup} & \text{in} & \text{demana} \end{array}$$

(9.39)

$$m_g c_g \frac{dT_g}{dt} = W c_g (T_{hot} - T_{cold}) - P_{ext},$$

where  $m_g$  is the mass of coolant in the steam generator and  $c_g$  is its specific heat. We again need an average temperature definition, which is

$$T_g = \frac{T_{hot} + T_{cold}}{2}. \quad (9.40)$$

- e. *Piping.* Due the finite transit time of coolant flowing through the pipes, it may take from 2 to 15 seconds for a temperature change in the reactor or steam generator to be felt by the other. If we ignore this factor, we see that the average reactor and steam generator temperatures must be identical, so that we can effectively lump the mass of coolant in the reactor and steam generator together and treat them as one. If this approximation is not valid, then the actual time delay must be used or it must be approximated by another differential equation.
- f. *Reactivity Feedback* from reference temperatures  $T_{fo}$  and  $T_{mo}$ . The temperature coefficient is defined as the change in reactivity per degree change in temperature. Hence, we must compute the temperature change from a reference point. We take this point to be the steady state, hot, critical, at-power situation. Hence, the reactivity expression becomes

$$\rho = \rho_{ext} + \alpha_f (T_f - T_{fo}) + \alpha_m (T_m - T_{mo}). \quad (9.41)$$

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The above simplified lumped system model contains four ordinary differential equations plus some algebraic equations, all coupled together. In order to solve this system, we need a set of initial conditions, which we take to be the steady state operating point.

**Steady State.** Steady state is the condition where all time derivatives are zero. We append a subscript of zero to each variable to denote this state. The reactor steady state equations become

$$\frac{\rho_0 - \bar{\beta}}{\Lambda} P_0 + \lambda_{c0} = 0, \quad (9.42)$$

and

$$\frac{\bar{\beta}}{\Lambda} P_0 - \lambda_{c0} = 0. \quad (9.43)$$

The steady state condition obtained from the above equations is that

$$\rho_0 = 0, \quad (9.44)$$

i.e., there is *no reactivity* when the system is *critical*.

Looking at the feedback equations, we have

$$\rho_0 = \rho_{ext0} + \alpha_f(T_{f0} - T_{fo}) + \alpha_m(T_{m0} - T_{mo}). \quad (9.45)$$

Hence, by setting the reference for the feedback terms at the steady state values, we obtain the fact that  $\rho_{ext0} = 0$ . If another reference point had been chosen, then the external reactivity term would have had to balance this feedback.

For the fuel temperature, moderator temperature, and steam generator temperature, we have the equations

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$$P_0 - hA(T_{fo} - T_{mo}) = 0,$$

$$hA(T_{fo} - T_{mo}) - Wc_m(T_{hot0} - T_{cold0}) = 0,$$

and

$$Wc_g(T_{hot0} - T_{cold0}) - P_{ext0} = 0.$$

Hence, since  $c_m = c_g$ , we conclude that the power produced just equals the power demanded, i.e.,

$$P_0 = P_{ext0}. \quad (9.46)$$

**Incremental System Equations.** Rather than deal with the actual system equations which have a set of given initial conditions, it is often easier to deal with equations describing the *variations* from an initial state, having zero initial conditions. Furthermore, although not completely obvious, the system of equations as given is nonlinear. We have the product  $\rho P$  appearing in the neutron balance, but since  $\rho$  is a function of  $T_f$  and  $T_m$ , which are functions of  $P$  in turn, we have a nonlinear product. However, if the variations about the steady state are not large, the system is approximately linear and we can formally linearize it.

We expand all variables about their steady state values. We have

$$\delta P_{ext} = P_{ext} - P_{ext0}.$$

and

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$$\begin{aligned}
 \delta T_f &= T_f - T_{fo}, \\
 \delta T_m &= T_m - T_{mo}, \\
 \delta P &= P - P_0, \\
 \delta c &= c - c_0, \\
 \delta \rho &= \rho - \rho_0 = \rho, \\
 \delta T_g &= T_g - T_{go},
 \end{aligned} \tag{9.47}$$

Formally, we subtract the steady state balance equations from the differential equations to obtain a set of equations entirely in the incremental variables. Since the time derivative of a steady state quantity is zero, we obtain the incremental reactor equations

$$\frac{d(\delta P)}{dt} = \frac{P_0 \delta \rho}{\Lambda} - \frac{\bar{\beta}}{\Lambda} \delta P + \lambda \delta c, \tag{9.48}$$

and

$$\frac{d(\delta c)}{dt} = \frac{\bar{\beta}}{\Lambda} \delta P - \lambda \delta c. \tag{9.49}$$

The nonlinear term is treated by expanding the product  $\rho P$  and ignoring second-order terms, i.e., by letting

$$\begin{aligned}
 \rho P &= (\rho_0 + \delta \rho)(P_0 + \delta P) \\
 &= \rho_0 P_0 + \rho_0 \delta P + P_0 \delta \rho + \delta \rho \delta P \\
 &\approx P_0 \delta \rho,
 \end{aligned} \tag{9.50}$$

because  $\rho_0 = 0$ .

The incremental fuel temperature equation becomes

$$m_f c_f \frac{d(\delta T_f)}{dt} = \delta P - hA(\delta T_f - \delta T_m). \tag{9.51}$$

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Since there is no time delay in the pipes,  $\delta T_m = \delta T_g$ , which can be obtained from a single differential equation that lumps the mass of coolant in the reactor and steam generator together. The resulting differential equation for the incremental water temperature is

$$(m_m + m_g)c_m \frac{d(\delta T_m)}{dt} = hA(\delta T_f - \delta T_m) - \delta P_{ext} , \quad (9.52)$$

Finally, the incremental feedback equation becomes

$$\delta \rho = \delta \rho_{ext} + \alpha_f \delta T_f + \alpha_m \delta T_m . \quad (9.53)$$

To summarize, after linearization we have a coupled set of four inhomogeneous first-order ordinary differential equations with constant coefficients. All of the incremental variable initial conditions are zero. We know the values of  $P_0$  (the operating point),  $\delta \rho_{ext}$  (the inhomogeneous term representing operator control), and  $\delta P_{ext}$  (the inhomogeneous term representing externally supplied load variations). We seek values for the variables  $\delta P$ ,  $\delta c$ ,  $\delta T_f$ , and  $\delta T_m = \delta T_g$ , plus the auxiliary variables  $\delta T_{hot}$  and  $\delta T_{cold}$  that are algebraically related to the primary variables.

The linear system indeed possesses a solution, and furthermore the solution is given as the sum of four exponential factors corresponding to the homogeneous solutions of the set of equations. A sufficient condition for system stability is that the real parts of all of the exponentials must be negative so that the corresponding incremental solutions decay with time. The entire set of equations can be put into the vector-matrix form

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$$\dot{\underline{X}} = \underline{B}\underline{X} + \underline{D}\underline{u}, \quad (9.54)$$

which is recognized to be the general State Variable form for a controlled dynamic system. The state vector and the control vector are defined as

$$\underline{X} \equiv \begin{bmatrix} \delta P \\ \delta c \\ \delta T_f \\ \delta T_m \end{bmatrix}, \quad \underline{u} \equiv \begin{bmatrix} \delta \rho_{\text{ext}} \\ \delta P_{\text{ext}} \end{bmatrix}.$$

The system matrix is defined as the 4 x 4 square matrix

$$\underline{B} \equiv \begin{bmatrix} -\frac{\bar{\beta}}{\Lambda} & \lambda & \frac{P_0 \alpha_f}{\Lambda} & \frac{P_0 \alpha_m}{\Lambda} \\ \frac{\bar{\beta}}{\Lambda} & -\lambda & 0 & 0 \\ \frac{1}{m_f c_f} & 0 & -\frac{hA}{m_f c_f} & \frac{hA}{m_f c_f} \\ 0 & 0 & \frac{hA}{(m_m + m_g) c_m} & \frac{-hA}{(m_m + m_g) c_m} \end{bmatrix},$$

and the control matrix is defined as the 4 x 2 non-square matrix

$$\underline{D} \equiv \begin{bmatrix} \frac{P_0}{\Lambda} & 0 \\ \Lambda & 0 \\ 0 & 0 \\ 0 & -1 \\ 0 & \frac{1}{(m_m + m_g) c_m} \end{bmatrix}.$$

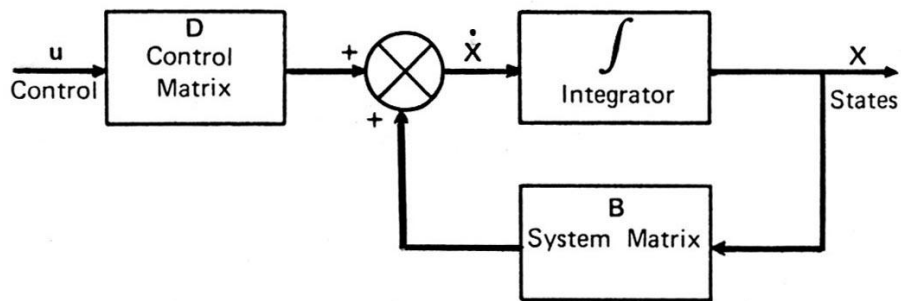
The entire system can be symbolically pictured using a feedback control diagram, as shown in Figure 9.14, where the heavy lines represent the fact that the interconnections are vectors.

The solution can be obtained by analog computer, digital computer, or in this case by analytic means. When the equations have constant coefficients, as they do here, the solutions are given as a sum of exponentials. For system stability, which is



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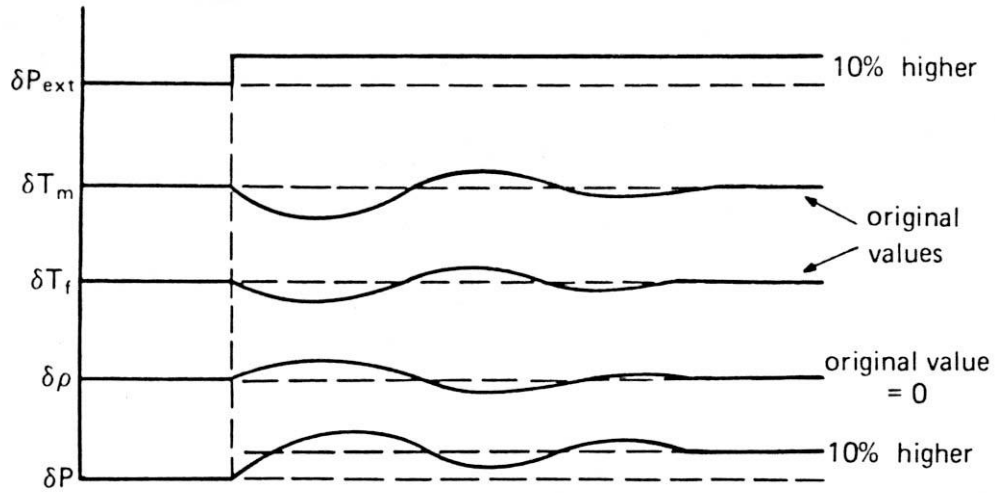
the condition that the system returns to steady state after a small perturbation, it is sufficient that the exponentials all have negative real parts. We can find these exponents by looking at the system matrix  $\underline{\underline{B}}$ . Specifically, we look for the eigenvalues of the  $\underline{\underline{B}}$  matrix by setting the determinant  $|\underline{\underline{B}} - \omega \underline{\underline{I}}| = 0$ . If  $\underline{\underline{B}}$  is an  $n$ th-order matrix, we obtain a polynomial of degree  $n$  in the variable  $\omega$ , whose solutions are the exponents,  $\omega_i$ ,  $i = 1, n$ . That is, we obtain the form  $(\omega - \omega_1)(\omega - \omega_2)(\omega - \omega_3) \cdots (\omega - \omega_n) = 0$ . Suffice it to say that in the present case, the condition for stability reduces to requiring that the overall power coefficient of reactivity,  $\alpha_p$ , be negative.



**Fig. 9.14** State Variable Feedback Control System

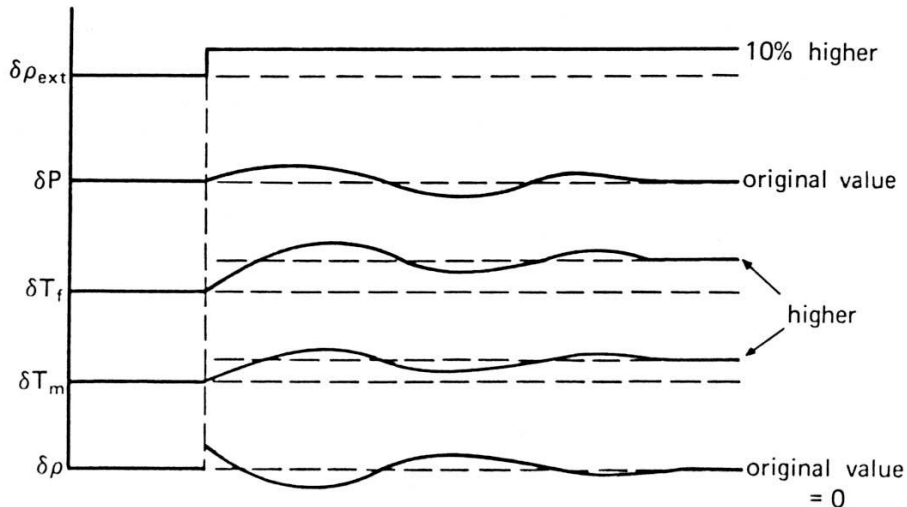
We illustrate the response of our stable reactor system to a step load increase, and also to a step positive increase in reactivity brought about by operator control, by means of diagrams of the incremental system response vs. time. For the step load increase we have the situation shown in Figure 9.15. As a result of the increased power demand, the temperatures are temporarily decreased causing a positive reactivity feedback and subsequent increased reactor power production. There is an overshoot, followed by a period of settling down, until eventually the reactor produces 10% more power, as demanded.

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**Fig. 9.15** Response to a 10% Step Increase in  $P_{\text{ext}}$

For the step increase in external reactivity, we have the situation shown in Figure 9.16. As a result of the increased external reactivity, the reactor power increases temporarily, until the fuel and coolant temperatures rise sufficiently to produce enough temperature feedback to balance the external reactivity. The system eventually settles down at the higher temperatures and continues to produce the original amount of power.



**Fig. 9.16** Response to a 10% Step Increase in  $\rho_{\text{ext}}$

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Instead of using the vector-matrix approach, the system of linear equations can also be solved using the technique of Laplace transforms. The algebraic ratio between an output variable and its corresponding input variable in the  $s$  domain is known as the Transfer Function. If the Laplace variable  $s$  is replaced by the variable  $i\omega$ , where  $i$  is the imaginary number and  $\omega$  is an angular frequency, then we obtain what is known as the "frequency domain". Transfer functions are often measured by supplying sinusoidal system excitation at a range of frequencies, or by applying autocorrelation or cross correlation operations to systems that are excited by random noise. Unfortunately, the resulting frequency response diagrams are often difficult to interpret.

It should be pointed out that the State Variable technique is the modern computational version of the analog computer approach. Solutions are obtained in the "time domain", i.e., we see the direct response of the system to a system perturbation. The connection between a given output variable and its corresponding input variable is a type of "transfer function" between the two, which is actually a convolution integral. The State Variable approach is also amenable to direct digital computer application of the ideas of optimal control. At present, it is the preferred method of solution of dynamic systems problems.

### 9.9 Depletion

Depletion is the process whereby fuel atoms are consumed and other atom species are produced. It is composed of two quite distinct aspects. The first one deals with the burnup of fissile atoms of uranium and plutonium, plus the production of new fissile atoms from fertile atoms of thorium, uranium, and

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plutonium. The total number of such atom species to be followed is of the order of ten. The second aspect is the treatment of the hundreds of radioactive fission products produced in fission.

In principle, depletion calculations are nothing more than repeated solutions of coupled sets of ordinary differential equations similar to the xenon and samarium equations. Each chain may have up to six or seven members, with various cross-links and direct fission yields. These equations are amenable to vector-matrix techniques and solution by digital computer. One such commonly used computer code is called ORIGEN; it is very useful for calculating the average amounts of different atoms for the purpose of evaluating the magnitude of the waste disposal problem for a given reactor.

Unfortunately, core depletion is a spatially-dependent problem. Typical cores may be depleted over tens of thousands of individual volume regions. Naturally, it would be very costly to solve hundreds of equations, thousands of times per depletion step. A compromise must be made. What is usually done is to solve the relevant burnup and production equations for the fissile and fertile species, plus a few of the important fission product chains such as xenon and samarium, plus equations for burnable poisons such as boron. All of the other fission products are lumped into one or two effective "gross fission product" equations. This brings the number of equations solved per reactor volume region down to the order of fifteen.

In order to fully appreciate the magnitude of the depletion problem, a brief description of the important factors is in order. More is involved than just calculating the buildup of some nuclides and the burnout of others; to the extent that the relative distribution of absorbers varies with time, the detailed spectrum of neutrons varies, which affects the averaging process used to obtain the macroscopic cross sections. Furthermore, we operate with the constraint that the reactor remains critical and

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produces a constant amount of power. This implies corrective control rod motion as a function of time, and also implies that the flux level must rise as the amount of remaining fuel decreases. One must also take into account the process by which the original fuel pin cells were homogenized to obtain the cross sections for the volume regions used in the diffusion calculation. This means that fuel pin self-shielding as a function of depletion must be correctly treated.

The larger the core, the more sensitive it is to spatial flux shifts caused by control rod motion and depletion. If the control rods are moved into the core center, the flux balloons to the outside. If the rods are kept in the top of the core, the flux peaks in the bottom. And if the control rods are moved into the bottom of the core, the flux moves up towards the top. Depending upon where the flux peaks, the burnup is a maximum, and so on.

As seen from the above considerations, the flux at any given point in the reactor is far from being constant with respect to time. Furthermore, since depletion is an initial value problem, small errors made early in the calculation may compound each other to create large errors at the end of the calculation. In the early days of commercial reactor design, the error in a depletion calculation at end-of-life (EOL) could have been as large as several hundred percent. In fact, by making an appropriate three-dimensional solution (synthesis method) and properly simulating control rod motion, recent depletion calculations have been carried out that predict the operating history of a prototype reactor to a very high degree of accuracy.

One sometimes discusses the accuracy in terms of a few inches difference in predicted and actual control rod positions near the end of core life.

In order to mathematically state the entire depletion problem, we must quantify the constraints and the various

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depletion equations that make up our problem. The criticality equation is simply the static reactor balance equation,

$$L(\vec{r}, t)\phi(\vec{r}, t) = \frac{1}{\lambda_0} M(\vec{r}, t)\phi(\vec{r}, t),$$

where  $\lambda_0 = 1.000$  for criticality. Embedded within the flux calculation is the control rod position iteration to maintain criticality, and the power normalization which is proportional to the total fission rate in the reactor from all fissile materials present, e.g.,

$$Power \propto \int_{\text{volume}}^{\text{Reactor}} \{ N_{25}(\vec{r}) f \sigma_{f25}^T \phi(\vec{r}) + N_{49}(\vec{r}) f \sigma_{f49}^T \phi(\vec{r}) + N_{41}(\vec{r}) f \sigma_{f41}^T \phi(\vec{r}) \} d\vec{r}. \quad (9.55)$$

Here, the quantity  $\mathbf{f}$ , which is *symbolically* included in the cross-section vector, is a self-shielding factor that indicates that not all of the atoms are available on an equal basis to cause fission. The self-shielding factor is time-dependent to the extent that as the outer layers of a self-shielded poison deplete, the neutrons can penetrate further into the lump. Judicious use of lumping can in fact allow us to tailor the depletion history at a given location in the core within certain limits. A detailed discussion of self-shielding factors and a practical prescription for including them in a depletion calculation appears in the *Naval Reactors Physics Handbook*.

Using the subscript a for absorption and the subscript c for radiative capture, and retaining the individual self-shielding factors, we can write the balance equations for the U-235 and U-238 chains at any spatial position as:

U-235 Chain,  $^{235}\text{U}$ ,

$$\frac{dN_{25}}{dt} = -N_{25} f \sigma_{a25}^T \phi \quad (9.56)$$

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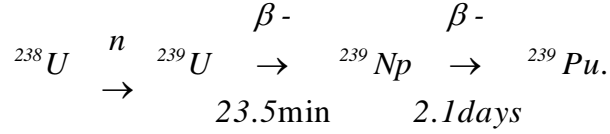
and  $^{236}\text{U}$ ,

$$\frac{dN_{26}}{dt} = -N_{26}f\sigma_{a26}^T\phi + N_{25}f\sigma_{c25}^T\phi. \quad (9.57)$$

U-238 Chain,  $^{238}\text{U}$ ,

$$\frac{dN_{28}}{dt} = -N_{28}f\sigma_{a28}^T\phi. \quad (9.58)$$

Assuming essentially direct production of  $^{239}\text{Pu}$ , by ignoring the short double  $\beta^-$  decay process which follows the scheme



we obtain the additional equations:

$^{239}\text{Pu}$ ,

$$\frac{dN_{49}}{dt} = -N_{49}f\sigma_{a49}^T\phi + N_{28}f\sigma_{c28}^T\phi \quad (9.59)$$

$^{240}\text{Pu}$ ,

$$\frac{dN_{40}}{dt} = -N_{40}f\sigma_{a40}^T\phi + N_{49}f\sigma_{c49}^T\phi. \quad (9.60)$$

and  $^{241}\text{Pu}$ ,

$$\frac{dN_{41}}{dt} = -\lambda_{41}N_{41} - N_{41}f\sigma_{a41}^T\phi + N_{40}f\sigma_{c40}^T\phi. \quad (9.61)$$

We must add to the above equations the effects due to the insertion of lumped burnable poisons (LBP) such as  $^{10}\text{B}$ , namely, the poison depletion equation

$$\frac{dN_B}{dt} = -N_Bf\sigma_{aB}^T\phi. \quad (9.62)$$

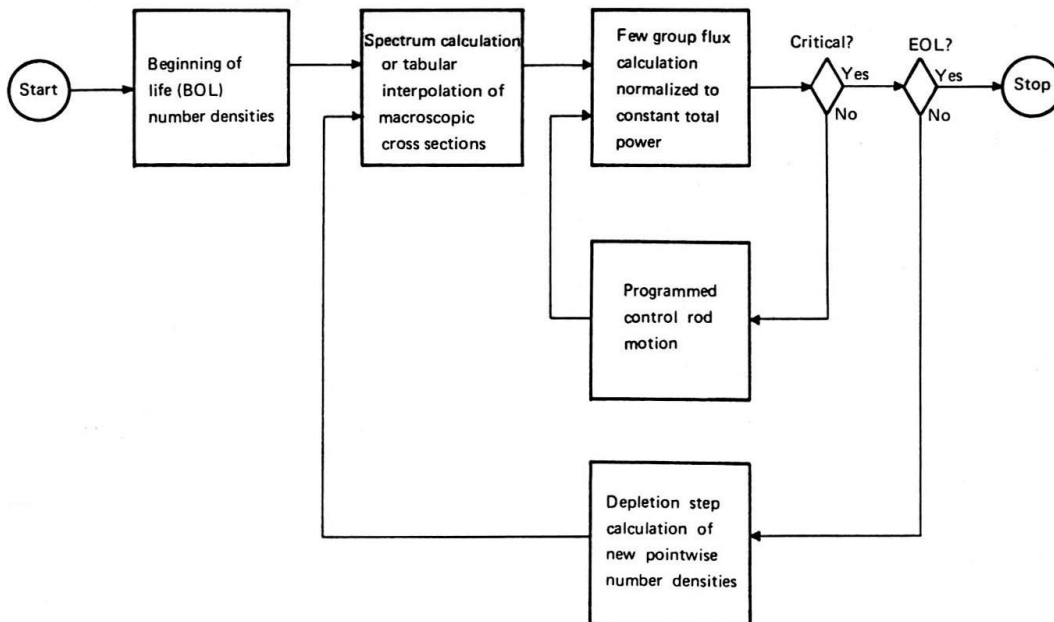
And finally, we must add equilibrium xenon and samarium as

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derived previously, plus some prescription to account for the gross buildup of a myriad of fission products which have, on the average, a 50 barn cross section per atom.

The above set of equations is not difficult to solve numerically over a time step of a few days to a few weeks, assuming that the flux is constant over the interval. The primary problem is that the equations must be solved separately over each spatial region in the core. Then, when the depleted number densities are obtained, new macroscopic cross sections must be computed so that the flux calculation can be repeated to obtain the flux and control rod positions for use in the next depletion step, and so on. The process is symbolically shown in Figure 9.17.

Unfortunately it is impractical to repeat the fast and thermal spectrum calculations for each of the thousands of volume regions in the reactor. Therefore, spectra are pre-calculated for typical mixtures of water, cladding, fuel enrichments, etc.



**Fig. 9.17** Block Diagram of Depletion Calculations



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These calculations are then fit by multi-parameter least squares techniques, such that all of the various region-wise few-group macroscopic cross sections can be interpolated for compositions in-between those calculated. Typical fitting parameters are: 1) fraction of  $^{235}\text{U}$  remaining in the fuel; 2) fuel-to-water ratio; and roddeed or unroddeed condition, etc.

During the entire depletion history of the core, any operating limits that have been imposed on the design must never be exceeded. Such limits are:

1. *Thermal-Hydraulic*. Peak fuel or cladding temperatures, or local boiling percentages must not be exceeded;
2. *Metallurgical*. Radiation damage to cladding or structural materials must not approach failure limits;
3. *Ceramic*. Radiation damage, thermal cycling, and fission gas production must not interrupt the integrity of the oxide, carbide, etc., compounds used as fuels.

These considerations imply that detailed thermal-hydraulic calculations must be done at each depletion step to check for hot spots, etc. We need detailed spatial power distributions for this work, and these must be culled from the flux solution performed at each depletion step. If limits are exceeded, the fuel distribution or control rod program must be modified to correct the problem. Likewise, gross accumulated irradiation histories must be kept and evaluated to check for potential materials problems. The appearance of such problems would also require design modifications. Needless to say, the design of a reactor with significant depletion is not a trivial problem.

**Fuel Management.** Superimposed upon the depletion calculation is the question of how to initially pick the core fuel loading, and after burnup begins, how to shift fuel in such

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a way as to obtain relatively uniform fuel burnup. Ideally, each fuel element should last exactly as long as all the others, regardless of where in the core it is placed. This would minimize the fuel costs. In addition, we would like each fuel assembly to reach the end of its useful life on a convenient schedule such as a year, or a year-and-a-half, etc. Table 9.1 shows the components of the design  $k_{\text{eff}}$  at Beginning-of-life (BOL).

We attain our objectives by proper fuel management. Typically, we load the core in three separate enrichment zones, with the highest enrichment in the outer region and the lowest in the center. A typical sequence of enrichments for a PWR would be 3%, 2.5% and 2%. The effect of this placement is to flatten the flux shape and the radial power distribution, except near the outer edge of the core where the boundary conditions force the flux to go to zero.

**Table 9.1**

PWR Design Reactivity at BOL

Reactivity Source	Value
Critical Condition	1.000
Depletion to Next Refueling	0.05 to 0.08
Temperature Swing, Cold to Hot	0.02 to 0.05
Power Swing, 0% to 100%	0.01 to 0.02
Xenon and Samarium Poisoning	0.025 to 0.03
Xenon Shutdown Override	0.01 to 0.02
Total $k_{\text{eff}}$ at BOL	1.115 to 1.120

After one burnup period of perhaps a year, the central zone fuel assemblies are removed, the outer fuel assemblies are moved to the second zone, and new fuel is placed in the outer zone. If we recognize that not all of the inner assemblies are uniformly

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burned, then we can scatter load them in their respective zones to optimize the subsequent burnup. If the reloading scheme is properly done, the core will eventually reach an equilibrium cycle where subsequent refueling will lead to identical burnup patterns.

In closing, it should be noted that even small gains in the uniformity of fuel burnup can translate to millions of dollars in reduced fuel costs. Therefore, there is a very strong incentive for Utilities to optimize their fuel management procedures.

### Problems

**9.1** Assume that  $^{135}\text{I}$  has a thermal neutron absorption cross section of  $\sigma_{aI} = 1 \times 10^6$  barns.

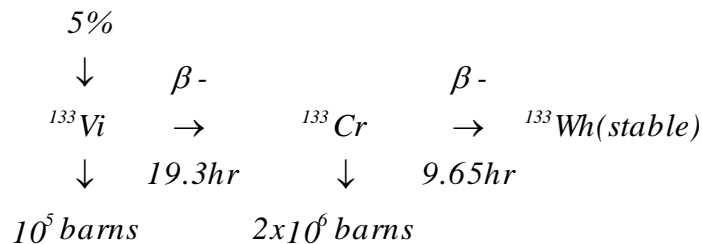
- a) Write the differential equations governing iodine and xenon in this case.
- b) Write a general expression for the equilibrium reactivity worth of the mass-135 chain.
- c) In the high flux limit, say  $\phi \approx 10^{15}$  n/cm<sup>2</sup>-s, what is the total reactivity worth of this chain. Let  $\gamma_x = 0.3\%$ ,  $\gamma_I = 6.1\%$ ,  $\nu = 2.42$ , and  $\beta = 0.0075$ .
- d) If the reactor is shut down from the equilibrium condition, write expressions for the xenon and iodine concentrations as a function of time after shutdown.

**9.2** A reactor has been operating at a constant flux level for a week.

- a) Derive an expression for the time  $t_{\max}$  at which peak xenon will be reached after shutdown.
- b) Show that  $t_{\max}$  is of the order of 11 hours for a range of flux levels between  $10^{12}$  and  $10^{15}$  n/cm<sup>2</sup>-s in a reactor fueled with  $^{235}\text{U}$ .

## NUCLEAR REACTOR THEORY AND DESIGN

- 9.3** The fictitious fission product Virginium ( $^{133}\text{Vi}$ ) is produced with a direct yield of  $\gamma_v = 5\%$  and decays with a 19.3-hr half-life ( $\lambda_v = 10^{-5} \text{ s}^{-1}$ ) to Cavalierium ( $^{133}\text{Cv}$ ). Cavalierium has an average thermal neutron absorption cross section of  $\sigma_{ac} = 2 \times 10^6$  barns and also decays but with a shorter 9.65-hr half life ( $\lambda_c = 2 \times 10^{-5} \text{ s}^{-1}$ ) to Wahooium ( $^{133}\text{Wh}$ ), which is stable. Virginium, unfortunately, also has a very high thermal neutron absorption cross section of  $\sigma_{av} = 10^5$  barns.

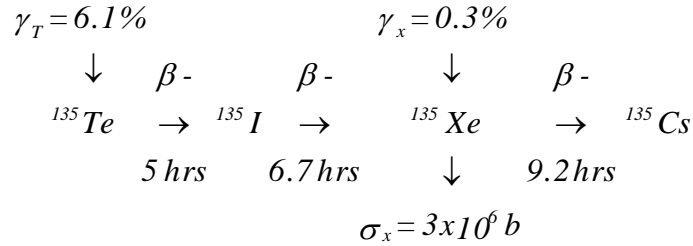


If the reactor is infinitely large and operates at an average thermal flux level of  $10^{14} \text{ n/cm}^2\text{-s}$ , answer the following:

- a) Write differential equations governing the number densities of  $^{133}\text{Vi}$  and  $^{133}\text{Cv}$  as a function of time.
  - b) Write an expression for the equilibrium reactivity worth of this chain and obtain an approximate numerical value for  $\rho_\infty$ .
  - c) If the reactor is shut down from equilibrium operation at the given flux level, what is the peak reactivity worth of this fission product chain.
- 9.4** Assume that the  $A = 135$  Chain for  $^{235}\text{U}$  fission starts with Tellurium, and that the half life of Tellurium is 5 hours instead of the actual value of 0.5 m. Iodine is formed exclusively by the decay of Tellurium, and the capture cross

# **NUCLEAR REACTOR THEORY AND DESIGN**

section of Tellurium is negligible. Take  $\Sigma_f = 0.05 \text{ cm}^{-1}$ .



Answer the following:

- a) Find an expression for the equilibrium reactivity worth of the  $A = 135$  chain in the high flux limit.
- b) Find the solution for  $X(t)$  after reactor shutdown from a steady state flux level of  $5 \times 10^{13} \text{ n/cm}^2\text{-s}$ . Plot this solution and compare with the solution given in Figure 9.1.

**9.5\*** You are given the xenon oscillation data shown in the accompanying figure for a core which uses  ${}^{235}\text{U}$  as fuel. Assume that the core is one-dimensional, has uniform properties everywhere and is describable by one group diffusion theory.

The core has the following parameters:

$$k_\infty = 1.06$$

$$L^2 = 60 \text{ cm}^2$$

height = 300 cm including extrapolation

$$\nu = 2.42$$

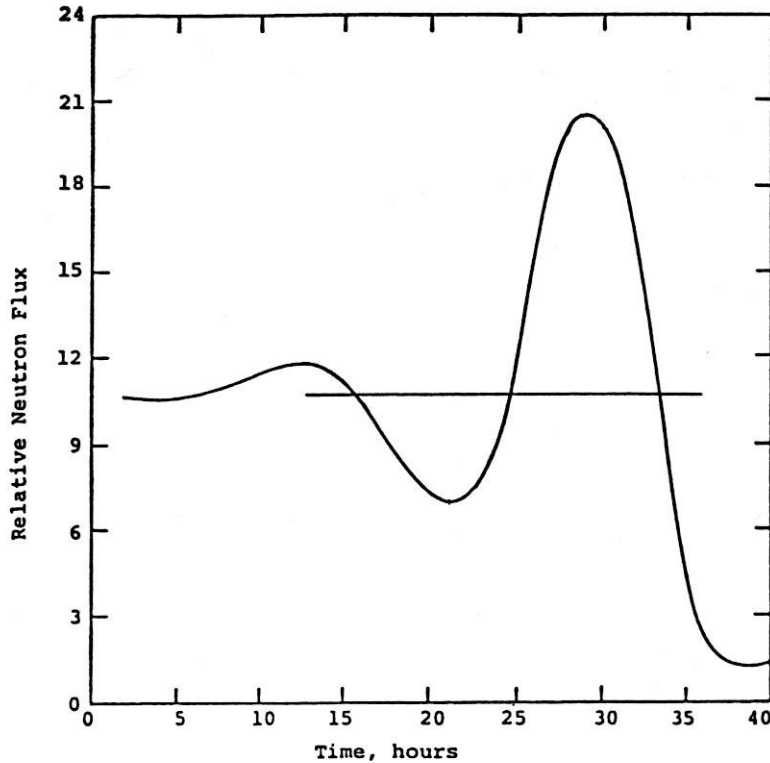
$$\sigma_x = 3 \times 10^6 \text{ barns}$$

$$\lambda_x = 2.1 \times 10^{-5} \text{ s}^{-1}$$

$$c = 3 \times 10^{10} \text{ fissions/s-watt}$$

For this core, find the dimensionless effective flux level  $\eta$ , the average flux ( $\text{n/cm}^2\text{-s}$ ) and the average power density  $Q'''$  ( $\text{watts/cm}^3$ ).

## NUCLEAR REACTOR THEORY AND DESIGN



- 9.6 Discuss the various factors that would tend to make the effects of equilibrium xenon and samarium differ in reactors fueled with  $^{233}\text{U}$ ,  $^{235}\text{U}$ , and  $^{239}\text{Pu}$ . For a flux of  $\phi = 5 \times 10^{13}$  n/cm<sup>2</sup>-s, estimate the relative worths in \$ for  $^{233}\text{U}$  and  $^{239}\text{Pu}$  fueled reactors compared to a  $^{235}\text{U}$  fueled reactor. Use the data in the table below.

quantity	$^{235}\text{U}$	$^{233}\text{U}$	$^{239}\text{Pu}$
$\beta$	.0065	.0026	.0021
$\gamma_I$	.0617	.0479	.0612
$\gamma_x$	.0024	.0105	.0108

- 9.7 A 1000 MWT reactor operating near its rated power undergoes a fuel temperature change of 0.2°F per megawatt and a moderator temperature change of 0.06°F per megawatt. If the

## NUCLEAR REACTOR THEORY AND DESIGN

moderator temperature coefficient at BOL is  $+3 \times 10^{-4} \Delta k/k/^{\circ}\text{F}$ , what range of values must the Doppler coefficient have for the reactor to be stable?

- 9.8\*** Use the reactor model given in Section 9.8, but apply the prompt-jump approximation to simplify the equations. Also assume that  $\alpha_f = 0$  so that only the moderator temperature coefficient is effective.

Do the following:

- a) Write the resulting set of equations in State Variable form, and define all the terms in the resulting vectors and matrices.
- b) The parameters have the following numerical values:

$$\Lambda = 10^{-5} \text{ s}$$

$$\beta = .007$$

$$P_o = 2000 \text{ MWT}$$

$$\alpha_m = -1.0 \times 10^{-4}/^{\circ}\text{F}$$

$$\lambda = 0.3 \text{ s}^{-1}$$

$$m_f = 100,000 \text{ kg}$$

$$c_f = 300 \text{ J/kg-}^{\circ}\text{C}$$

$$m_m = 500,000 \text{ lb}_m$$

$$c_m = 1.4 \text{ Btu/lb}_m\text{-}^{\circ}\text{F}$$

$$h = 5000 \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{F}$$

$$A = 50,000 \text{ ft}^2$$

Calculate the characteristic equation for the system and determine if the system is stable by evaluating the characteristic eigenvalues.

Determine the natural frequency of oscillation of the system.

- c) Set up the solution form for obtaining the

## NUCLEAR REACTOR THEORY AND DESIGN

response of the system to a +10% change in power demand. Do not actually evaluate these expressions, but explain how you would go about evaluating the solutions and sketch what you think the response would look like.

- 9.9 You are given the three following equations describing a reactor system with prompt thermal feedback:

$$\frac{dP}{dt} = \frac{\rho}{\Lambda} P \quad (\text{prompt reactor kinetics});$$

$$\frac{dT}{dt} = P - P_0 \quad (\text{fuel with constant heat removal } P_0);$$

$$\rho = \alpha_f (T - T_0) \quad (\text{temperature feedback reactivity}).$$

- Find the steady state operating point conditions  $P(0)$ ,  $T(0)$ , and  $\rho(0)$ .
- Linearize the above equations about the steady state operating point  $P(0)$ ,  $T(0)$ , and  $\rho(0)$ , writing the results in terms of the incremental variables  $\delta P$ ,  $\delta T$ , and  $\delta \rho$ .
- Write the system of equations in vector-matrix form. What kind of equation is this? What kind of solutions does it possess?
- Derive the required condition for system stability.

- 9.10\* In problem 9.9, assume that the reactivity  $\rho(t) = \rho_{\text{feedback}}(t) + \rho_{\text{ext}}(t)$ . Also assume that  $\alpha_f$  is negative. Using Laplace transforms, calculate the transfer function between the external reactivity and the reactor temperature, defined as



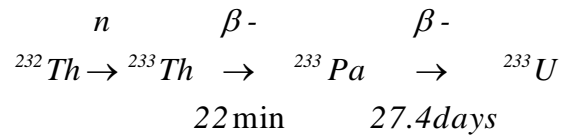
## NUCLEAR REACTOR THEORY AND DESIGN

$$H(s) = \frac{T(s)}{\rho_{ext}(s)}.$$

Using  $s = i\omega$ , calculate and plot the magnitude,  $|H(i\omega)|$ , of the transfer function versus the angular frequency  $\omega$ . Also calculate and plot the phase angle,  $P(\omega) = \tan^{-1} \left( \frac{\text{imag} H(i\omega)}{\text{real} H(i\omega)} \right)$ , versus frequency. Comment on the results.

- 9.11** Assume that a power reactor has been operating at full power in the steady state. The operator is requested to make a rapid change to 50% power and hold the reactor critical at the new state. Take into account that the reactor has a negative power coefficient of reactivity, and that the xenon level will have to adjust to a new equilibrium value. Sketch the time-dependent changes of the reactor flux, temperature, control rod position, and iodine and xenon concentrations in terms of their fractional deviations from the initial states. Explain the shapes of the curves.
- 9.12** Using the fact that 1 watt =  $3.1 \times 10^{10}$  fissions/s in  $^{235}\text{U}$ , calculate the amount of  $^{235}\text{U}$  in grams consumed in one day of operation of the UVAR Reactor at 2 megawatts of power. Remember that not all absorptions in  $^{235}\text{U}$  lead to fission, e.g.,  $\sigma_a = 681$  barns and  $\sigma_f = 582$  barns for thermal neutrons. Assume that all fissions occur at thermal (0.025 eV) energy. Avagadro's number =  $0.6023 \times 10^{24}$  atoms/gm-mole.
- 9.13** Assume a constant thermal flux for the production of the fissile isotope  $^{233}\text{U}$  from the fertile isotope  $^{232}\text{Th}$  through the chain

## NUCLEAR REACTOR THEORY AND DESIGN



- a) Write the differential equations governing the concentrations of  ${}^{232}\text{Th}$ ,  ${}^{233}\text{Th}$ ,  ${}^{233}\text{Pa}$ , and  ${}^{233}\text{U}$  in the reactor assuming that all isotopes have a significant absorption cross section.
- b) Make appropriate assumptions based on half-lives to simplify the governing equations.
- c) Derive the concentration of  ${}^{233}\text{Pa}$  as a function of time in a reactor operated at a constant flux based on the equations derived in part b.

**9.14\*** A thermal reactor fueled with natural uranium operates at a constant flux level. Derive expressions for the atom densities of  ${}^{235}\text{U}$ ,  ${}^{238}\text{U}$ ,  ${}^{239}\text{Pu}$ ,  ${}^{240}\text{Pu}$  and  ${}^{241}\text{Pu}$  as a function of time using the Laplace transform method.

### References

- J.R. Lamarsh**, *op. cit.* Chapter 18.  
**A. Radkowsky**, *op. cit.*, Chapter 4.  
**P.M. DeRusso, R.J. Roy and C.M. Close**, *State Variables for Engineers*, (John Wiley and Sons, New York, NY 1967) Chapters 4 and 5.

## NEUTRON MODERATION

Thus far we have treated reactors using few-group diffusion theory (2 to 4 groups) to find  $k_{\text{eff}}$  for various geometrical configurations. The macroscopic cross sections for each of these groups, which are averages of the actual cross sections (e.g., from the BNL-325 book) over appropriate energy spectra, have been supplied to us. We must now turn to the problem of calculating the spectra used in the averaging process, and this implies going back to some of the basic physics of elastic and inelastic scattering of neutrons by various materials.

Here we treat the *space-independent* case because the problem becomes cumbersome otherwise, and to a good approximation space and energy are separable over small core regions. We consider the energy range from fission down to the point where upscatter is possible, i.e., where the neutron can gain energy in a collision with a thermally vibrating atom. Hence, we treat the range from 10 MeV down to about 1 eV. This fortunately happens to include the resonance region. The flux that we deal with is  $\phi(E)$  n/cm<sup>2</sup>-s-eV, the differential flux per unit energy. The energy range from 1 eV down to essentially zero is treated later when we discuss neutron thermalization.

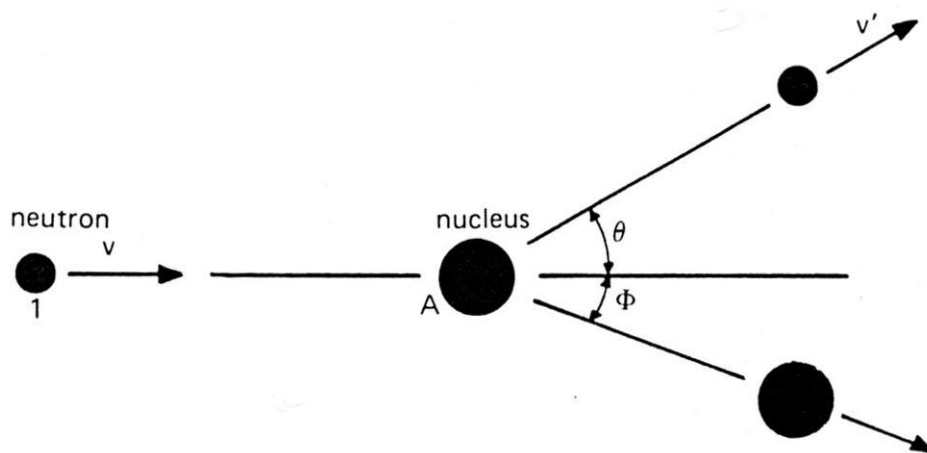
The cases that are treated in this chapter comprise most of the special situations where an analytic solution to the slowing down problem can readily be found. These specific cases serve to illustrate the method of solving the integral equation obtained from the energy-dependent balance equation. Some general characteristics of the flux solution are observed, including a transient behavior near and below the energies of neutron

## NUCLEAR REACTOR THEORY AND DESIGN

sources, and sinks such as resonances. For a carbon moderator, the transient behavior can affect the amount of resonance absorption. The asymptotic flux,  $\phi(E)$ , is found to vary as  $1/E$  for most cases of interest, including those where mixtures of different isotopes are present and where absorption occurs during slowing down.

### 10.1 Scattering Collisions

At this point, it is useful to review and expand upon the material given in Chapter 2 on the mechanics of scattering in the LAB and CM systems. In the laboratory system, a neutron of velocity  $v$  approaches a stationary atom of mass  $A$ ; the neutron scatters through an angle  $\theta$  and has a resulting velocity  $v'$ , as shown in Figure 10.1. Given the masses, plus the initial neutron velocity and the scattering angle  $\theta$ , one can *completely* specify the recoil angle  $\Phi$  and the final energy of both particles using conservation of energy and momentum.



**Fig. 10.1** Collision in the LAB System

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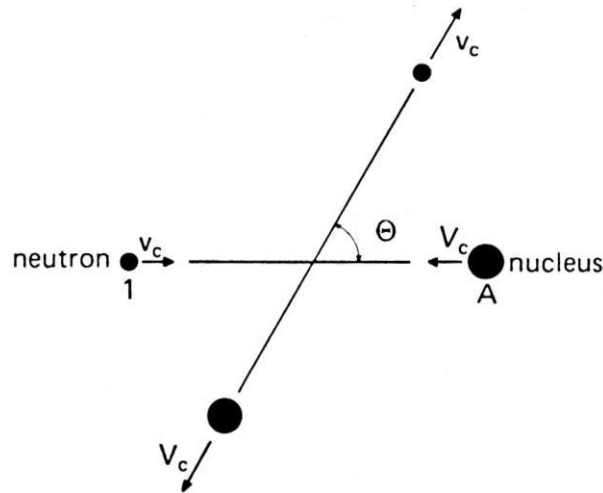
In the CM system, both particles approach each other. The atom has the velocity of the center of mass, but goes in the opposite direction, i.e.,

$$V_c = -V_{CM} = \frac{-v}{A + 1},$$

while the neutron has the velocity

$$v_c = v - V_{CM} = \frac{A}{A + 1}v.$$

After the collision, both particles scatter through the *same* angle  $\Theta$ , and if the collision is elastic, both have the *same* velocities as they had originally, as shown in Figure 10.2. This is a zero momentum system. In the LAB System, the center of mass moves, while in the CM system it is stationary.



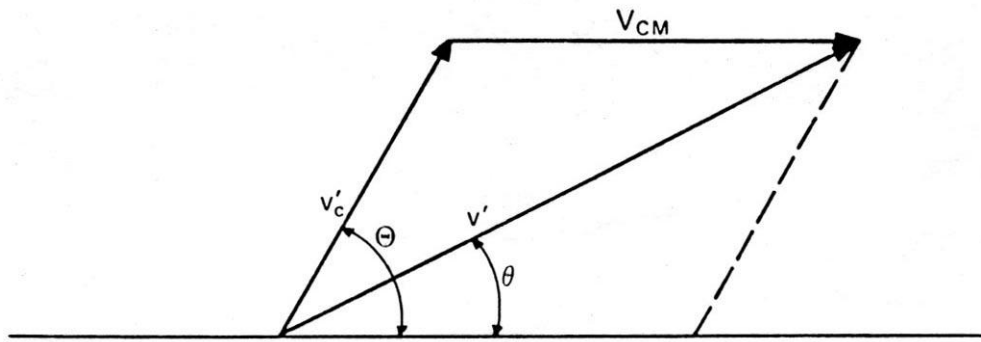
**Fig. 10.2** Elastic Collision in the Center-of-Mass System

Since we observe the collision in the laboratory, why does one treat the CM system at all? The primary reason is that the nucleus considers itself to be residing at the center of the

## NUCLEAR REACTOR THEORY AND DESIGN

universe, and the probability of a reaction being *isotropic* in the CM system is high. It is easier to convert the collision to the CM system than to convert the angular cross section to the LAB system. There is a simple relationship between the two systems given by the vector diagram shown in Figure 10.3. Use of the law of cosines allows one to derive an expression between the initial lab velocity of the neutron and its final velocity as a function of the CM scattering angle  $\Theta$ . The energy-equivalent of this expression is

$$E' = E \left[ \frac{A^2 + 2A \cos \Theta + I}{(A + I)^2} \right]. \quad (10.1)$$



**Fig. 10.3** Diagram Relating Laboratory and CM Systems

Actually, in the general case, which includes inelastic scattering, a similar expression results. Of course  $v \neq v_c$  in an inelastic encounter since a  $Q$  value is involved. Also, not all of the kinetic energy of the neutron can be used, since some of it goes into motion of the center of mass. The available kinetic energy in the CM system is

$$E_c = E \left( \frac{A}{A + I} \right), \quad (10.2)$$

which decreases as  $A$  decreases. One can define the term  $\gamma$  for

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the general reaction as

$$\frac{v_c'}{V_{CM}} = \frac{I}{\gamma} \equiv \left( A^2 + \frac{A(A+1)Q}{E} \right)^{1/2}. \quad (10.3)$$

In an elastic collision,  $Q = 0$ , and  $\gamma$  reduces to

$$\gamma_{elastic} = \frac{I}{A}. \quad (10.4)$$

The general relationship between the initial and final neutron energy is

$$E' = E \left[ \frac{\gamma^2 + 2\gamma \cos \Theta + I}{\gamma^2 (A+1)^2} \right]. \quad (10.5)$$

This expression reduces to the simple expression given previously for elastic scattering.

Look carefully at the scattering equation. We know intuitively that the maximum energy transfer occurs for a "head-on" collision, which gives the minimum energy to the scattered neutron. Setting  $\Theta = 180^\circ$ , so that  $\cos \Theta = -1$ , gives

$$E'_{min} = E \left[ \frac{A^2 - 2A + I}{(A+1)^2} \right] = E \left[ \frac{A - I}{A + I} \right]^2. \quad (10.6)$$

Define the term alpha as

$$\alpha \equiv \left[ \frac{A - I}{A + I} \right]^2. \quad (10.7)$$

For elastic scattering of neutrons on atoms of mass  $A$ , we obtain the expression

$$E'_{min} = \alpha E. \quad (10.8)$$

We can therefore rewrite the energy transfer equation in terms of  $\alpha$ , obtaining

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$$E' = \frac{E}{2} [(1 + \alpha) + (1 - \alpha) \cos \Theta]. \quad (10.9)$$

We can also write an expression for the general case, but this expression is considerably more complicated than the one given above, except for the fact that  $E'$  is still only a function of  $E$ ,  $\alpha$ ,  $\Theta$  and  $Q$ .

For hydrogen,  $\alpha = 0$  and  $E'$  can have any energy between  $E$  and 0 eV. For carbon,  $A = 12$  and  $\alpha = 0.716$ . Hence, the scattered neutron will have at least as much as 71.6% of its original energy. For uranium,  $\alpha = 0.983$ , and only 1.7% of the neutron's energy is lost, at most, in an elastic collision. In the elastic scattering case, we can find out how  $E'$  varies with  $\Theta$  by differentiation of Eq. (10.9). The result is

$$dE' = -\frac{E}{2}(1 - \alpha) \sin \Theta d\Theta. \quad (10.10)$$

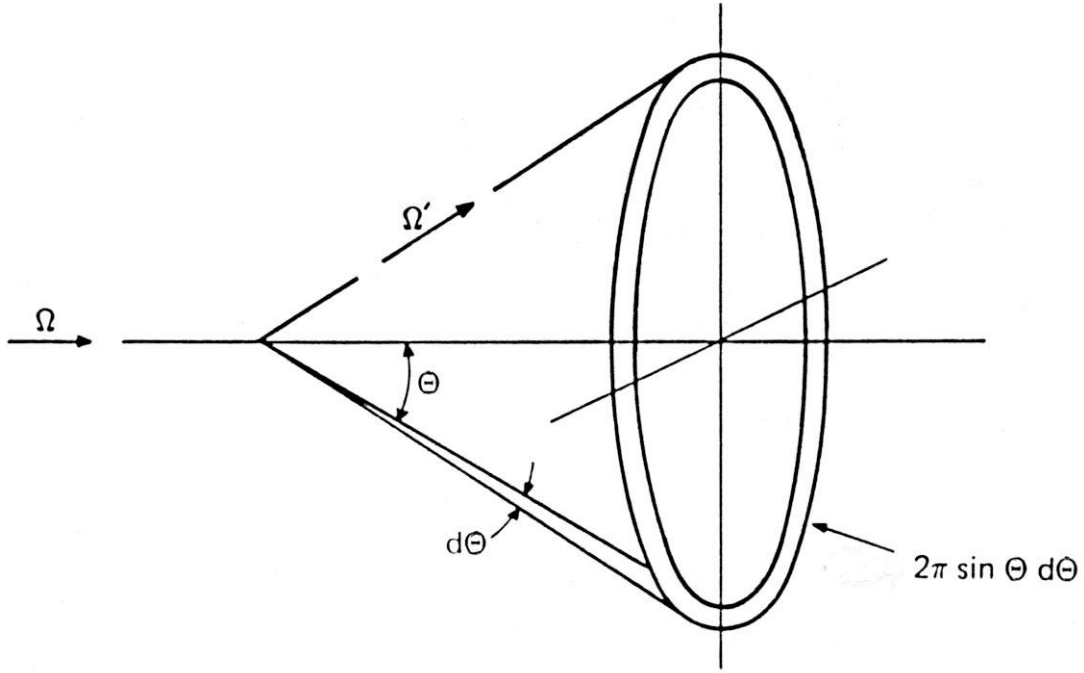
All of the above information is obtained from the conservation laws alone and tells us *nothing* about the probability that a neutron will scatter through an angle  $\Theta$ . For this we must look at the cross sections that are determined by the nuclear properties of the atoms that do the scattering. Consider the diagram in Figure 10.4. Most neutron scattering reactions possess rotational symmetry, that is to say the result for  $\vec{\Omega} \rightarrow \vec{\Omega}'$  depends only upon  $\Theta$  and is independent of the rotational angle  $\Psi$ . All of the neutrons that scatter through the polar angle  $\Theta$  and end up in a ring-shaped solid angle element, change their energies from  $E$  to  $E'$  within an energy interval  $dE'$ . Since  $E'$  decreases as  $\vec{\Omega}'$  increases, this can be written as the probability equivalence,

$$P(\vec{\Omega} \rightarrow \vec{\Omega}') d\Omega' = -\frac{1}{2\pi} P(E \rightarrow E') dE' d\psi, \quad (10.11)$$

where  $P$  is a probability which is normalized to unity over the



range of the variable.



**Fig. 10.4** Neutron Scattering in the CM System with Rotational Symmetry

The angular probability can be obtained directly from the ratio of the differential angular scattering cross section to the total scattering cross section so that

$$P(\vec{\Omega} \rightarrow \vec{\Omega}') d\Omega' = \frac{P(\Theta)}{2\pi} \sin \Theta d\Theta d\psi, \quad (10.12)$$

where

$$P(\Theta) \equiv \frac{\sigma_s(\Theta)}{\sigma_s}. \quad (10.13)$$

Hence,

$$P(E \rightarrow E') dE' = - \frac{\sigma_s(\Theta)}{\sigma_s} \sin \Theta d\Theta. \quad (10.14)$$

But we already have an expression from the conservation laws

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relating  $dE'$  and  $d\Theta$ , given by Eq. (10.10). Combining the two we obtain the general elastic scattering relationship

$$P(E \rightarrow E') dE' = \begin{cases} \frac{2\sigma_s(\Theta)}{\sigma_s(1-\alpha)E}; & \alpha E < E' < E \\ 0 & 0 < E' < \alpha E. \end{cases} \quad (10.15)$$

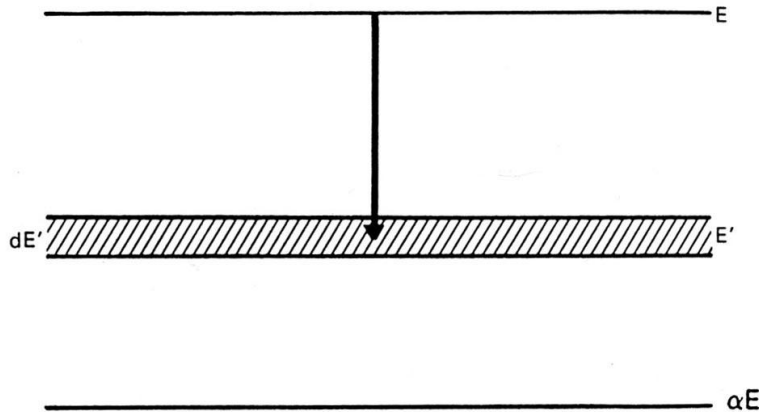
For the important and often-encountered case of isotropic scattering in the CM system we have the relationship

$$\sigma_s(\Theta) = \frac{\sigma_s}{2}. \quad (\text{isotropic}) \quad (10.16)$$

This gives

$$P(E \rightarrow E') dE' = \begin{cases} \frac{1}{(1-\alpha)E}; & \alpha E < E' < E \\ 0 & 0 < E' < \alpha E. \end{cases} \quad (10.17)$$

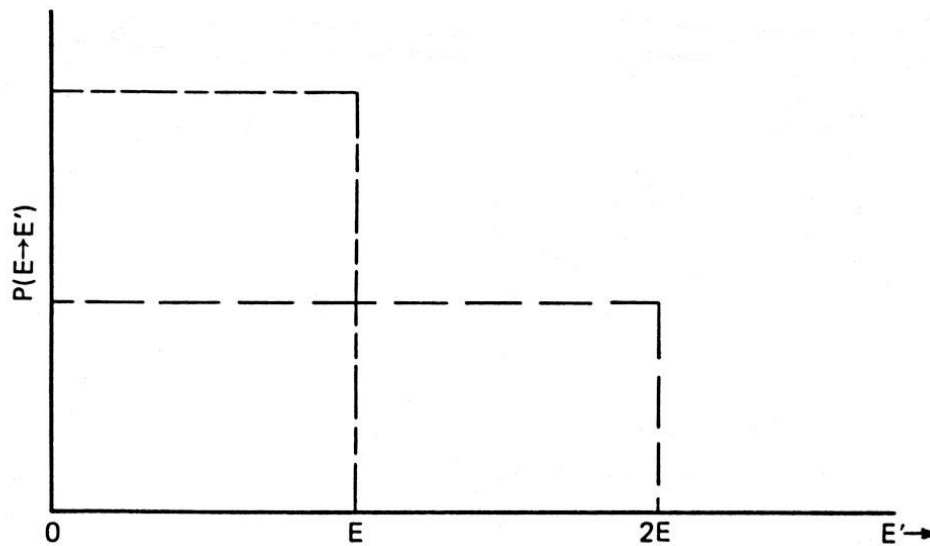
This expression states that the probability of obtaining any energy  $E'$  between  $E$  and  $\alpha E$  is uniform and is independent of  $E'$ . The corresponding energy scattering diagram is given in Figure 10.5.



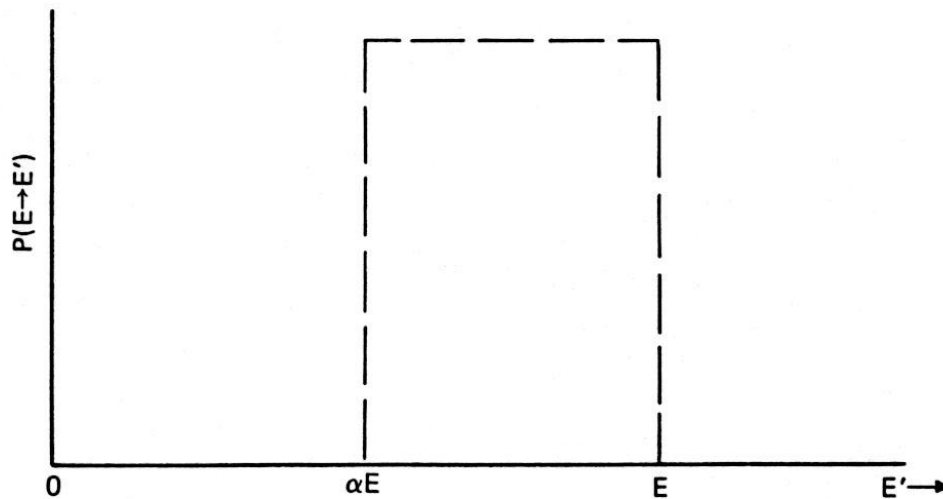
**Fig. 10.5** Scattering of a Neutron from Energy  $E$  to  $E'$

## NUCLEAR REACTOR THEORY AND DESIGN

For hydrogen,  $\alpha = 0$  and  $P(E \rightarrow E') = 1/E$ . Plotted, this looks like a uniform rectangular distribution extending downward from the initial energy of the incident neutron to zero as shown in Figure 10.6.



**Fig. 10.6** Isotropic Scattering Probabilities for Hydrogen



**Fig. 10.7** Scattering Probabilities for  $A > 1$

## NUCLEAR REACTOR THEORY AND DESIGN

For  $A > 1$ , the diagrams are similar but the scattering range is restricted as shown in Figure 10.7. The difficulty met in using this scattering theory arises when one must consider the superposition of the results of multiple scattering, which must be treated by writing an integral balance equation.

### 10.2 Slowing Down Problem

In order to treat the slowing down problem in a medium, one must write a neutron balance equation describing the behavior of the neutrons. The proper form of this equation for downscatter only is the time-independent Boltzmann equation, which is of the form,

$$\begin{array}{c}
 \text{leakage} \qquad \text{absorption and outscatter} \\
 \\
 \vec{\Omega} \cdot \nabla \Phi(\vec{r}, \vec{\Omega}, E) + \Sigma_T(\vec{r}, E) \Phi(\vec{r}, \vec{\Omega}, E) \\
 \\
 \text{source} \qquad \qquad \qquad \text{inscatter} \\
 \\
 = S(\vec{r}, \vec{\Omega}, E) + \int_E^\infty \int_{4\pi} \Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \Phi(\vec{r}, \vec{\Omega}', E') d\Omega' dE'.
 \end{array}
 \tag{10.18}$$

Now, recall that the scattering angle and the change in energy of the scattered neutron are *not independent* of one another. To make the problem tractable, take the special case of an infinite medium (no leakage) having uniformly distributed isotropic sources in it. For this case, we can average over all angles by integrating out the  $\vec{\Omega}$  dependence. The result is a diffusion-theory type equation of the form

$$\Sigma_T(E) \phi(E) = S(E) + \int_E^\infty \Sigma_s(E' \rightarrow E) \phi(E') dE. \tag{10.19}$$

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This is the equation that will be specialized to handle moderation in hydrogen and other materials, with and without absorption.

### 10.3 Slowing Down in Hydrogen With No Absorption

The first case that we examine is the case where the reactor is composed entirely of hydrogen, which is not a very practical case. We make the following additional conditions:

- (1) The source emits neutrons at a single energy  $E_0$ . Hence, using the energy-loss probability derived previously for a single scattering event, we have

$$S(E) = S_0 P(E_0 \rightarrow E). \quad (10.20)$$

- (2) The energy loss scattering cross section can be replaced by the total scattering cross section times the energy loss probability, i.e.,

$$\Sigma_s(E' \rightarrow E) = \Sigma_s(E') P(E' \rightarrow E). \quad (10.21)$$

- (3) There is no absorption, and hence in this case

$$\Sigma_T(E) = \Sigma_s(E).$$

Using these conditions, we obtain the balance equation in the form

$$\Sigma_s(E) \phi(E) = S_0 P(E_0 \rightarrow E) + \int_E^{E_0} \Sigma_s(E') P(E' \rightarrow E) \phi(E') dE', \quad (10.22)$$

where we already know that for hydrogen,

$$P(E' \rightarrow E) = \frac{1}{E'}.$$

Furthermore, we can define a term called the *collision density*,

## NUCLEAR REACTOR THEORY AND DESIGN

which is just the scattering rate per cubic centimeter, as follows:

$$F_s(E) \equiv \sum_s(E)\phi(E). \quad (10.23)$$

Hence, we obtain the balance equation

$$F_s(E) = \frac{S_0}{E_0} + \int_E^{E_0} F_s(E') \frac{dE'}{E'}. \quad (10.24)$$

This is an integral equation known as a Volterra equation of the second kind. It can be solved by differentiation, remembering the rules for treating the integral when the quantity to be differentiated occurs in one of the limits. The result is

$$\frac{dF_s}{dE} = -\frac{d(E)F_s(E')}{dE E'} \bigg|_E = -\frac{F_s(E)}{E}. \quad (10.25)$$

The equation is separable, and upon integration gives the result

$$F_s(E) = \frac{C}{E}, \quad (10.26)$$

where C is an arbitrary constant of integration to be determined. Replacing this solution in the integral equation and evaluating the equation at  $E = E_0$ , one finds the constant to be simply

$$C = S_0. \quad (10.27)$$

Therefore, we can state immediately for this case that the flux is

$$\phi(E) = \frac{S_0}{\sum_s(E)E}. \quad (10.28)$$

If  $\Sigma_s(E)$  is approximately constant, which is a good assumption for hydrogen, then we obtain the well-known  $1/E$  flux behavior. Note that if E varies over seven decades (10 MeV down to 1 eV)

## NUCLEAR REACTOR THEORY AND DESIGN

then the *magnitude* of  $\phi(E)$  also varies over seven decades.

To improve upon this situation, we define a dimensionless logarithmic energy variable called the lethargy  $u$ , as follows:

$$u \equiv \ln \left[ \frac{E_0}{E} \right], \quad (10.29)$$

where  $E_0$  is customarily taken to be 10 MeV. Taking the derivative of both sides, we find that the lethargy increases as the energy decreases,

$$du = -\frac{dE}{E}. \quad (10.30)$$

More important, however, is the effect on the flux. Since

$$\phi(E)dE = -\phi(u)du, \quad (10.31)$$

we find that

$$E\phi(E) = \phi(u) = \frac{S_0}{\Sigma_s(u)}, \quad (10.32)$$

or

$$F_s(u) = S_0. \quad (10.33)$$

Therefore, we have obtained a flux function that is essentially *constant* in magnitude and is given in terms of a *linear* variable  $u$ .

It is also interesting to look at the form of the energy-loss probability in terms of lethargy. This function is

$$\begin{aligned} P(u' \rightarrow u)du &= -P(E' \rightarrow E)dE \\ &= -\frac{dE}{E'}. \end{aligned} \quad (10.34)$$

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Hence,

$$\begin{aligned} P(u' \rightarrow u) &= -\frac{1}{E'} \left( \frac{dE}{du} \right) \\ &= \frac{E}{E'} = e^{(u'-u)}. \end{aligned} \tag{10.35}$$

This function will be fairly useful in some of our subsequent work. It is easier to see the integration ranges and limits when the energy variable is used, but the mathematics is often easier in terms of lethargy.

### 10.4 The Slowing Down Density in Hydrogen, No Absorption

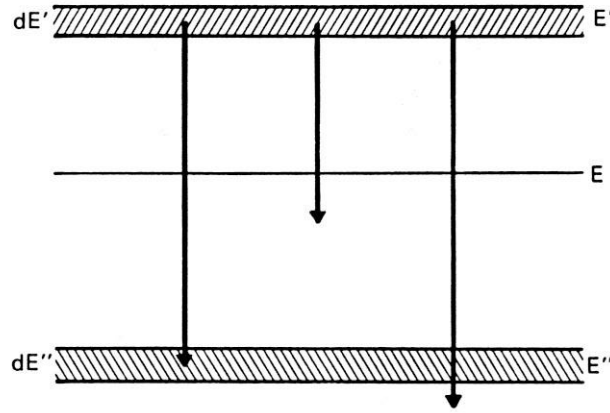
We now define a new quantity called the slowing down density,  $q(E)$ , which is analogous to a volumetric flow rate. This quantity represents the number of neutrons per cubic centimeter whose energy falls below the value of  $E$  per second. Consider for the moment that the only source of neutrons is those that have just scattered in the energy interval  $dE'$  about  $E'$ . Refer to the diagram in Figure 10.8, where the scattering medium is assumed to be hydrogen so that the scattering probability is  $P(E' \rightarrow E) = 1/E'$ . From the definition, the differential number of neutrons per  $\text{cm}^3\text{-s}$  that had their last collision in the interval  $dE'$  and scatter to *any* energy  $E''$  below  $E$  is the following integral,

$$dq(E, E') = \left[ \int_0^E \Sigma_s(E') \phi(E') P(E' \rightarrow E'') dE'' \right] dE'. \tag{10.36}$$

Note that the integration is to all *final* energies  $E''$  less than  $E$ .



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**Fig. 10.8** Scattering from Energy  $E'$  Past Energy  $E$

To obtain the total slowing down density we must now integrate over all *initial* energies  $E'$  above  $E$ . Upon integration over  $dE'$ , the slowing down density becomes the double integral

$$q(E) = \int_E^\infty \int_0^E [\Sigma_s(E') \phi(E') \frac{1}{E'} dE''] dE'. \quad (10.37)$$

The integral over  $dE''$  can now be done immediately to give

$$q(E) = E \int_E^\infty \Sigma_s(E') \phi(E') \frac{1}{E'} dE'. \quad (10.38)$$

In terms of lethargy, which is a dimensionless variable, the corresponding equation is

$$q(u) = \int_{-\infty}^u \Sigma_s(u') \phi(u') e^{(u'-u)} du'. \quad (10.39)$$

This expression could have been derived directly.

Now, consider that the *primary source* of neutrons is located at energy  $E_0$ . The slowing down density will consist of two contributions, which are:

- (1) **direct contribution**, which comes from the *first* scattering collision of a source neutron. Since the probability of scattering is uniform for all energies

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below the source energy  $E_0$ , the fraction of the source appearing below  $E$  is simply  $E/E_0$ , the ratio of the energy ranges. Hence, the first collision contribution is  $S_0 E/E_0$ ;

- (2) **multiple-collision contribution**, which is the integral term given by Eq. (10.38) with an upper limit of  $E_0$ . Hence, in the case of a direct source, the slowing down density is given by the equation

$$q(E) = \frac{S_0 E}{E_0} + E \int_E^{E_0} \Sigma_s(E') \phi(E') \frac{dE'}{E'}. \quad (10.40)$$

Comparing this result to Eq. (10.24) for the collision density,  $F_s(E)$ , one finds that the entire right-hand side of the equation is simply  $E \Sigma_s(E) \phi(E)$ . We can therefore use our previous solution of the integral equation to write down the answer,

$$q(E) = E \Sigma_s(E) \phi(E) = S_0 = \text{constant} \quad (10.41)$$

Since  $\phi(u) = E \phi(E)$ , the corresponding result in terms of lethargy is

$$q(u) = \Sigma_s(u) \phi(u) = S_0. \quad (10.42)$$

This result is physically obvious. Since there is no absorption, all neutrons from the source must eventually slow down past any chosen energy  $E$ . The usefulness of the slowing down density is that even when there is absorption, the slowing down density remains relatively constant and varies slowly with energy.

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### 10.5 Moderation for $A > 1$ , No Absorption

When  $A > 1$ , there exists a *minimum* energy that a neutron can attain in a single scattering event. The net effect is to limit the allowable ranges on the integrals in the balance equation, which produces a discontinuity in the direct source contribution to the collision density at the energy  $\alpha E_0$  for a mono-energetic source at  $E_0$ . This in turn produces a transient behavior over an energy range immediately below the source energy.

If we consider for the moment that the total collision density is made up of neutrons from the source that have had one collision, plus those that have scattered twice, plus those that have scattered three times, etc., we obtain the following series expansion:

$$F_s(E) = F_1(E) + F_2(E) + F_3(E) + \dots \quad (10.43)$$

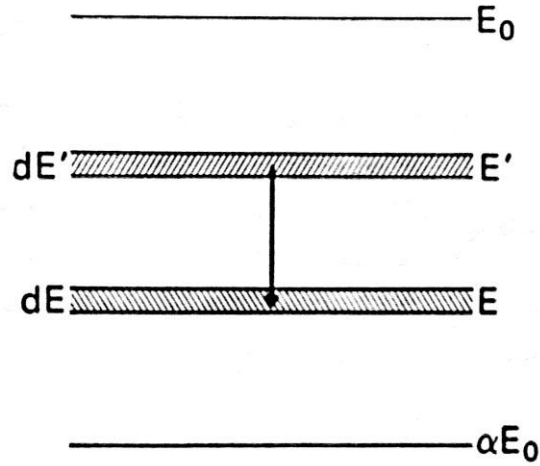
The partial collision densities,  $F_i(E)$ , are to be determined. We can accomplish this without solving the integral equation. We know that the first term is the direct source contribution of once-scattered neutrons, namely,

$$F_1(E) = \begin{cases} \frac{S_0}{(1-\alpha)E_0} & \alpha E_0 < E < E_0, \\ 0 & 0 < E < \alpha E_0. \end{cases} \quad (10.44)$$

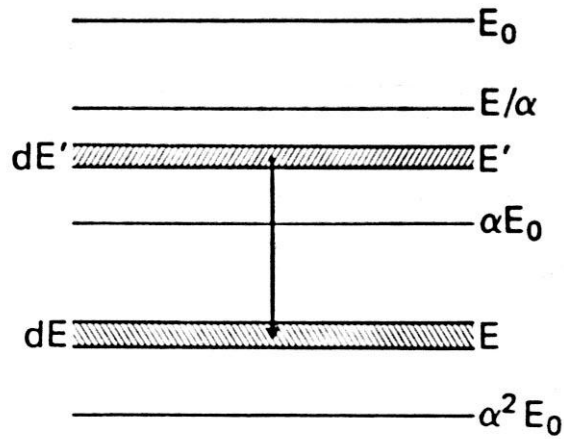
We have two possibilities for the second collision:

- (1) Scattering to an energy  $E$ , which is in the original energy range  $\alpha E_0 < E < E_0$ , as shown in Figure 10.9.
- (2) Scattering to an energy below  $\alpha E_0$ , but only as far as  $\alpha^2 E_0$ , as shown in Figure 10.10.

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**Fig. 10.9** Scattering Within the Energy Range  $E_0$  to  $\alpha E_0$ .



**Fig. 10.10** Scattering in the Energy Range Between  $\alpha E_0$  and  $\alpha^2 E_0$

These two possibilities are taken care of by properly specifying the limits of the integral equation. For the former, where  $E > \alpha E_0$ , the expression is

$$F_2(E) = \int_E^{E_0} \frac{F_1(E') dE'}{(1-\alpha)E'}; \quad \alpha E_0 < E < E_0. \quad (10.45)$$

For the latter case, where  $E < \alpha E_0$ , the scattering has a limited upper range giving

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$$F_2(E) = \int_{\alpha E_0}^{E/\alpha} \frac{F_1(E') dE'}{(1-\alpha)E'}; \quad \alpha^2 E_0 < E < \alpha E_0. \quad (10.46)$$

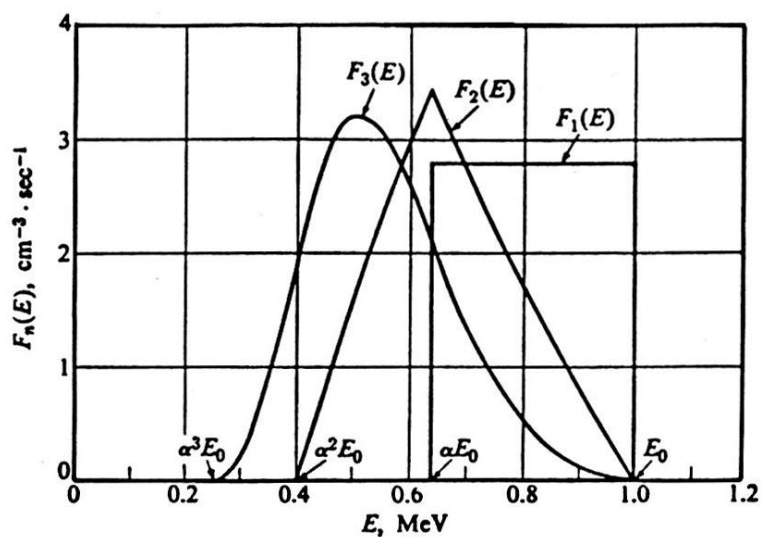
These two integrals can be evaluated giving

$$F_2(E) = \begin{cases} \frac{S_0}{(1-\alpha)^2 E_0} \ln\left[\frac{E_0}{E}\right] & \alpha E_0 < E < E_0, \\ \frac{S_0}{(1-\alpha)^2 E_0} \ln\left[\frac{E}{\alpha^2 E_0}\right]; & \alpha^2 E_0 < E < \alpha E_0, \\ 0 & 0 < E < \alpha^2 E_0. \end{cases} \quad (10.47)$$

The next term,  $F_3(E)$ , can be obtained using  $F_2(E)$  as the source and properly specifying the limits in the three allowed energy intervals. After a succession of these calculations, one finds that the general behavior of the  $i$ th function,  $F_i(E)$ , becomes a Gaussian. The first few terms are plotted in Figure 10.11.

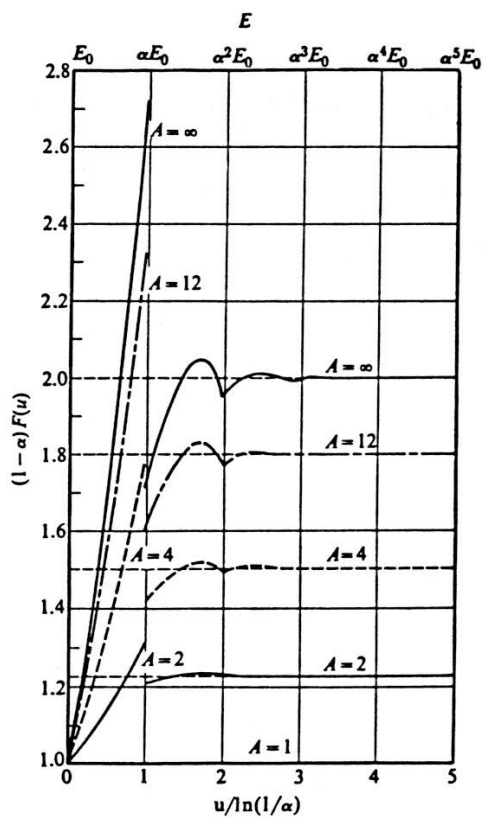
The total collision density as a function of lethargy is relatively constant after an initial transient behavior near the source energy. This is shown in Figure 10.12. Note that there is an asymptotic region that begins at a value of about  $\alpha^3 E_0$  below the source energy  $E_0$ . This asymptotic behavior gives us the possibility of treating only collided neutrons if the source energy is high with respect to the energy region of interest. Furthermore, if the source is distributed over a range of energies, the convolution of the above results over the source distribution will give a considerably smoother collision density as a function of energy than does a mono-energetic source.

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**Fig. 10.11** Partial Collision Densities vs. Energy

(From *Introduction to Nuclear reactor Theory* by J. Lamarsh, 1966, Addison Wesley)



**Fig. 10.12** Collision Density vs. Energy

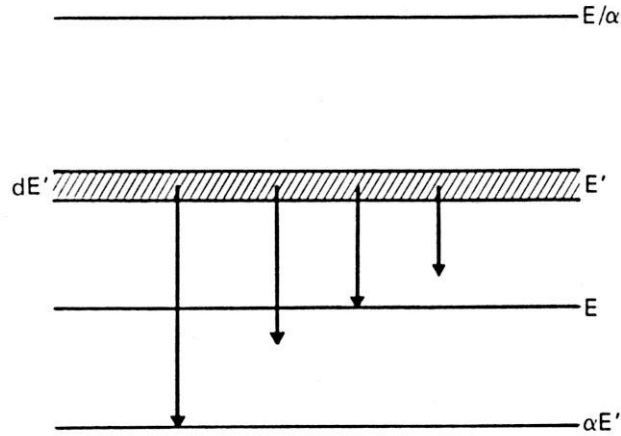
(From *The Physical Theory of Neutron Chain Reactors* by A.M. Weinberg and E.P. Wigner, 1958, University of Chicago Press)

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The solution shown in Figure 10.12 can also be obtained directly by solving the integral equation for one collision interval at a time, starting at the source energy and moving downward. This method is illustrated in a problem at the end of the chapter.

### 10.6 Asymptotic Slowing Down Theory, $A > 1$ , No Absorption

In the asymptotic case, at energies far below the source energy, the slowing down density  $q(E)$  is governed only by neutrons that come from the adjacent energy range,  $E/\alpha > E' > E$ , and these neutrons can only be scattered down to an energy of  $\alpha E'$ , at most. The diagram is shown in Figure 10.13.



**Fig. 10.13** Slowing Down in the Asymptotic Range

The equation for the asymptotic slowing down density becomes

$$q(E) = \int_E^{E/\alpha} F_s(E') \left[ \frac{E - \alpha E'}{E' - \alpha E'} \right] dE'. \quad (10.48)$$

The quantity in the brackets is the fraction of neutrons that pass below energy  $E$  for an assumed uniform scattering

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distribution. If we next assume that the *solution* to the collision density balance equation is also asymptotic, we can test our assumption by direct substitution. The form chosen is

$$F_s(E) = C/E, \quad (10.49)$$

where the constant  $C$  is to be determined.

Upon substitution and integration, we obtain the following result for the slowing down density:

$$q(E) = C(1 + \frac{\alpha}{1 - \alpha} \ln[\alpha]) \equiv C\xi. \quad (10.50)$$

On the other hand, if there is no absorption, then  $q(E) = S_0$ . Substituting, we find that in the asymptotic region

$$C = \frac{S_0}{\xi}. \quad (10.51)$$

Hence, by replacing  $C$  in the assumed collision density solution, we obtain a result very similar to the result obtained for hydrogen, namely,

$$\phi(E) = \frac{S_0}{\xi \sum_s(E)E}. \quad (10.52)$$

In terms of lethargy,

$$\phi(u) = \frac{S_0}{\xi \sum_s(u)}, \quad (10.53)$$

which is essentially constant, and hence

$$F_s(u) = \frac{S_0}{\xi} = \text{constant}. \quad (10.54)$$

It remains to relate the new constant  $\xi$  to the other variables of interest. Let us calculate the average change in lethargy,  $\overline{\Delta u}$  per collision over any allowed energy region in the



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asymptotic range. The change in lethargy from energy  $E$  to  $E'$  is

$$\Delta u = \ln \left[ \frac{E_0}{E'} \right] - \ln \left[ \frac{E_0}{E} \right] = \ln \left[ \frac{E}{E'} \right]. \quad (10.55)$$

Hence,

$$\begin{aligned} \overline{\Delta u} &= \overline{\ln \left( \frac{E}{E'} \right)} = \int_{\alpha E}^E \ln \left( \frac{E}{E'} \right) P(E \rightarrow E') dE' \\ &= \frac{1}{E(1 - \alpha)} \int_{\alpha E}^E \ln \left( \frac{E}{E'} \right) dE' \\ &= 1 + \frac{\alpha}{1 - \alpha} \ln[\alpha] \equiv \xi. \end{aligned} \quad (10.56)$$

Therefore, the constant  $\xi$  is equal to the average lethargy change per collision. When  $\alpha$  is inserted in terms of its definition as a function of the mass of the scattering atom,  $A$ , we obtain

$$\xi = 1 - \frac{(A - 1)^2}{2A} \ln \left( \frac{A + 1}{A - 1} \right). \quad (10.57)$$

When  $A$  is not too small,

$$\xi \approx \frac{2}{A + (2/3)}. \quad (10.58)$$

One finds that the average number of collisions required for a neutron to scatter from the source energy  $E_0$  down to energy  $E$  is simply equal to the ratio  $u/\overline{\Delta u}$ , or

$$n = \frac{\ln \left( \frac{E_0}{E} \right)}{\xi} = \frac{u}{\overline{\Delta u}}. \quad (10.59)$$

The slowing down parameters for several isotopes are tabulated in

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Table 10.1. We can think of  $\xi$  as a type of scattering efficiency factor, where heavy atoms are not as efficient as hydrogen in slowing neutrons down.

**Table 10.1**  
Typical Slowing Down Parameters

Material	Mass	$\alpha$	$\xi$	$n^*$
Hydrogen	1	0	1.000	14.5
H <sub>2</sub> O	—	—	0.920	15.8
Deuterium	2	0.111	0.725	20.0
D <sub>2</sub> O	—	—	0.509	28.5
Beryllium	9	0.640	0.209	69.4
Carbon	12	0.716	0.158	91.3
Oxygen	16	0.779	0.120	121.
Sodium	23	0.840	0.0825	176.
Iron	56	0.931	0.0357	407.
Uranium	238	0.983	0.00838	1730.

\*Slowing down from 2 MeV to 1 eV

The asymptotic slowing down density results are easily extended to the case of a mixture of different scattering isotopes because the equations are *linear*. Basically, we obtain the same result as before with  $\xi$  replaced by an appropriate average. Hence, the solution for the flux is simply

$$\phi(E) = \frac{S_0}{\xi \sum_s (E) E}. \quad (10.60)$$

The average value of  $\xi$  is a function of energy because of the

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way in which the different isotopes are weighted by their macroscopic scattering cross sections. The result can be shown to be

$$\bar{\xi}(E) = \frac{\sum_{i=1}^N \xi_i \Sigma_s^i(E)}{\sum_{i=1}^N \Sigma_s^i(E)}. \quad (10.61)$$

When the cross sections are relatively constant, the value of  $\bar{\xi}$  is also relatively constant. However, it should be noted that this averaging procedure is *not* strictly correct when hydrogen is present in the mixture since the hydrogen scattering contribution is *not* really asymptotic, i.e., some neutrons can scatter directly from the source. Therefore, hydrogen is often treated separately from the other materials in a mixed medium.

### 10.7\* Slowing Down in Hydrogen With Absorption

The Boltzmann equation for the space- and time-independent case, with uniformly distributed isotropic sources plus absorption, can be written in terms of lethargy, where the maximum source lethargy is  $u = 0$ . The balance equation is the following,

$$\text{removal} \quad \text{source} \quad \text{inscatter} \quad (10.62)$$

$$\Sigma_T(u)\phi(u) = S(u) + \int_0^u \Sigma_s(u')\phi(u')P(u' \rightarrow u)du'.$$

Consider the case of hydrogen atoms mixed with absorber atoms that are in essence "infinitely heavy," so that little energy transfer occurs in a scattering event. The equation can be written so that there is a separate contribution for each

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scattering term. For the heavy atoms, the highest possible energy providing scattering to  $E$  is  $E/\alpha$ , which corresponds to  $(u - \ln 1/\alpha)$ . Using the superscript H for hydrogen and A for absorber, we have the expanded balance equation,

$$\begin{aligned}
 & [\Sigma_s^H + \Sigma_a^H + \Sigma_s^A + \Sigma_a^A] \phi(u) = S(u) \\
 & + \int_0^u \Sigma_s^H(u') \phi(u') e^{u'-u} du' + \int_{u-\ln 1/\alpha}^u \Sigma_s^A(u') \phi(u') \frac{e^{u'-u}}{1-\alpha} du'.
 \end{aligned} \tag{10.63}$$

Now, if the absorber atom is infinitely heavy,  $\alpha \rightarrow 1$  and the amount of energy transferred in an elastic collision approaches 0. The range on the second integral term becomes very small, and therefore the product  $\Sigma_s^A(u) \phi(u)$  can be factored out of the integral giving

$$\begin{aligned}
 & \int_{u-\ln 1/\alpha}^u \Sigma_s^A(u') \phi(u') \frac{e^{u'-u}}{1-\alpha} du' \\
 & \approx \Sigma_s^A(u) \phi(u) \int_{u-\ln 1/\alpha}^u \frac{e^{u'-u}}{1-\alpha} du' \rightarrow \Sigma_s^A(u) \phi(u).
 \end{aligned} \tag{10.64}$$

Hence, the second integral term approaches the total scattering rate for the absorber atoms. As far as the original balance equation is concerned, the scattering due to the heavy absorber atoms appears in the same way on both sides of the equation, which means that it cancels out and we can ignore it. The balance equation then becomes

$$(\Sigma_s^H + \Sigma_a^H + \Sigma_a^A) \phi(u) = S(u) + \int_0^u \Sigma_s^H(u') \phi(u') e^{u'-u} du'. \tag{10.65}$$

It will simplify our work to define a new total removal cross section, excluding heavy atom scattering, as

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$$\Sigma_T' \equiv \Sigma_s^H + \Sigma_a^H + \Sigma_a^A.$$

Also

$$\Sigma_a \equiv \Sigma_a^H + \Sigma_a^A = \Sigma_T' - \Sigma_s^H.$$

**Conversion to a Differential Equation.** In order to solve the above integral equation, we must convert it to a differential equation. We accomplish this by a complicated series of steps. Recall that the slowing down density in pure hydrogen is given by Eq. (10.39). This is equal to the integral term that appears in Eq. (10.65). We, therefore, represent this integral by  $q(u)$ , i.e.,

$$q(u) = \int_0^u \Sigma_s^H(u') \phi(u') e^{u'-u} du', \quad (10.66)$$

because in this case all the slowing down is accomplished by scattering by hydrogen. We differentiate the above expression obtaining

$$\frac{dq}{du} = \Sigma_s^H(u) \phi(u) - \int_0^u \Sigma_s^H(u') \phi(u') e^{u'-u} du'. \quad (10.67)$$

Since the integral term reappears, we can add Eqs. (10.66) and (10.67) to eliminate the integral and obtain

$$q(u) + \frac{dq}{du} = \Sigma_s^H(u) \phi(u). \quad (10.68)$$

We return to the balance equation and replace the integral term by  $q(u)$ . This gives

$$q(u) = \Sigma_T'(u) \phi(u) - S(u). \quad (10.69)$$

By defining the total collision density as  $F(u) \equiv \Sigma_T'(u) \phi(u)$ , which now contains absorption, one obtains the form

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$$q(u) = F(u) - S(u). \quad (10.70)$$

The derivative of this expression is

$$\frac{dq}{du} = \frac{dF}{du} - \frac{dS}{du}. \quad (10.71)$$

Now, we have one expression that contains both  $q(u)$  and  $dq/du$ . We also have an expression derived from the balance equation for each of these quantities. Combining Eqs. (10.68), (10.70), and (10.71) to eliminate terms in  $q$ , we obtain the form

$$F(u) - S(u) + \frac{dF}{du} - \frac{dS}{du} = \frac{\Sigma_s^H(u)}{\Sigma_T'(u)} F(u). \quad (10.72)$$

This can be rearranged into a separable differential equation of the form

$$\frac{dF}{du} + \frac{\Sigma_a(u)}{\Sigma_T'(u)} F(u) = \frac{dS}{du} + S(u). \quad (10.73)$$

**Nonabsorption Probability for Constant  $\Sigma_a/\Sigma_T'$ .** The above equation is a first-order, inhomogeneous ordinary differential equation with variable coefficients. We have succeeded in converting the integral equation into a differential equation, just as we did for the case where there was no absorption. However, we can't really go much further unless we specify the source and simplify the cross section dependence on energy. Hence, we will assume that  $\Sigma_a/\Sigma_T' = \text{constant}$ , and also assume that the source is mono-energetic and of strength  $S_0$  at energy  $E_0$ .

Take the energy-dependent first-collision source to be

$$S(u) = S_0 e^{-u}. \quad (10.74)$$

The derivative of this expression is

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$$\frac{dS}{du} = -S_o e^{-u}. \quad (10.75)$$

Hence, if we apply our two restrictions, Eq. (10.73) reduces to a first-order equation with constant coefficients, namely,

$$\frac{dF}{du} + \frac{\Sigma_a}{\Sigma_T} F = 0. \quad (10.76)$$

This equation can be solved using the integrating factor

$$\rho(u) = e^{\frac{\Sigma_a}{\Sigma_T} u}, \quad (10.77)$$

to obtain the solution

$$F(u) = C e^{-\frac{\Sigma_a}{\Sigma_T} u}. \quad (10.78)$$

To find the constant of integration, we evaluate Eqs. (10.78) and (10.74) at  $u = 0$  to obtain

$$F(0) = C = S(0) = S_0. \quad (10.79)$$

Hence, the final result is

$$F(u) = S_o e^{-\frac{\Sigma_a}{\Sigma_T} u}, \quad (10.80)$$

or

$$\phi(u) = \frac{S_o e^{-\frac{\Sigma_a}{\Sigma_T} u}}{\Sigma_T(u)}. \quad (10.81)$$

Note that this is the same  $1/E$  flux distribution obtained previously for hydrogen, multiplied by a factor

$$p(u) = e^{-\frac{\Sigma_a}{\Sigma_T} u}. \quad (10.82)$$

We can refer to  $p(u)$  as being the *non-absorption probability*,

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since it approaches unity as  $\Sigma_a$  approaches zero, and approaches zero as  $\Sigma_a$  becomes very large.

We can also write down a *direct physical definition* for the non-absorption probability by integrating the total absorption rate down to lethargy  $u$  normalized to the corresponding total source emission rate. This gives the equation

$$p(u) = 1 - \frac{\int_0^u \Sigma_a(u') \phi(u') du'}{\int_0^\infty S(u') du'}. \quad (10.83)$$

The above result is *always* valid, but the calculation depends upon first knowing  $\phi(u)$ . Another useful result of the same type can be obtained by combining Eqs. (10.68) and (10.69), which gives

$$\frac{dq}{du} = S(u) - \Sigma_a(u) \phi(u). \quad (10.84)$$

This equation states that the change in slowing down density in a lethargy interval  $du$  wide is equal to the source contribution minus the absorption taking place in the interval.

Unfortunately, if the absorption varies rapidly in the interval, the flux usually also varies rapidly making it difficult to calculate  $dq/du$  accurately.

### 10.8\* Special Cases of Slowing Down With Absorption, $A > 1$ .

In the general case, we cannot analytically solve the slowing down equation for moderators having  $A > 1$  in the presence of absorption. However, we can obtain approximate results for certain special cases, and these serve to give us some insight into the types of solutions expected in general.



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**Constant  $\Sigma_a/\Sigma_s$ .** For example, let us look at the asymptotic case where the ratio of absorption to scattering is constant as a function of energy. We assume that  $\Sigma_a(u)/\Sigma_s(u) = \text{constant}$  and  $\Sigma_a$  is small compared to  $\Sigma_s$ . We then solve the integral equation in the asymptotic region, far from the source energy. In terms of collision density, the balance equation is

$$\begin{array}{cc} \text{removal} & \text{inscatter} \\ F(u) = \int_{u-\ell n l/\alpha}^u \frac{\Sigma_s(u') F(u') e^{u'-u}}{\Sigma_T(u') (1 - \alpha)} du' & (10.85) \end{array}$$

The key point, which makes a solution possible, is the fact that the ratio  $\Sigma_s/\Sigma_T$  is constant and can be taken outside of the integral. Then, as shown in Ferziger and Zweifel, a Laplace transform method leads to the approximate asymptotic solution,

$$F(u) \approx \frac{\exp\left(-\frac{\Sigma_a}{\xi \Sigma_T} u\right)}{\xi}. \quad (10.86)$$

Instead of deriving this solution directly, we simply insert it into the integral equation and derive the conditions for its validity. Upon substitution, one obtains

$$\begin{aligned} \frac{\exp\left(-\frac{\Sigma_a}{\xi \Sigma_T} u\right)}{\xi} &\approx \frac{\Sigma_s e^{-u}}{\Sigma_T \xi} \int_{u-\ell n l/\alpha}^u \frac{\exp\left(1 - \frac{\Sigma_a}{\xi \Sigma_T} u'\right)}{1 - \alpha} du' \\ &= \left(\frac{\Sigma_s}{\xi \Sigma_T - \Sigma_a}\right) \left[ \frac{\exp\left(-\frac{\Sigma_a}{\xi \Sigma_T} u\right)}{1 - \alpha} \right] \left[ 1 - \alpha \exp\left(\frac{\Sigma_a}{\xi \Sigma_T} \ell n \frac{l}{\alpha}\right) \right]. \end{aligned} \quad (10.87)$$

Now, if the absorption is small, so that  $\Sigma_a \ll \Sigma_s$  and  $\Sigma_t \approx \Sigma_s$ ,

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then

$$\frac{\Sigma_s}{\xi \Sigma_T - \Sigma_a} \rightarrow \frac{1}{\xi}$$

and

$$\exp\left(\frac{\Sigma_a}{\xi \Sigma_T} \ln \frac{1}{\alpha}\right) \rightarrow 1,$$

leading to an equality.

For the case where absorption is small and the ratio of absorption to scattering is not a function of energy, the slowing down density indeed varies slowly with lethargy. For this case we can compute the non-absorption probability directly from Eq. (10.83). For a unit source at  $u = 0$ ,

$$p(u) = 1 - \int_0^u \Sigma_a(u') \phi(u') du'. \quad (10.88)$$

Inserting  $\phi(u) = F(u) / \Sigma_T(u)$ , we obtain

$$\begin{aligned} p(u) &= 1 - \int_0^u \frac{\Sigma_a}{\xi \Sigma_T} \exp\left(-\frac{\Sigma_a}{\xi \Sigma_T} u'\right) du' \\ &= \exp\left(-\frac{\Sigma_a}{\xi \Sigma_T} u\right). \end{aligned} \quad (10.89)$$

Note that this result is very similar to the result obtained for the case of hydrogen mixed with a non-scattering absorber. We have simply multiplied  $\Sigma_T$  in the denominator by  $\xi$ . Therefore, the average logarithmic decrement enters whenever  $A > 1$ , both in the collision density and in the non-absorption probability. The corresponding flux varies as

$$\phi(u) = \frac{S_0 p(u)}{\xi \Sigma_T(u)}. \quad (10.90)$$

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**Slowly Varying Capture.** Another special case is the case of slowly varying capture. We use the Grueling-Goertzel approximation, which consists of employing a truncated Taylor series expansion for the collision density in the asymptotic slowing down region. Recall that the slowing down density is strictly a function of the scattering rate in the medium, which is defined as

$$F_s(u) \equiv \sum_s(u) \phi(u).$$

As before, we write the asymptotic balance equation

$$q(E) = \int_E^{E/\alpha} F_s(E') \left[ \frac{E - \alpha E'}{E' - \alpha E'} \right] dE'.$$

In terms of lethargy this becomes

$$q(u) = \int_{u-\ln 1/\alpha}^u F_s(u') \left[ \frac{e^{u'-u} - \alpha}{1 - \alpha} \right] du', \quad (10.91)$$

where the transition between forms is trivial when one recalls that

$$\frac{E}{E'} = e^{u'-u}.$$

A second useful equation can be obtained by taking the derivative of  $q$  with respect to  $u$  in a manner similar to that used for hydrogen mixed with a non-scattering absorber. Using Leibniz's rule, the result is

$$\frac{dq}{du} = F_s(u) - \frac{1}{1 - \alpha} \int_{u-\ln 1/\alpha}^u F_s(u') e^{u'-u} du'. \quad (10.92)$$

Now, we make the approximation that  $F_s(u')$  varies slowly in a lethargy width so that it can be expanded in a truncated Taylor series about  $F_s(u)$  in both equations. What happens, of course, is that  $F_s(u')$  is essentially brought outside of the integral

# NUCLEAR REACTOR THEORY AND DESIGN

leaving an easily integrated function. Let

$$F_s(u') \approx F_s(u) + (u' - u) \frac{dF_s}{du}. \quad (10.93)$$

Equation (10.91) becomes

$$\begin{aligned} q(u) = & F_s(u) \int_{u-\ell n l / \alpha}^u \left[ \frac{e^{u'-u} - \alpha}{1 - \alpha} \right] du' \\ & + \frac{dF_s}{du} \int_{u-\ell n l / \alpha}^u (u' - u) \left[ \frac{e^{u'-u} - \alpha}{1 - \alpha} \right] du'. \end{aligned} \quad (10.94)$$

We have already evaluated the first integral in Eq. (10.94). Its value is

$$\int_{u-\ell n l / \alpha}^u \left[ \frac{e^{u'-u} - \alpha}{1 - \alpha} \right] du' = 1 + \frac{\alpha}{1 - \alpha} \ell n[\alpha] \equiv \xi. \quad (10.95)$$

The second integral is

$$\begin{aligned} & \int_{u-\ell n l / \alpha}^u (u' - u) \left[ \frac{e^{u'-u} - \alpha}{1 - \alpha} \right] du' \\ & = \frac{\alpha + \alpha \ell n \frac{1}{\alpha} + \frac{1}{2} \alpha \left( \ell n \frac{1}{\alpha} \right)^2 - 1}{1 - \alpha} \equiv a. \end{aligned} \quad (10.96)$$

In terms of the above definitions, we have the result,

$$q(u) = \xi F_s(u) + a \frac{dF_s}{du}. \quad (10.97)$$

The second equation, Eq. (10.92), becomes

## NUCLEAR REACTOR THEORY AND DESIGN

$$\frac{dq}{du} = F_s(u) - F_s(u) \int_{u-\ell n 1/\alpha}^u \frac{e^{u'-u}}{1-\alpha} du' \quad (10.98)$$

$$- \frac{dF_s}{du} \int_{u-\ell n 1/\alpha}^u \frac{(u' - u)e^{u'-u}}{1-\alpha} du'.$$

The first integral in Eq. (10.98) is unity and the second is in fact equal to  $-\xi$ , so that we obtain the differential equation

$$\frac{dq}{du} = \xi \frac{dF_s}{du}. \quad (10.99)$$

We can therefore combine Eqs. (10.97) and (10.99), eliminating the derivative  $dF_s/du$  to obtain the single equation

$$-a \frac{dq}{du} + \xi q(u) = \xi^2 F_s(u). \quad (10.100)$$

In order to proceed further, we require another equation describing  $dq/du$ . Recall that, in the absence of sources, Eq. (10.84) states that the slowing down density varies as

$$\frac{dq}{du} = -\Sigma_a(u)\phi(u). \quad (10.101)$$

Insertion of this result into Eq. (10.100) gives

$$a \Sigma_a(u)\phi(u) + \xi q(u) = \xi^2 \Sigma_s(u)\phi(u). \quad (10.102)$$

If we now divide through by  $\xi$  and define  $\gamma$  as

$$\gamma \equiv -\frac{a}{\xi}, \quad (10.103)$$

we obtain the flux expression for slowly varying capture, namely,

## NUCLEAR REACTOR THEORY AND DESIGN

$$\phi(u) = \frac{q(u)}{\xi \Sigma_s + \gamma \Sigma_a}. \quad (10.104)$$

By combining this result with Eq. (10.101) for  $dq/du$ , we obtain a separated differential equation in  $q(u)$ , namely,

$$\frac{dq}{q(u)} = \left[ \frac{\Sigma_a(u)}{\xi \Sigma_s(u) + \gamma \Sigma_a(u)} \right] du. \quad (10.105)$$

This equation can readily be integrated using the initial condition that  $q(0) = S_0$  to obtain

$$q(u) = S_0 \exp \left[ - \int_0^u \frac{\Sigma_a(u')}{\xi \Sigma_s(u') + \gamma \Sigma_a(u')} du' \right]. \quad (10.106)$$

The exponential term is easily recognized as a form of the non-absorption probability

$$p(u) = \frac{q(u)}{S_0} = \exp \left[ - \int_0^u \frac{\Sigma_a(u')}{\xi \Sigma_s(u') + \gamma \Sigma_a(u')} du' \right]. \quad (10.107)$$

Hence, the final form for the flux solution is

$$\phi(u) = \frac{S_0 p(u)}{\xi \Sigma_s + \gamma \Sigma_a}. \quad (10.108)$$

Note the similarity to previous equations. The primary difference is that  $\Sigma_a$  has its own coefficient. Values of the coefficients for several common moderators are given in Table 10.2. One sees that the magnitudes of  $\xi$  and  $\gamma$  are not greatly different, so that using the quantity  $\xi \Sigma_T$  is not a bad approximation to using the sum of  $\xi \Sigma_s$  and  $\gamma \Sigma_a$  in the non-absorption probability expression, especially if  $\Sigma_a$  is small compared to  $\Sigma_s$ .

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**Table 10.2**

Slowing Down Parameters for Selected Moderators

Element	A	$\alpha$	$\xi$	$\gamma$
Hydrogen	1	0	1.000	1.000
Deuterium	2	0.111	0.725	0.583
Beryllium	9	0.640	0.209	0.149
Carbon	12	0.716	0.158	0.116

### 10.9 Final Comments

The net conclusion from all of the analytic solutions obtained thus far is that the flux over most of the energy range of interest varies as approximately  $1/E$ . This is caused by the basic nature of the scattering process. Smooth absorption acts to slowly decrease the flux as energy decreases relative to the flux solution without absorption. Hence, the use of a  $1/E$  weighting function to process multi-group cross section libraries is quite reasonable.

Up to this point we have examined cases where  $\Sigma_a$  is small, or where it is essentially constant ( $\Sigma_a/\Sigma_T = \text{constant}$ ), or where it varies slowly in the energy range of  $E$  to  $\alpha E$ . A resonance violates all of these conditions. In a resonance, the absorption is large, it does not vary in proportion to the scattering cross section and it varies rapidly in a small energy interval. Hence, a more sophisticated treatment is required. The treatment of resonances, and slowing down in the presence of resonances, is covered in Chapter 11.

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### Problems

- 10.1 Suppose that the differential elastic scattering cross section for hydrogen at some energy is given by the expression

$$\sigma_s(\Theta) = a + b \cos \Theta + c \cos^2 \Theta,$$

where  $\Theta$  is the CM scattering angle.

- a) Derive the total scattering cross section at this energy.
  - b) Derive the average logarithmic energy decrement  $\xi$ , i.e., the average increase in lethargy per collision, assuming that the differential cross section for hydrogen is as given above.
  - c) What is the energy distribution of once scattered neutrons given a mono-energetic neutron source of energy  $E_0$ ? Plot this probability distribution,  $P(E_0 \rightarrow E)$  vs.  $E$ , if  $E_0 = 1$  MeV, for assumed values of  $a$ ,  $b$  and  $c$ .
- 10.2 Show that the elastic scattering probability  $P(E \rightarrow E')$  is normalized to unity, irrespective of whether or not the scattering is isotropic in the CM system.
- 10.3\* Consider a mono-energetic neutron source which is uniformly distributed in a non-absorbing infinite medium of mass  $A > 1$ . For the successive collisions method, the balance equation governing the collision density of all neutrons that have suffered three collisions after emission from a mono-energetic source at energy  $E_0$  is of the form

$$F_3(E) = \int_0^E \frac{F_2(E') dE'}{(1 - \alpha)E'},$$



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valid over ? > E > ?

- a) For each region which contributes to  $F_3(E)$ , draw the appropriate energy scattering diagram or diagrams which allow determination of the limits of the integral. Replace all question marks with the appropriate values.
- b) Derive an analytical expression for  $F_3(E)$  which is valid over each allowable collision interval.
- c) Evaluate  $F_3(E)$  and its first two derivatives at the boundaries of each allowable collision interval, and comment on the results.

**10.4\*** Consider a mono-energetic neutron source at energy  $E_0$  which is uniformly distributed in a non-absorbing medium of mass  $A > 1$ . We shall make a separate neutron balance over each successive collision interval.

- a) Derive the integral balance equation for the collision density in the first collision interval,  $F^{(1)}(E)$ , valid between  $E_0$  and  $\alpha E_0$ .
- b) Differentiate the integral equation found in part a) and then integrate the resulting differential equation to obtain an expression for  $F^{(1)}(E)$ .
- c) The balance equation for the collision density in the second collision interval is of the form

$$F^{(2)}(E) = \int_{?}^{?} \frac{F^{(?)}(E') dE'}{(1 - \alpha)E'};$$

valid over ? > E > ?

Draw the appropriate energy scattering diagrams that allow determination of the limits of the integrals. Replace all question marks with the appropriate values.

- d) Differentiate this equation and integrate the

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resulting differential equation to find an expression for  $F^{(2)}(E)$ .

- e) Discuss the consequences of having a mixture of two scattering isotopes instead of just one.

**10.5** Derive the expression for  $\xi$  given by Eq. (10.50) by evaluating the integral given in Eq. (10.48). Show that  $\overline{\Delta u} = \xi$  by evaluating the integral in Eq. (10.56).

**10.6** Assume that the ratio of scattering to absorption is equal to 100 in a material having the moderating properties of beryllium, independent of energy. For moderation from 10 MeV to 1 eV, what is the non-absorption probability computed according to the constant  $\Sigma_a/\Sigma_s$  and slowly-varying capture models?

## References

- S. Glasstone** and **M.C. Edlund**, op. cit., Chapter 6.  
**J.R. Lamarsh**, op. cit., Chapter 6.  
**J.H. Ferziger** and **P.F. Zweifel**, op. cit., Chapter 2.  
**A.M. Weinberg** and **E.P. Wigner**, op. cit., Chapter 11.

## SLOWING DOWN IN THE PRESENCE OF RESONANCES

Reactors are composed of a combination of fuel, coolant and structural materials. For a typical reactor, there is an energy range from 10 MeV down to approximately 10 KeV where essentially pure slowing down takes place. In this region, the problem can be treated using the methods of Chapter 10. Below 10 KeV, many important materials possess resonances, requiring a modified treatment. For example, all reactors contain fissile and fertile materials, such as uranium, plutonium and thorium, each of which has a large number of closely spaced resonances above approximately 5 eV. Many control poisons, such as silver, indium, cadmium, gadolinium and hafnium have significant resonances in the eV range. Even sodium, a coolant for fast reactors, has some important resonances.

Before proceeding to the calculation of resonance absorption during slowing down, we must first examine the structure of a single resonance. To complicate matters, the absorber atoms are in thermal motion with speeds comparable to those of the neutron.

This relative motion gives rise to a Doppler effect, which must also be included. Fortunately, the Doppler effect is an inherent safety feature of nuclear reactors that helps to mitigate the effects of an accidental positive-reactivity power excursion. Under these circumstances, the fuel heats up, resonance absorption increases and this provides a negative reactivity insertion that reduces the power again.

To complicate matters even more, fuel and moderator materials are usually heterogeneously arranged in order to allow

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some of the neutrons to bypass the resonances by having a portion of their scattering collisions occur in the moderator region rather than in the fuel. The formulation of the heterogeneous neutron balance equation in a spatial cell requires the development of ideas such as region escape probabilities, Dancoff corrections for the presence of adjacent cells, and the concept of spatial reciprocity.

Finally, all of these ideas are put together into the formulation of a set of slowing down equations that can be solved by computer. The equations described here are used in the GAM code, and form what is known as a multi-group  $P_1$  treatment. We use the GAM code separately for each type of fuel assembly or reflector region to obtain the few-group cross sections for the fast groups of a multidimensional reactor design code such as EXTERMINATOR or VENTURE. The method of obtaining the corresponding few-group cross sections for the single thermal group of each assembly is the subject of Chapter 12.

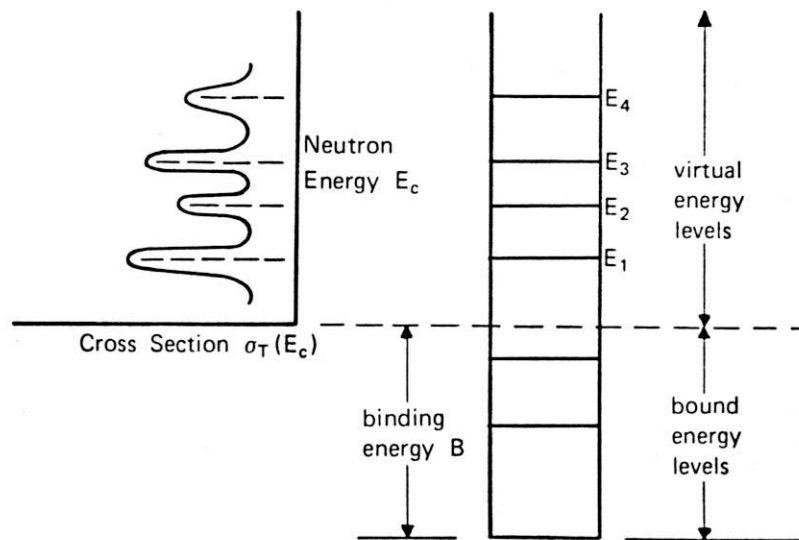
### 11.1 Resonance Cross Sections

Most neutron reactions in the energy range of interest for nuclear reactors proceed via a two-step process. First, the neutron is absorbed, thus forming an excited compound nucleus. Subsequently, the compound nucleus decays through various exit channels such as scattering, radiative capture, fission, etc. The interaction of the neutron with the nucleus is wave-mechanical in nature, and can be modeled by solving the Schrödinger wave equation both inside and outside of the compound nucleus taking into account an appropriate potential energy distribution. Since neutrons are uncharged particles, there is no Coulomb barrier to be overcome, so that the potential energy distribution can be approximated by a uniform square potential

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well existing inside the nuclear volume.

The resulting cross section curve as a function of incident neutron energy exhibits a resonance structure, as seen symbolically in Figure 11.1. The resonance peaks are related to the virtual energy levels in the compound nucleus, which are a function of the angular momentum  $I$ , binding energy  $B$  and the nuclear radius  $R$  of the nucleus in question. A detailed examination of an actual cross-section curve indicates that the values of the cross sections in the resonance peaks may be several orders of magnitude greater than in the valleys. In heavy nuclei, the levels are narrowly spaced and many low-energy resonances are observed. In light nuclei, the levels are widely spaced and the behavior of the cross sections is relatively smooth over a wide range of energies.



**Fig. 11.1** Resonance Cross section vs. Virtual Levels in the Compound Nucleus

A standard source of experimental cross section data in graphical form is the Brookhaven National Laboratory BNL-325 report, which is sometimes referred to as the "barn book". For

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computational purposes, numerical data are extracted from evaluated nuclear data files such as the American ENDF-B file or the European JEF file.

### Formation of the Compound Nucleus

In the case of narrowly-spaced resonances, which are close enough to overlap, the solution to the Schrödinger equation is fairly complicated. However, for a single isolated resonance, located at energy  $E_r$ , the solution can be put into a fairly simple form, namely,

$$\sigma_{CN}(E_c) = \pi \lambda_r^2 g \left( \frac{E_r}{E_c} \right)^{1/2} \left( \frac{\Gamma_n' \Gamma}{(E_c - E_r)^2 + \Gamma^2/4} \right). \quad (11.1)$$

The factors that appear in the equation are defined as follows:

$E_c$  is the kinetic energy of the neutron in the CM system;  
 $\lambda_r = \hbar p_r$  is the neutron wavelength, where the quantity  $p_r$  is the momentum of the system at the resonance energy computed using the reduced mass;  
 $g$  is defined as

$$g = \begin{cases} 1 & \text{for } I = 0 \\ 1/2 \left( \frac{2J+1}{2I+1} \right) & \text{for } I \neq 0 \end{cases},$$

and it is a statistical spin factor which is proportional to the angular momentum of the target nucleus,  $I$ , and the angular momentum of the compound nucleus  $J$ ;

$\Gamma$  is the total level width of the resonance in energy units, defined as the total decay constant for de-exciting the level multiplied by  $\hbar$ , which is the rationalized Planck's constant. The total level width is the sum of the partial level widths, i.e.,

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$$\Gamma = \Gamma_{\gamma} + \Gamma_n^r + \Gamma_f + \dots;$$

$\Gamma_{\gamma}$  is the radiative capture width;

$\Gamma_n^r$  is the neutron emission width evaluated at the resonance energy; and

$\Gamma_f$  is the fission width.

The above equation is known as the Breit-Wigner single level formula, originally derived in 1936. Other forms, such as the R-Matrix representation, exist for the more complicated cases.

If one evaluates the Breit-Wigner expression at the resonance energy, that is at  $E_c = E_r$ , one obtains a value for the maximum cross section for the formation of the compound nucleus, namely,

$$\sigma_{CN}(E_r) \equiv \sigma_r = 4\pi \lambda_r^2 g \frac{\Gamma_n^r}{\Gamma}. \quad (11.2)$$

Furthermore if the resonance is fairly narrow so that the factor  $\sqrt{E_r/E_c} \approx 1$ , then the cross section evaluated at an energy of  $E_c = E_r \pm \Gamma/2$  is approximately

$$\sigma_{CN}\left(E_r \pm \frac{\Gamma}{2}\right) \approx \frac{\sigma_r}{2}. \quad (11.3)$$

In principle, one can obtain the total emission width  $\Gamma$  experimentally by measuring the width of the resonance peak at  $\frac{1}{2}$  the maximum cross section value. In practice because of the finite resolution of available neutron monochromators and detectors, the determination must be made indirectly by measuring the neutron transmission through both thin samples and thick samples and relating the results to the area under the resonance curve. It can be shown quite generally that the area under a narrow resonance, where  $\sqrt{E_r/E_c} \approx 1$ , is

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$$\int_{-\infty}^{+\infty} \sigma_{CN}(E_c) dE_c \approx \frac{\sigma_r \Gamma \pi}{2}. \quad (11.4)$$

This is true irrespective of instrumental resolution or broadening caused by thermal agitation of the absorber atoms.

**Radiative Capture.** The de-excitation of the compound nucleus is directly proportional to the ratio of the level width of the particular exit channel under consideration to the total level width. Hence, for radiative capture the appropriate expression is

$$\sigma_c(E_c) = \frac{\Gamma_\gamma}{\Gamma} \sigma_{CN}(E_c) = \pi \lambda_r^2 g \left( \frac{E_r}{E_c} \right)^{1/2} \frac{\Gamma_n^r \Gamma_\gamma}{(E_c - E_r)^2 + \Gamma^2/4}. \quad (11.5)$$

A similar expression can also be written for fission, when it is energetically possible. The capture cross section can be written in a fairly convenient form by defining a new dimensionless quantity  $y$  as

$$y \equiv \frac{2}{\Gamma} (E_c - E_r). \quad (11.6)$$

In terms of the maximum total cross section, the capture cross-section expression becomes

$$\sigma_c(E_c) = \frac{\sigma_r \Gamma_\gamma}{\Gamma} \left( \frac{E_r}{E_c} \right)^{1/2} \left( \frac{1}{1 + y^2} \right). \quad (11.7)$$

At low energy, well below the resonance energy, all of the factors in the equation are essentially constant except for  $E_c$ . The factor  $(E_c - E_r)^2$  is large and almost constant so that the low-energy behavior is approximately

$$\sigma_c(E_c) \approx \frac{\text{constant}}{v}. \quad (11.8)$$



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This is the well-known  $1/v$  cross section behavior that is exhibited by reactions such as  $^{10}\text{B}$ ,  $^{109}\text{Ag}$ ,  $^6\text{Li}$ ,  $^{197}\text{Au}$ ,  $^{113}\text{Cd}$ , and  $^{115}\text{In}$  at energies well below their lowest resonance.

Since the neutron wavelength is inversely proportional to velocity, the wavelength of a slow neutron is very much greater than the size of the target nucleus and essentially all such neutron interactions are s-wave, i.e., head-on collisions with zero angular momentum.

**Elastic Scattering.** In the case of elastic scattering another quantum-mechanical effect appears that does not proceed through the formation of a compound nucleus. This is scattering from the nuclear surface. It is called potential scattering, and it corresponds to a billiard ball effect. The cross section at low energy is  $\sim 4\pi R^2$ , which is the surface area of a hard impenetrable sphere with a radius equal to the nuclear radius  $R$ . The projected area of the sphere is  $\pi R^2$ ; the factor 4 appears due to quantum effects.

Unfortunately, the formation of a compound nucleus competes with the potential scattering, leading to an interference term in the cross section formula. For s-wave scattering, the equation is

$$\sigma_s(E_c) = \frac{\text{compound nucleus}}{\frac{\pi \tilde{\chi}_r^2 g \Gamma_n^2}{(E_c - E_r)^2 + \Gamma^2/4}} + \frac{\text{interference}}{\frac{4\pi \tilde{\chi}_r g R (E_c - E_r) \Gamma_n^r}{(E_c - E_r)^2 + \Gamma^2/4}} + \frac{\text{potential}}{4\pi R^2}. \quad (11.9)$$

In terms of  $y$  and  $\sigma_r$ , this equation becomes

$$\sigma_s(E) = \frac{\sigma_r \Gamma_n^r}{\Gamma} \left( \frac{1}{1 + y^2} \right) + \frac{2\sigma_r R}{\tilde{\chi}_r} \left( \frac{y}{1 + y^2} \right) + 4\pi R^2. \quad (11.10)$$

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In the equations for radiative capture and elastic scattering, the wavelength and the neutron width are both *evaluated* at the resonance energy  $E_r$ . As a matter of fact, the neutron width is *not* a constant for a given resonance, but varies directly proportional to the neutron velocity. This accounts for the factor  $\sqrt{E_r/E_c}$  appearing in the radiative capture equation. The Breit-Wigner equation is often written in terms of the actual wavelength and the actual neutron width. The form is very similar to that given above because the factors containing energy conveniently cancel, i.e.,

$$\Gamma_n \tilde{\lambda} = \Gamma_n' \tilde{\lambda}_r. \quad (11.11)$$

Hence, we have an equation for radiative capture,

$$\sigma_c(E_c) = \pi \tilde{\lambda}^2 g \frac{\Gamma_n \Gamma_\gamma}{(E_c - E_r)^2 + \Gamma^2/4}, \quad (11.12)$$

and for elastic scattering,

$$\sigma_s(E_c) = \frac{\pi \tilde{\lambda}^2 g \Gamma_n^2}{(E_c - E_r)^2 + \Gamma^2/4} + \frac{4\pi \tilde{\lambda} g R (E_c - E_r) \Gamma_n}{(E_c - E_r)^2 + \Gamma^2/4} + 4\pi R^2. \quad (11.13)$$

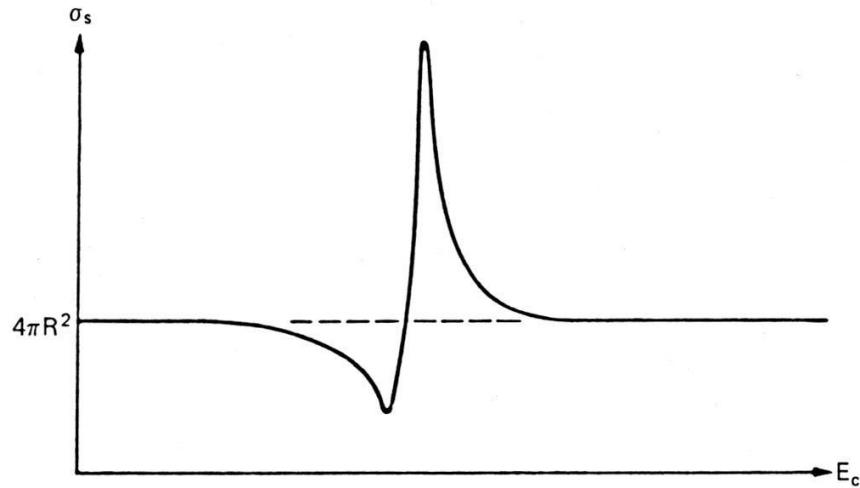
The sum of the two, when  $\Gamma_f = 0$ , is the total cross section

$$\sigma_T(E_c) = \frac{\pi \tilde{\lambda}^2 g \Gamma_n \Gamma}{(E_c - E_r)^2 + \Gamma^2/4} + \frac{4\pi \tilde{\lambda} g R (E_c - E_r) \Gamma_n}{(E_c - E_r)^2 + \Gamma^2/4} + 4\pi R^2. \quad (11.14)$$

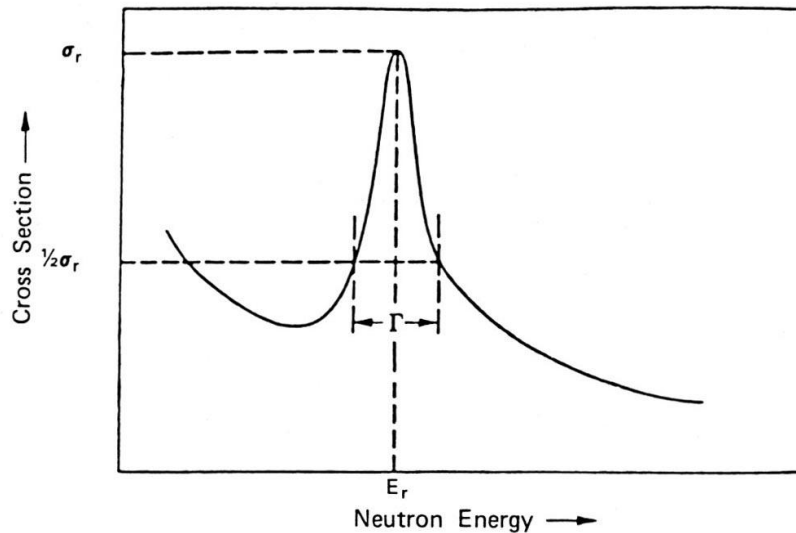
One sees that the interference term, if it is large, makes the elastic scattering cross section curve quite non-symmetric, while the potential scattering term provides a constant background cross section. A typical scattering cross section curve in the vicinity of a single isolated scattering resonance is shown in Figure 11.2. On the other hand, the absorption cross section due to radiative capture is almost symmetric except for the effect of the  $\sqrt{E_r/E_c}$  dependence, which gives a  $1/v$  tail at low energy as shown in Figure 11.3.

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Naturally, the total cross section is the sum of all of the possible modes of interaction, so that any given resonance is some linear combination of the two curves. The predominant form of interaction can often be discerned by examining the symmetry of an experimentally measured resonance curve.



**Fig. 11.2** Elastic Scattering Cross Section vs. Energy



**Fig. 11.3** Radiative Capture Cross Section vs. Energy for Pure Capture

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### 11.2 Doppler Effect

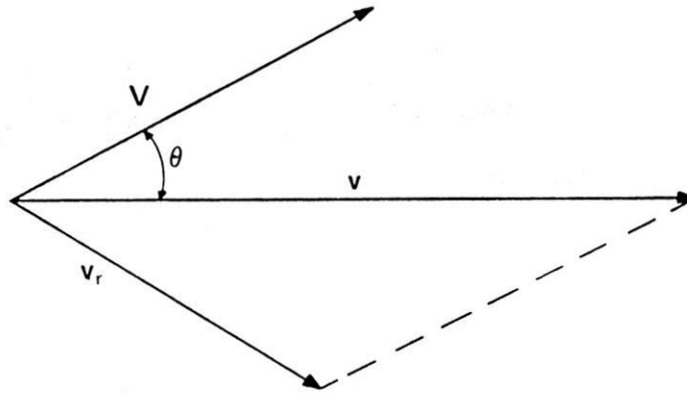
At energies in the resonance region of  $^{238}\text{U}$ , that is, from about 6 eV up to a few keV, the interaction rate of neutrons with uranium atoms may be influenced by the thermal motion of the atoms. Specifically, we have to calculate the reaction rate taking into account the *relative* velocity between the atom and the neutron that strikes it. This is called the Doppler effect.

For the moment, assume that all of the neutrons are traveling in a beam along the x-axis. This can be relaxed later by superposition of neutrons traveling in all directions. In this restricted case the velocity diagram for an interaction with a given atom is a vector diagram, as shown in Figure 11.4. We know that the kinetic energy of the two particles in the CM system is given in terms of their reduced mass  $\mu_r$  and the relative velocity between the particles. It is

$$E_c = \frac{1}{2} \mu_r v_r^2, \quad (11.15)$$

where  $v_r^2$  is a scalar, equal to

$$v_r^2 = \vec{v}_r \bullet \vec{v}_r = |\vec{v} - \vec{V}|^2. \quad (11.16)$$



**Fig. 11.4** Relative Velocity Diagram for a Neutron-Nucleus Interaction

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Expanding out, we obtain

$$\begin{aligned}
 v_r^2 &= v^2 + V^2 - 2\vec{V} \cdot \vec{v} \\
 &= v^2 + V^2 - 2vV \cos \theta \\
 &= v^2 + V^2 - 2vV_x \\
 &\approx v^2 - 2vV_x, \text{ since } V \ll v, \text{ usually.}
 \end{aligned}
 \tag{11.17}$$

Hence, we can express the CM energy in terms of the scalar neutron velocity and the x component of the velocity of the atom in the LAB system. In addition, for atoms such as uranium, the reduced mass is essentially equal to the neutron mass, i.e.,  $\mu_r \approx m$ . The CM energy is then related to the neutron energy and the x component of the atom velocity by the expression

$$E_c \approx E - \sqrt{2mE}V_x. \tag{11.18}$$

Now we examine the reaction rate assuming that we have a large number of atoms whose velocities are distributed according to some statistical law. What we would really like to do is to define an effective or average cross section such that the product of the neutron flux and the effective cross section gives the same reaction rate as the case where the relative velocity between the neutron and the atom is considered over the entire distribution of atom velocities. The defining expression is

$$\begin{aligned}
 \text{Reaction rate} &= \frac{\text{effective flux}}{\text{macroscopic sigma}} \equiv \frac{\text{relative sigma}}{\text{flux distribution}} \\
 (nv) N_0 \bar{\sigma}(E, T) &= \int_{-\infty}^{+\infty} n v_r N(\vec{V}) \sigma(E_c) d\vec{V}.
 \end{aligned}
 \tag{11.19}$$

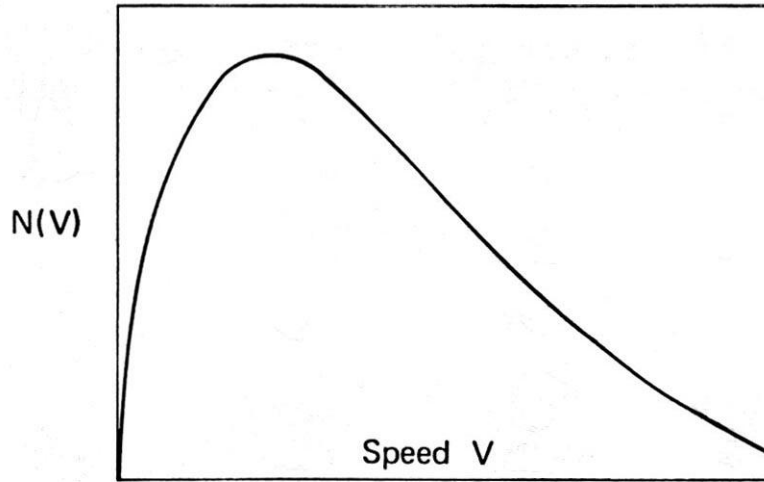
We know  $E_c$  in terms of  $V_x$ . Furthermore, we know  $v_r$  in terms of  $V_x$ . Hence, all we need is the vector velocity distribution of the atoms,  $N(\vec{V})$ , in order to carry out the integration. You are

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probably most familiar with the scalar Maxwellian distribution, which gives the number of particles having a given speed as a function of speed. This particular function is obtained by weighting a Gaussian distribution function by the volume element in velocity space, that is,

$$N(V)dV = \left[ N_0 \left( \frac{M}{2\pi kT} \right)^{3/2} e^{-MV^2/2kT} \right] 4\pi V^2 dV, \quad (11.20)$$

where  $M$  is the mass of the atom,  $k$  is Boltzmann's constant, and  $T$  is the absolute temperature of the medium. The scalar distribution, which has a nonzero mean, is plotted in Figure 11.5.



**Fig. 11.5** Scalar Maxwellian Distribution of Atom Velocities

In our specific application, we are interested in the directed distribution, which is the portion given above in square braces. This can be expanded into the form

$$N(\vec{V})d\vec{V} = N_0 \left( \frac{M}{2\pi kT} \right)^{3/2} e^{-MV_x^2/2kT} e^{-MV_y^2/2kT} e^{-MV_z^2/2kT} dV_x dV_y dV_z. \quad (11.21)$$

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Naturally,  $\vec{V} = \hat{i}V_x + \hat{j}V_y + \hat{k}V_z$ . The directed distribution has a zero mean, which simply states that as many particles go in one direction as go in exactly the opposite direction. This expression is separable in each of the three directions and has the normalization

$$\int_{-\infty}^{+\infty} N(\vec{V}) d\vec{V} = N_0. \quad (11.22)$$

Since only the x component of velocity appears in the reaction rate integral, the integrals over y and z can be done immediately, giving unity. The remaining integral contains just the x component and is of the form

$$nvN_0\bar{\sigma}(E,T) = \int_{-\infty}^{\infty} n_{V_r} N_0 \left( \frac{M}{2\pi kT} \right)^{1/2} e^{-MV_x^2/2kT} \sigma(E_c) dV_x. \quad (11.23)$$

The expression for the effective cross section can then be obtained by canceling common terms and dividing through by v.

All of the terms inside the integral are now known as a function of  $V_x$ . If we use the Breit-Wigner form for the cross section, the integral can be evaluated by making an appropriate change of variable. We must evaluate the expression separately for  $\bar{\sigma}_c$  and for  $\bar{\sigma}_s$ . For radiative capture, the expression becomes

$$\bar{\sigma}_c(E,T) = \left( \frac{M}{2\pi kT} \right)^{1/2} \left( \frac{\sigma_r \Gamma_\gamma}{\Gamma} \right) \quad (11.24)$$

$$x \int_{-\infty}^{\infty} \left( \frac{m E_c}{\mu_r E} \right)^{1/2} \left( \frac{E_r}{E_c} \right)^{1/2} \frac{e^{-MV_x^2/2kT}}{\left[ \frac{2(E_c - E_r)}{\Gamma} \right]^2 + 1} dV_x.$$

Recall that  $\mu_r \approx m$  and  $M/m = A$ , which is the atomic mass number of the atom.

Let the following substitutions be made:

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$$x \equiv \frac{2}{\Gamma}(E - E_\gamma), \quad (11.25)$$

$$y \equiv \frac{2}{\Gamma}(E_c - E_r).$$

Upon subtraction,

$$(x - y) = \frac{2}{\Gamma}(E - E_c) \approx \frac{2}{\Gamma}\sqrt{2mE} V_x. \quad (11.26)$$

Since  $x$  is not dependent upon  $V_x$ , the derivative of this expression is

$$dy = -\frac{2}{\Gamma}\sqrt{2mE} dV_x. \quad (10.27)$$

The integration over  $V_x$  can now be replaced by an equivalent integration over the variable  $y$ . The limits remain the same as before because the minus sign is absorbed in the variable change. The factor in the exponential term is expressed in terms of  $(x - y)$  as follows. Write

$$\frac{MV_x^2}{2kT} = \frac{M}{2kT} \frac{(x - y)^2 \Gamma^2}{8mE} \quad (11.28)$$

and define a new coefficient

$$\zeta^2 \equiv \frac{\Gamma^2 \left( \frac{M}{m} \right)}{4EkT} = \frac{\Gamma^2 A}{4EkT}. \quad (11.29)$$

In terms of this coefficient,

$$\frac{MV_x^2}{2kT} = \frac{\zeta^2}{4}(x - y)^2. \quad (11.30)$$

Using the above definitions, a final form of the expression



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for the effective capture cross section is obtained. The result is the temperature-dependent cross section,

$$\bar{\sigma}_c(E,T) = \frac{\sigma_r \Gamma_\gamma}{\Gamma} \sqrt{\frac{E_r}{E}} \frac{\zeta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{1}{4}\zeta^2(x-y)^2\right]}{1+y^2} dy \quad (11.31)$$

$$\equiv \frac{\sigma_r \Gamma_\gamma}{\Gamma} \sqrt{\frac{E_r}{E}} \psi(\zeta, x).$$

The Doppler function,  $\psi(\zeta, x)$ , has been computed numerically. It is given in Table 11.1, and it is also available in the form of a graph.

It is also convenient to define the term  $\Gamma_D$ , called the Doppler width, in the following fashion:

$$\Gamma_D \equiv \left(\frac{4EkT}{A}\right)^{1/2} \approx \left(\frac{4E_r kT}{A}\right)^{1/2}. \quad (11.32)$$

This is a measure of the width of a narrow energy line due to pure thermal agitation of the atoms. By comparison, one sees that the factor

$$\zeta = \frac{\Gamma}{\Gamma_D} \quad (11.33)$$

is a measure of the actual width of the resonance compared to a temperature-broadened line.

The important thing to notice is that the Doppler effect competes with the natural line width and hence there should exist some limiting functional dependence. When  $\Gamma_D \gg \Gamma$ , which could occur at high temperature, the natural shape of the resonance is masked by the Doppler effect and the cross-section curve is a Gaussian peak. When  $\Gamma_D \ll \Gamma$ , The Doppler effect is negligible

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and the cross-section curve has the pure Breit-Wigner shape.

The latter point can be proven fairly easily. As  $T$  approaches absolute zero,  $\Gamma_D$  becomes very small compared to  $\Gamma$  and  $\zeta \rightarrow \infty$ . The function

$$\lim_{\zeta \rightarrow \infty} \frac{\zeta}{2\sqrt{\pi}} \exp\left(-\frac{\zeta^2}{4}(x-y)^2\right) = \delta(x-y), \quad (11.34)$$

where  $\delta$  is the Dirac delta function. Hence,

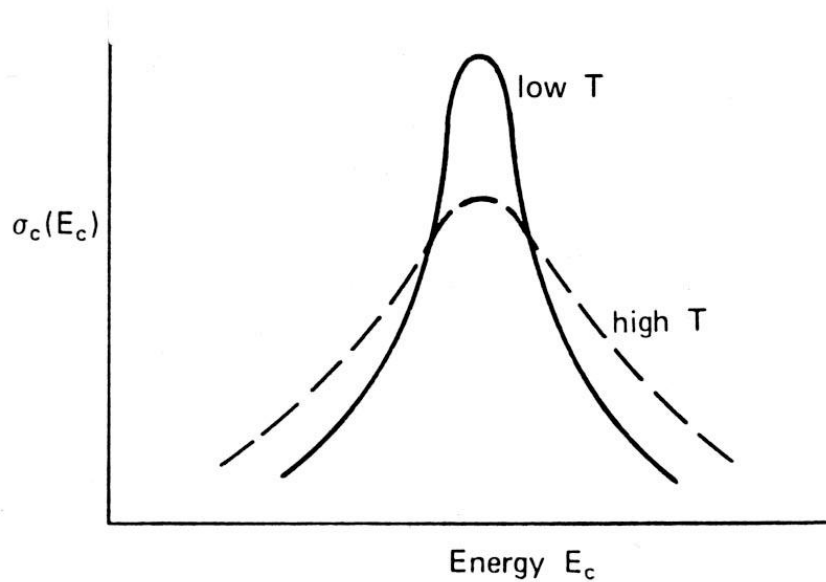
$$\lim_{\zeta \rightarrow \infty} \psi(\zeta, x) = \frac{I}{I + x^2}, \quad (11.35)$$

which is the natural line shape.

Furthermore, the area under the Doppler shape function is independent of  $x$ , and in particular is given by the integral

$$\int_{-\infty}^{+\infty} \psi(\zeta, x) dx = \pi. \quad (11.36)$$

The effect of changing the temperature is shown in Figure 11.6, where the area under the two curves is the same.



**Fig. 11.6** Capture Cross Section vs. Temperature

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The interference part of the scattering cross section is also Doppler broadened. Following a similar derivation, we obtain the interference Doppler shape function

$$\chi(\zeta, x) \equiv \frac{\zeta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left(-\frac{\zeta^2}{4}(x-y)^2\right)}{1+y^2} 2y dy. \quad (11.37)$$

$\chi(\zeta, x)$  is related to  $\psi(\zeta, x)$  by the differential equation

$$\psi(\zeta, x) = 2x\psi(\zeta, x) + \frac{4}{\zeta^2} \frac{d\psi(\zeta, x)}{dx}. \quad (10.38)$$

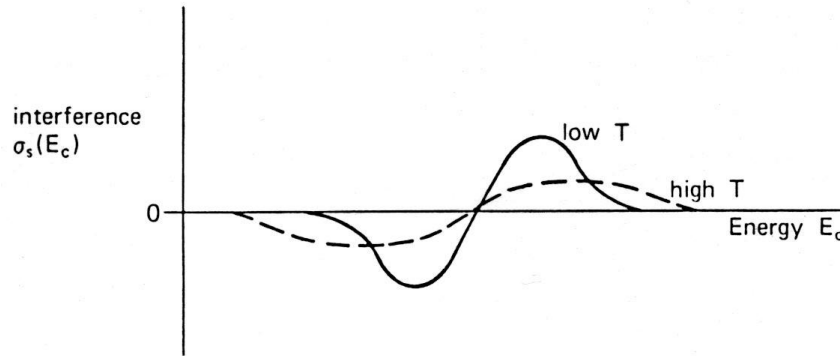
This function has also been tabulated and is given in Table 11.1. When the Doppler width is small,  $\chi(\zeta, x)$  approaches the natural line shape, i.e.,

$$\lim_{\zeta \rightarrow \infty} [\chi(\zeta, x)] = \frac{2x}{1+x^2}. \quad (11.39)$$

Furthermore,  $\chi(\zeta, x)$  is an odd function, so that

$$\int_{-\infty}^{+\infty} \chi(\zeta, x) dx = 0. \quad (11.40)$$

For the interference term, the effect of changing the temperature is shown in Figure 11.7.



**Fig. 11.7** Interference Scattering Contribution vs. Temperature.

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If we define  $\sigma_p \equiv 4\pi R^2$  for the potential scattering, then the complete Doppler-broadened scattering term becomes the temperature-dependent cross section,

$$\bar{\sigma}_s(E,T) = \frac{\sigma_r \Gamma_n^r}{\Gamma} \psi(\zeta, x) + \left( \sigma_r \sigma_p g \frac{\Gamma_n^r}{\Gamma} \right)^{1/2} \chi(\zeta, x) + \sigma_p. \quad (11.41)$$

We have derived the Doppler effect based upon the use of a Maxwellian distribution for an ideal gas. Actually, one can use other distributions, for example the Debye distribution that applies to solids. It can be shown that in this case, the same type of result is obtained but the temperature is replaced by an effective temperature  $T^*$ . For temperatures of interest in reactor fuel elements,  $T^* \approx T$ .

In actual practice, a nucleus has many resonances including some at high energy that are not resolved. The total effect upon the reactor is obtained by summing the effect of *each* resonance modified by the Doppler effect. The lowest energy resonances tend to be the most important, since this is where the thermal motion is comparable to the energy of the neutrons and where the Doppler effect is greatest.

### 11.3 Slowing Down in the Presence of Resonances

Now that we have obtained expressions for the absorption and scattering cross-section terms in a resonance, we must return to the problem of computing the flux and the absorption rate in the vicinity of a resonance. In the general case, for an arbitrary mixture of moderators and absorbers, an analytic solution is not possible. However, solutions can be obtained in certain special cases, notably when the resonance is narrow compared to an allowed scattering interval  $\Delta u = \ln 1/\alpha$ , and when the resonances are widely spaced so that the effect of one resonance does not

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interfere with the behavior of another resonance.

**Table 11.1**  
Tables of  $\psi(\zeta, x)$  and  $\chi(\zeta, x)$

$\zeta \backslash x$	0	0.5	1	2	4	6	8	10	20	40
0.05	0.04309	0.04308	0.04306	0.04298	0.04267	0.04216	0.04145	0.04055	0.03380	0.01639
0.10	0.08384	0.08379	0.08364	0.08305	0.08073	0.07700	0.07208	0.06623	0.03291	0.00262
0.15	0.12239	0.12223	0.12146	0.11989	0.11268	0.10165	0.08805	0.07328	0.01695	0.00080
0.20	0.15889	0.15854	0.15748	0.15331	0.13777	0.11540	0.09027	0.06614	0.00713	0.00070
0.25	0.19347	0.19281	0.19086	0.18324	0.15584	0.11934	0.08277	0.05253	0.00394	0.00067
0.30	0.22624	0.22516	0.22197	0.20968	0.16729	0.11571	0.07042	0.03880	0.00314	0.00065
0.35	0.25731	0.25569	0.25091	0.23271	0.17288	0.10713	0.05724	0.02815	0.00289	0.00064
0.40	0.28679	0.28450	0.27776	0.25245	0.17359	0.09604	0.04566	0.02109	0.00277	0.00064
0.45	0.31477	0.31168	0.30261	0.26909	0.17052	0.08439	0.03670	0.01687	0.00270	0.00064
0.50	0.34135	0.33733	0.32557	0.28286	0.16469	0.07346	0.03025	0.01446	0.00266	0.00063

THE  $\chi$ -FUNCTION

$\zeta \backslash x$	0	0.5	1	2	4	6	8	10	20	40
0.05	0	0.00120	0.00239	0.00478	0.00951	0.01415	0.01865	0.02297	0.04076	0.05221
0.10	0	0.00458	0.00915	0.01821	0.03573	0.05192	0.06626	0.07833	0.10132	0.05957
0.15	0	0.00986	0.01968	0.03894	0.07470	0.10460	0.12690	0.14096	0.12219	0.05341
0.20	0	0.01680	0.03344	0.06567	0.12219	0.16295	0.18538	0.19091	0.11754	0.05170
0.25	0	0.02515	0.04994	0.09714	0.17413	0.21909	0.23168	0.22043	0.11052	0.05103
0.30	0	0.03470	0.06873	0.13219	0.22694	0.26757	0.26227	0.23199	0.10650	0.05069
0.35	0	0.04529	0.08940	0.16976	0.27773	0.30564	0.27850	0.23236	0.10437	0.05049
0.40	0	0.05674	0.11160	0.20890	0.32442	0.33286	0.28419	0.22752	0.10316	0.05037
0.45	0	0.06890	0.13498	0.24880	0.36563	0.35033	0.28351	0.22223	0.10238	0.05028
0.50	0	0.08165	0.15927	0.28875	0.40075	0.35998	0.27979	0.21729	0.10185	0.05022

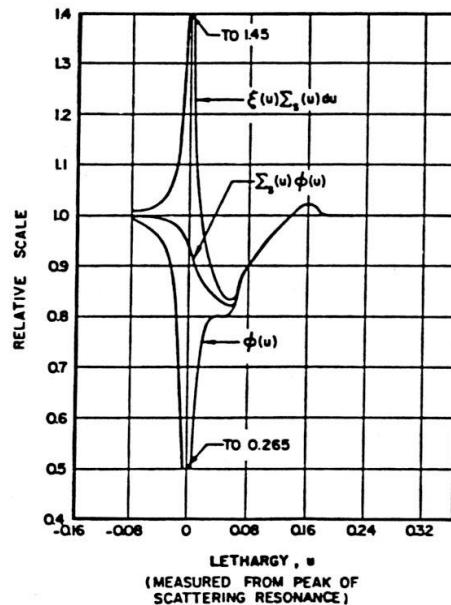
\*From T. D. Beynon and I. S. Grant, "Evolution of the Doppler-Broadened Single Level and Interference Functions," *Nucl. Sci. Eng.* 17, 547 (1963), with permission of the American Nuclear Society.

Qualitatively, in the vicinity of a resonance the flux will decrease, sometimes appreciably due to the significant increase in the total cross section. One can therefore expect at least three different types of complications to arise in the slowing down solution. These are:

1. *Transient solution behavior* - as noted previously, the collision density exhibits a transient behavior up to  $\sim \alpha^3 E'$  below an energy  $E'$  where there is a neutron source or sink;

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2. *Absorption effect* - as the flux decreases in a resonance, the absorption is lessened compared to that which would occur if the flux remained constant with lethargy. This is called energy shielding. If a lumped arrangement of fuel and moderator is assembled, the relative amount of absorption will be different from the case where the atoms are intimately mixed because of spatial self-shielding. This has consequences not only in reactor design but also in reactor safety because the Doppler coefficient of reactivity feedback is different in the two cases;
3. *Variation in  $\xi$*  - if the scattering cross section varies rapidly with  $E$ , the value of  $\xi(E)$ , which is averaged with respect to the macroscopic cross sections of the constituent atoms, will also vary. This in turn complicates the calculation of the collision density.



**Fig. 11.8** Slowing Down through a Scattering Resonance in an Iron-Sodium Mixture

(From *The Theory of Neutron Slowing Down in Reactors*, by J. Fertziger and P. Zweifel, 1960, Pergamon Press)

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As an example of the type of behavior that one would see in a single isolated scattering resonance, say a sodium resonance in an iron-sodium mixture in a fast reactor, refer to Figure 11.8. In addition to observing the characteristic asymmetric shape of the scattering resonance, one sees that the collision density decreases in the resonance region and then recovers because a greater proportion of neutrons actually scatter from the lighter sodium atoms in the iron-sodium mixture and hence lose more energy on the average than they do outside the resonance. The flux as a function of lethargy exhibits a marked decrease that is almost the inverse of the scattering cross section curve. However, the most important point is that the behavior of the collision density is not asymptotic, that is to say  $F(u)$  is not constant, and the entire solution must be obtained numerically.

**Single Isolated Absorption Resonance.** Consider now the case of a strong absorption resonance in a situation where the total scattering cross section is constant and absorption occurs only in the resonance. If an asymptotic flux is established one collision interval above the resonance, we can write a neutron balance equation about the interval that contains the resonance. If absorption begins at lethargy  $u_0$ , the in-scattering integral can be split into two parts and the first part can be integrated directly by assuming  $F(u) = 1/\xi$  and  $\Sigma_s = \Sigma_T$  for  $u < u_0$ . We have the expression

$$\begin{aligned}
 F(u) &= \int_{u-\ell n 1/\alpha}^{u_0} \frac{\Sigma_s(u')}{\Sigma_T(u')} F(u') \frac{e^{u'-u}}{1-\alpha} du' + \int_{u_0}^{\infty} \frac{\Sigma_s(u')}{\Sigma_T(u')} F(u') \frac{e^{u'-u}}{1-\alpha} du' \\
 &= \frac{e^{u_0-u} - \alpha}{\xi(1-\alpha)} + \int_{u_0}^{\infty} \frac{\Sigma_s(u')}{\Sigma_T(u')} F(u') \frac{e^{u'-u}}{1-\alpha} du'.
 \end{aligned}
 \tag{11.42}$$

This equation can be treated in the same manner as before. To solve for  $F(u)$ , we differentiate to convert the equation to a

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differential equation, and then integrate using an integrating factor. Note that the sharply varying ratio  $\Sigma_s/\Sigma_T$  appears inside the integral term to complicate the solution. By applying the method of successive collision intervals to obtain the solutions in lower-energy intervals, we can obtain a Placzek-type transient solution. However, because of the complexity of the results, reliance is usually placed on direct numerical solution of the integral equation.

### 11.4 Homogeneous-Medium Resonance Absorption

In general, the absorption rate in a single resonance is given by the integral

$$\text{Absorptionrate} = \int_{\text{resonance}} \Sigma_a(E) \phi(E) dE. \quad (11.43)$$

The form of the absorption cross section is known in terms of the Doppler-broadened Breit-Wigner formulation, but the flux as a function of energy is usually not known exactly so that it must be approximated.

As we have seen previously in the case of a broad scattering resonance, the collision density may vary significantly over the extent of the resonance, forcing us to solve the integral balance equation numerically to obtain the true collision density; the absorption rate must then be computed numerically using the collision density solution. On the other hand, if the resonance is not too broad, one can make some simplifying assumptions that allow a fairly straightforward semi-analytic treatment of the equations.

If the resonance can be considered to be narrow compared to the average energy loss in an elastic scattering collision with the atoms in the medium, then the neutrons entering the resonance



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will consist essentially of those neutrons that had their last scattering event in the collision interval just above the resonance. In other words, the neutron source can be considered to be asymptotic. The flux as a function of energy then has the simple approximate form,

$$\phi(E) = \frac{I}{\bar{\xi} \Sigma_r(E) E}, \quad (11.44)$$

which is the expression we shall use in the absorption rate equation. The implication of using this expression is that the collision density  $F(u) = 1/\bar{\xi}$  is constant over the range of the resonance, which is not exactly true.

We must now define what we mean by a "narrow" resonance. Specifically, let us define the "practical width,"  $\Gamma_p$ , as the width of the resonance measured from the values where the macroscopic resonance and macroscopic total potential scattering cross sections are just equal to one another. This is shown in Figure 11.9. There exist two readily treated cases:

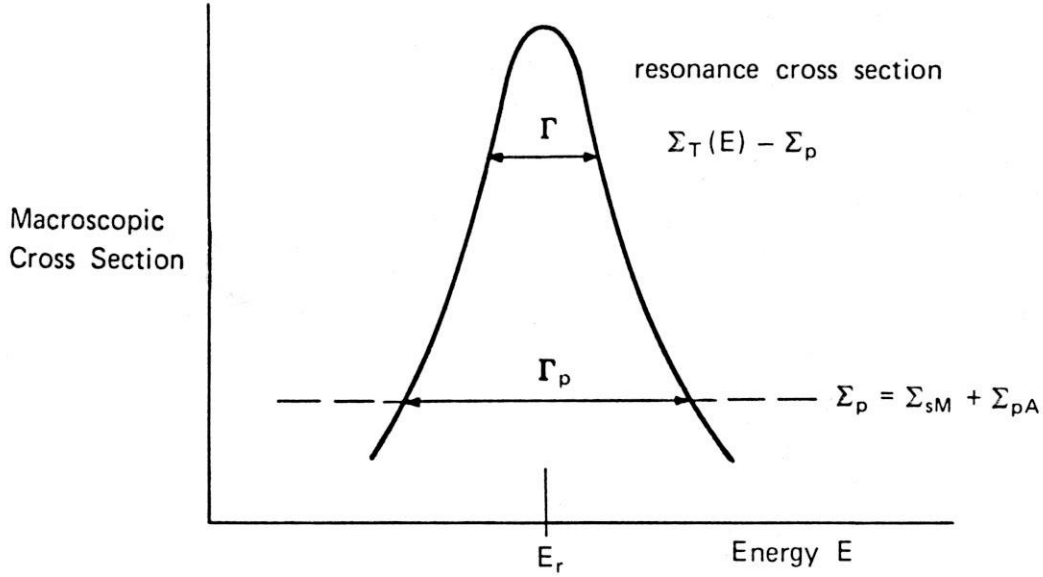
1. If the practical width is less than the average energy loss in scattering events in *both* moderator (M) and absorber (A), we have the narrow resonance (NR) approximation,

$$NR \text{ if } \Gamma_p \ll \frac{(1 - \alpha_A)E_r}{2} \ll \frac{(1 - \alpha_M)E_r}{2}.$$

2. If the practical width is less than the average energy loss in a moderator scattering collision but much greater than the average energy loss in an absorber atom scattering collision, we can *neglect* the scattering from the absorber atoms and we have the narrow resonance, infinite mass absorber (NRIM) approximation,

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$$NRIM \text{ if } \Gamma_p << \frac{(1 - \alpha_M)E_r}{2} \text{ but } \Gamma_p >> \frac{(1 - \alpha_A)E_r}{2}.$$



**Fig. 11.9** Diagram Defining the Practical Width  $\Gamma_p$

Naturally, there exist some cases where a certain amount of error is made using either approximation. A notable example is a graphite ( $A = 12$ ) moderated system. For these cases, an intermediate resonance treatment (IR) can be used, but this involves considerably more work because the slowing down effect must be included.

In either the NR or NRIM approximations, the form of the absorption rate equation is

$$\frac{\text{Resonance absorption}}{\text{probability}} \approx \int_{\text{resonance}} \frac{\Sigma_a(E') dE'}{\xi(E') \Sigma_T(E') E'}. \quad (11.45)$$

If the resonance is narrow and the scattering cross sections are fairly constant, then the product  $E_r$  can be extracted from the integral leaving an absorption rate equation of the form,

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$$\frac{\text{Resonance absorption}}{\text{probability}} \approx \frac{1}{\xi E_r} \int_{\text{resonance}} \frac{\Sigma_a(E')}{\Sigma_T(E')} dE'. \quad (11.46)$$

We now have a ratio of macroscopic cross sections that contain Doppler broadened terms in both the numerator and the denominator. This integral can be evaluated directly.

**NR Case.** We use the subscript A for absorber and the subscript M for moderator. If there is no absorption in the moderator, then the various macroscopic cross sections are defined in terms of the Doppler functions as

$$\Sigma_a \equiv N_A \sigma_r \frac{\Gamma_\gamma}{\Gamma} \psi(\zeta, x), \quad (11.47a)$$

and

$$\begin{aligned} \Sigma_T \equiv & N_M \sigma_{sM} + N_A \sigma_r \psi(\zeta, x) \\ & + N_A \left( \sigma_r \sigma_{pA} g \frac{\Gamma_n^r}{\Gamma} \right)^{1/2} \chi(\zeta, x) + N_A \sigma_{pA}. \end{aligned} \quad (11.47b)$$

For the Doppler functions, the integral over the resonance takes on the limits of  $-\infty$  to  $+\infty$ . Obviously, the integral containing the interference term,  $\chi(\zeta, x)$ , is a fairly complicated function. In many practical situations, interference can be neglected, in which case the absorption integral is a fairly simple expression of the form

$$\frac{\text{NR Resonance absorption}}{\text{probability}} \approx \frac{\Gamma_\gamma}{\xi E_r} \int_0^\infty \frac{\psi(\zeta, x) dx}{\psi(\zeta, x) + \beta_{NR}}, \quad (11.48)$$

where

$$\beta_{NR} \equiv \frac{N_M \sigma_{sM} + N_A \sigma_{pA}}{N_A \sigma_r}. \quad (11.49)$$

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$\beta_{NR}$  is the ratio of the total macroscopic potential scattering cross section to the peak macroscopic resonance cross section. Also, from the definition of  $x$ ,

$$dx = \frac{2}{\Gamma} dE.$$

The factor of 2 was absorbed in writing the limits on the integral from 0 to  $\infty$  instead of from  $-\infty$  to  $+\infty$ .

The integral term in the above equation has been evaluated numerically and is available in both tabular and graphical form. Dresner defines this integral as the J-function

$$J(\zeta, \beta) \equiv \int_0^\infty \frac{\psi(\zeta, x) dx}{\psi(\zeta, x) + \beta}. \quad (11.50)$$

It is given graphically in terms of a parameter  $j$ , where  $\beta \equiv 2^j \times 10^{-5}$ , as shown in Figure 11.10. A tabulation of  $J(\zeta, \beta)$  is given in ANL-5800, Reactor Physics Constants. Using the J-function, the NR resonance absorption can be written simply as,

$$\frac{\text{NR Resonance absorption}}{\text{probability}} \approx \frac{\Gamma_\gamma}{\xi E_r} J(\zeta, \beta_{NR}). \quad (11.51)$$

When the interference term is included, the absorption probability has the form,

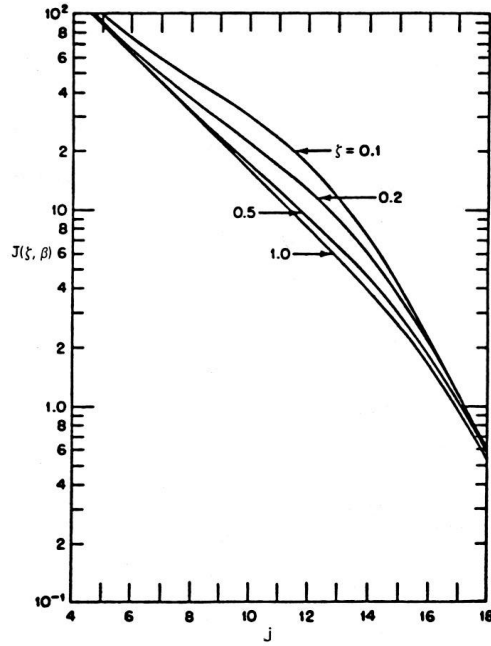
$$\frac{\text{NR Resonance absorption}}{\text{probability}} \approx \frac{\Gamma_\gamma}{\xi E_r} \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\zeta, x) dx}{\psi(\zeta, x) + (\beta_{NR} \gamma)^{1/2} \chi(\zeta, x) + \beta_{NR}}, \quad (11.52)$$

where the coefficient

$$\gamma \equiv \frac{N_A \sigma_{pA} \left( g \frac{\Gamma_n^r}{\Gamma} \right)}{N_A \sigma_{pA} + N_M \sigma_{sM}} \quad (11.53)$$

contains the ratio of the potential scattering in the absorber to the total non-resonance scattering.

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**Fig. 11.10** The Function  $J(\zeta, \beta)$  vs.  $j$ , where  $\beta = 2^j \times 10^{-5}$   
 (From *Resonance Absorption in Nuclear Reactors* by L. Dresner, 1960, Pergamon Press)

This equation can also be put into the form

$$\frac{\text{NR Resonance absorption}}{\text{probability}} \approx \frac{\Gamma_\gamma}{\xi E_r} J(\zeta, \beta_{NR}, \gamma), \quad (11.54)$$

where the modified J-function is defined as

$$J(\zeta, \beta_{NR}, \gamma) \equiv \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\zeta, x) dx}{\psi(\zeta, x) + (\beta_{NR} \gamma)^{1/2} \chi(\zeta, x) + \beta_{NR}}. \quad (11.55)$$

In the low-temperature limit where Doppler broadening is negligible,  $\zeta \rightarrow \infty$  and

$$\lim_{\zeta \rightarrow \infty} J(\zeta, \beta_{NR}, \gamma) = \frac{\pi}{2\sqrt{\beta_{NR}(1 + \beta_{NR} - \gamma)}}. \quad (11.56)$$

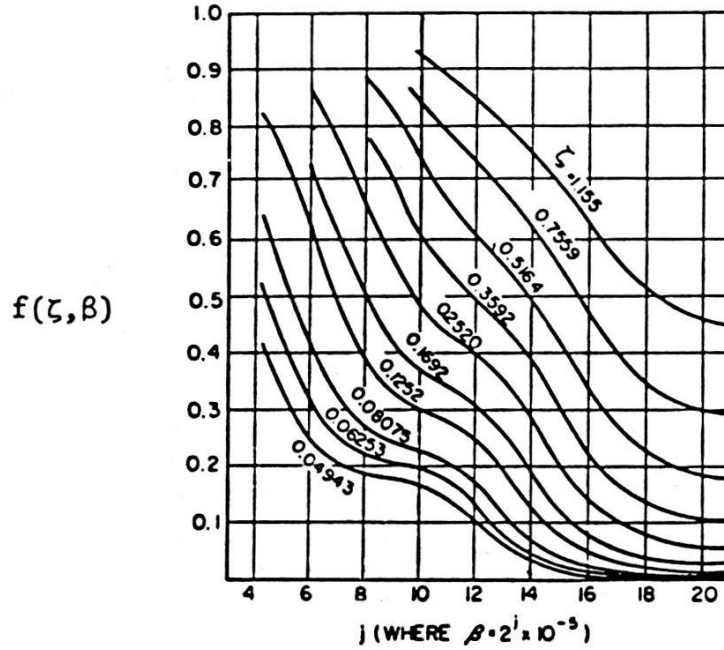
For intermediate cases, Rothenstein has computed a series expansion for the modified J-function in powers of  $\gamma$ . His

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results are of the form,

$$J(\zeta, \beta_{NR}, \gamma) = J(\zeta, \beta_{NR}) + \frac{\pi \beta_{NR} f(\zeta, \beta_{NR})}{4 \beta_{NR} (1 + \beta_{NR})^{3/2}} + \dots, \quad (11.57)$$

where the function  $f(\zeta, \beta_{NR})$  is given in Figure 11.11.



**Fig. 11.11** Plot of the Correction Factor  $f(\zeta, \beta)$ , Used in Calculating the Modified  $J(\zeta, \beta, \gamma)$

(From W. Rothenstein, *Nucl. Sci. Eng.*, 7, 162, 1960)

**NRIM Case.** When the average energy loss in a scattering collision with an absorber atom is small compared to the practical width, we can neglect this scattering contribution entirely and therefore the total cross section consists only of moderator scattering and resonance absorption: there is no potential scattering or interference term to worry about. In this case, again letting  $\sqrt{E_r/E} \approx 1$ , we have

$$\Sigma_a \equiv N_A \sigma_r \frac{\Gamma_\gamma}{\Gamma} \psi(\zeta, x). \quad (11.58a)$$

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and

$$\Sigma_{T\text{ }NRIM} \equiv N_M \sigma_{sM} + N_A \sigma_r \frac{\Gamma_\gamma}{\Gamma} \psi(\zeta, x). \quad (11.58b)$$

We form the ratio of  $\Sigma_a/\Sigma_T$ , as done previously in computing the absorption probability, and then divide through by  $N_A \sigma_r \Gamma_\gamma/\Gamma$  to obtain the expression

$$\frac{\text{NRIM Resonance absorption probability}}{\xi E_r} \approx \frac{\Gamma}{\xi E_r} \int_0^\infty \frac{\psi(\zeta, x) dx}{\psi(\zeta, x) + \beta_{NRIM}} = \frac{\Gamma}{\xi E_r} J(\zeta, \beta_{NRIM}). \quad (11.59)$$

In this case, the value of  $\beta_{NRIM}$  is different from  $\beta_{NR}$ , namely,

$$\beta_{NRIM} \equiv \frac{N_M \sigma_{sM} \Gamma}{N_A \sigma_r \Gamma_\gamma}. \quad (11.60)$$

**Limiting Cases.** There are some limiting cases which are useful to examine with regard to the  $J(\zeta, \beta)$  function. For example, when the mixture of absorber atoms is very dilute so that there are very few absorber atoms compared to moderator atoms, we would expect very little absorption to take place. In terms of the defining integral,

$$J(\zeta, \beta) = \int_0^\infty \frac{\psi(\zeta, x) dx}{\psi(\zeta, x) + \beta}.$$

the value of  $\beta$  becomes very large for dilute mixtures, and it is possible to neglect  $\psi(\zeta, x)$  in the denominator in comparison to  $\beta$ . Hence,

$$\lim_{\beta \rightarrow \infty} J(\zeta, \beta) \approx \frac{1}{\beta} \int_0^\infty \psi(\zeta, x) dx = \frac{\pi}{2\beta}. \quad (11.61)$$

Not only does the absorption rate become small, but the rate becomes *independent of* temperature.

At the other extreme, when the absorber becomes very

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concentrated, one can neglect  $\beta$  in the denominator with respect to  $\psi(\zeta, x)$ , and the absorption probability becomes large and independent of temperature. For intermediate cases,  $\partial J / \partial \beta$  is negative, so that the transition between extremes is monotonic.

It further can be shown that as the temperature increases,  $\zeta$  decreases and the partial derivative  $\partial J / \partial \zeta$  is negative, implying that  $\partial J / \partial T$  is positive and resonance absorption increases with increasing temperature. For  $^{238}\text{U}$ , the Doppler coefficient of reactivity is negative. However, for  $^{235}\text{U}$ , the Doppler coefficient is positive because resonance absorption also produces fission. The overall Doppler coefficient depends upon the relative contributions from each of these isotopes, and is a design concern in highly enriched cores.

Finally, at  $T = 0^\circ$ , which implies no Doppler broadening, the  $J$  function has the limiting value

$$J(\infty, \beta) = \frac{\pi}{2\sqrt{\beta(1 + \beta)}}. \quad (11.62)$$

This value is consistent with the result for the infinitely dilute case.

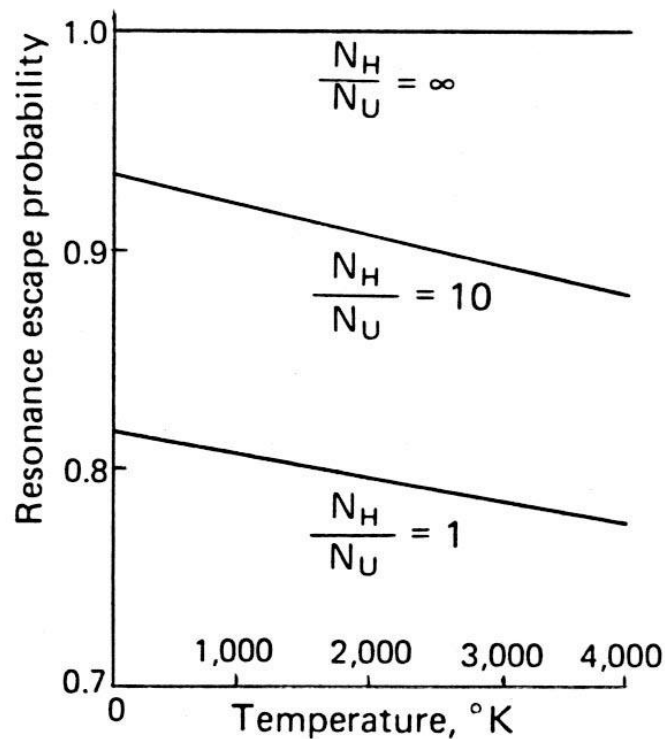
If one plots the resonance escape probability  $p$ , which is equal to 1.0 minus the resonance absorption probability, one obtains the curves shown in Figure 11.12 for hydrogen-uranium mixtures. These results are consistent with the above predictions. We can state that for a homogeneous system of moderator and resonance absorbers we have a negative Doppler coefficient of reactivity as a function of temperature. This can be considered to be a safety feature with respect to power excursions in such reactors. Doppler feedback acts independently of any moderator density effects.

Because of the factor of  $1/E_r$  in the denominator of the absorption rate equation, all other things being equal, the



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lowest energy resonances capture the most neutrons because the flux is largest there. This is illustrated in Table 11.2, where the exact solution and the NR and NRIM approximations are compared for various  $^{238}\text{U}$  resonances for a ratio of  $N_{\text{H}}/N_{\text{U}} = 1.0$ . Note that the lower energy resonances indeed have the highest capture rates, and that the accuracy of the NR and NRIM approximations is consistent with a comparison of the practical width to the scattering interval for the absorber. We see that the NR approximation should be used at high resonance energies and the NRIM approximation at low energies. Note also that some of the error is due to the use of an asymptotic collision density instead of the actual collision density.



**Fig. 11.12** Resonance Escape Probability for the 6.67 eV Resonance in Hydrogen-Uranium Mixtures

(From *Introduction to Nuclear Reactor Theory* by J.R. Lamarsh, 1966, Addison Wesley)

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**Table 11.2**

Absorption in Uranium-238 Resonances for  $N_H/N_U = 1$ .

Resonance Energy (eV)	$(1-\alpha_A)E_r$	$\Gamma$ (eV)	$\Gamma_p$ (eV)	Exact value NR absorption rate probability	NR	NRIM
418	7.0	.105	2.56	.0019	-6.9%	+97%
278	4.7	.065	1.87	.0035	-5.1	+41.
212	3.6	.085	2.63	.0050	-11.6	+53.
192	3.21	.165	5.66	.0071	-29.	+73.
117	1.97	.040	1.32	.0092	-1.5	+3.6
90	1.51	.025	10.13	.0011	+0.9	-9.6
81	1.36	.0271	0.76	.0096	+5.9	-15.5
36.9	.626	.0575	3.65	.0582	-18.6	+5.
21	.357	.0339	1.95	.0676	+10.4	+4.5
6.67	.113	.027	0.72	.1963	+20.	+1.7

(From K.T. Spiney, BNL-433)

### 11.5 Homogeneous Resonance Integrals

At this point we have computed the absorption rate per unit source, or alternately the absorption probability, for individual resonances. Using either approximation for widely spaced resonances, the form of the equation is,

$$\frac{\text{Resonance absorption}}{\text{probability}} \approx \int_{\text{resonance}} \frac{\sum_a(E) dE}{\xi \sum_T(E) E}.$$

If the resonance were absent entirely, then the flux would asymptotically have the value

$$\phi_{\text{Asy}}(E) = \frac{I}{\xi \sum_p E} \quad \text{or} \quad \phi_{\text{Asy}}(u) = \frac{I}{\xi \sum_p}, \quad (11.63)$$

where the scattering cross section is constant and equal to

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$$\Sigma_p = N_A \sigma_{pA} + N_M \sigma_{sM}.$$

We can use the above expression to define a new "point" quantity called the effective resonance integral (ERI). Let  $I_r$  be an effective microscopic cross section such that the product  $N_A I_r \phi_{Asy}(u)$  is equal to the resonance absorption probability. This expression is

$$\begin{array}{l} \text{Resonance} \\ \text{absorption} = \frac{N_A I_r}{\xi \Sigma_p} \equiv \int_{\text{resonance}} \frac{N_A \sigma_{cA}(E) dE}{\xi \Sigma_T(E) E}. \end{array} \quad (11.64)$$

*probability*

Rearranging, one has the definition, in units of barns,

$$I_r \equiv \Sigma_p \int_{\text{resonance}} \frac{\sigma_{cA}(E) dE}{\Sigma_T(E) E}. \quad (11.65)$$

This quantity is useful in defining the effective absorption over an energy band of width  $\Delta u$  containing the resonance in terms of the flux that would exist in  $\Delta u$  without the resonance. The corresponding Doppler-broadened effective resonance integral in the NR approximation has the form

$$I_r^{NR} = \frac{\Sigma_p \Gamma_\gamma}{N_A E_r} J(\zeta, \beta_{NR}). \quad (11.66)$$

When the system is infinitely dilute, so that there are very few absorber atoms present,  $\Sigma_T(E)$  approaches  $\Sigma_p$ , and the resonance integral approaches

$$I_r^\infty = \int_{\text{resonance}} \sigma_{cA}(E) \frac{dE}{E}. \quad (11.67)$$

This is called the resonance integral (RI).

It is possible to build a well-moderated irradiation facility that has a  $1/E$  flux over a wide range of energies. Hence, one may prepare small samples of absorber and moderator,

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approximating infinitely dilute mixtures for example, and measure the absorption rate in the sample by a means such as activation analysis. What one obtains, is a total resonance integral RI which is the *sum* of the absorption over all resonances, both resolved and unresolved, namely,

$$I^{\infty} = \sum_{r=1}^{\infty} I_r^{\infty}. \quad (11.68)$$

Likewise, for mixtures, the total effective resonance integral ERI is

$$I = \sum_{r=1}^{\infty} I_r. \quad (11.69)$$

By heating the samples, the total effect of Doppler broadening can also be measured. The important thing to note is that there is an experimental check available, at least for the total resonance integral, for comparison with the sum of the individual contributors.

Neutron cross sections as a function of energy have been measured in detail using a variety of means to obtain a monochromatic neutron beam. Among these devices are crystal spectrometers and neutron "choppers" with time-of-flight gating. An example of the data for  $^{238}\text{U}$  is shown in Figure 11.13. All of these devices have the property that their resolution worsens as energy increases. The net result is that the experimental curves are well resolved at low energy, say below 500 eV, and poorly resolved or unresolved above this energy. Unfortunately, for a material such as  $^{238}\text{U}$ , approximately 20% of the total measured resonance integral is due to the unresolved resonances. This absorption is significant and cannot be ignored; when doing multi-group calculations such absorption must be included in the higher-energy groups to properly account for capture in the

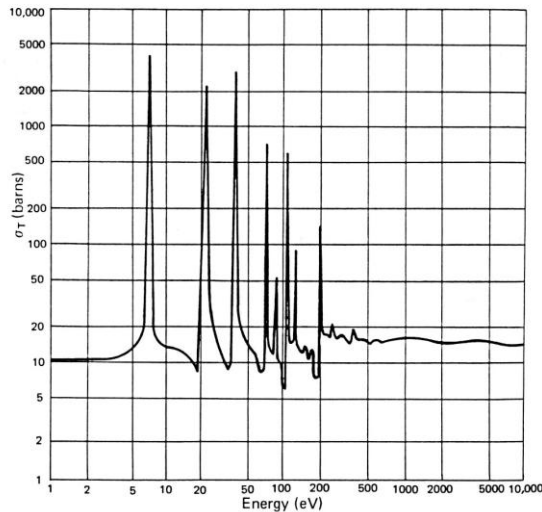
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unresolved resonances. Resonance overlap must also be considered, if significant.

It should be noted that the peak cross sections shown in Figure 11.13 are considerably smaller than the values obtained from the pure line shape. At  $0^\circ\text{K}$ ,  $\psi(0,0) = 1$ , while at room temperature  $\psi(0.05,0) = 0.341$ . Therefore, the experimental data are low by approximately a factor of 3, due to room-temperature Doppler broadening alone!

Fortunately, there is sufficient data in the resolved resonance region to allow one to evaluate the statistical properties of the resonance parameters. It is found, for example, that the radiation width  $\Gamma_\gamma$  is almost constant for a given nuclide while the neutron width has a statistical chi-square distribution about the mean value of  $\overline{\Gamma_n^r}$ . The chi-square distribution for one degree of freedom is called the Porter-Thomas distribution, and, for  $x \equiv \Gamma_n^r / \overline{\Gamma_n^r}$ , is of the form,

$$P(x) = \frac{1}{2\sqrt{\pi}} \sqrt{\frac{2}{x}} e^{-x/2}. \quad (11.70)$$



**Fig. 11.13** Total Cross Section of  $^{238}\text{U}$  in the Resonance Region

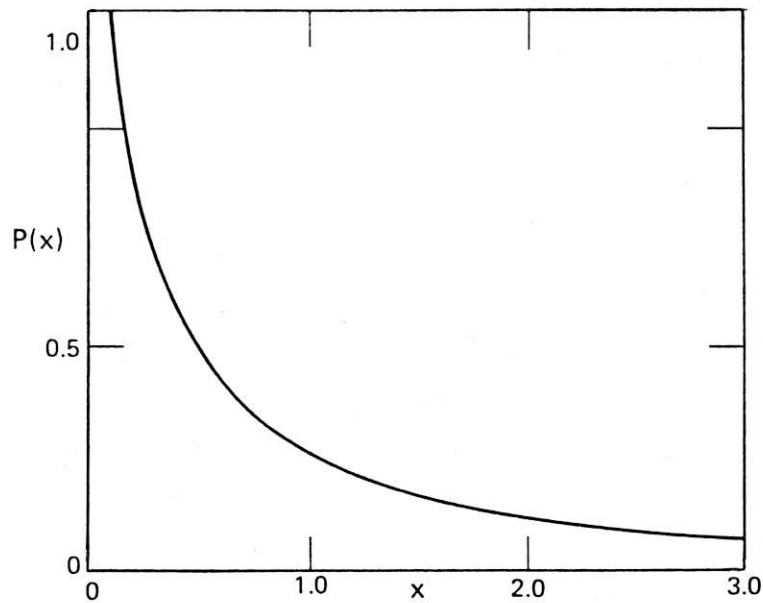
(From BNL-325)

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The function  $P(x)$  is shown in Figure 11.14. Furthermore, Wigner has suggested that the spacing of resonances has a distribution about the mean value  $\bar{D}$  of the form

$$P(z) = \frac{\pi z}{2} e^{-\pi z^2/4}, \quad (11.71)$$

where  $z \equiv D/\bar{D}$  ( $z$  is shown in Figure 11.15). Values are given for the average parameters in Table 11.3, based upon the resolved data.



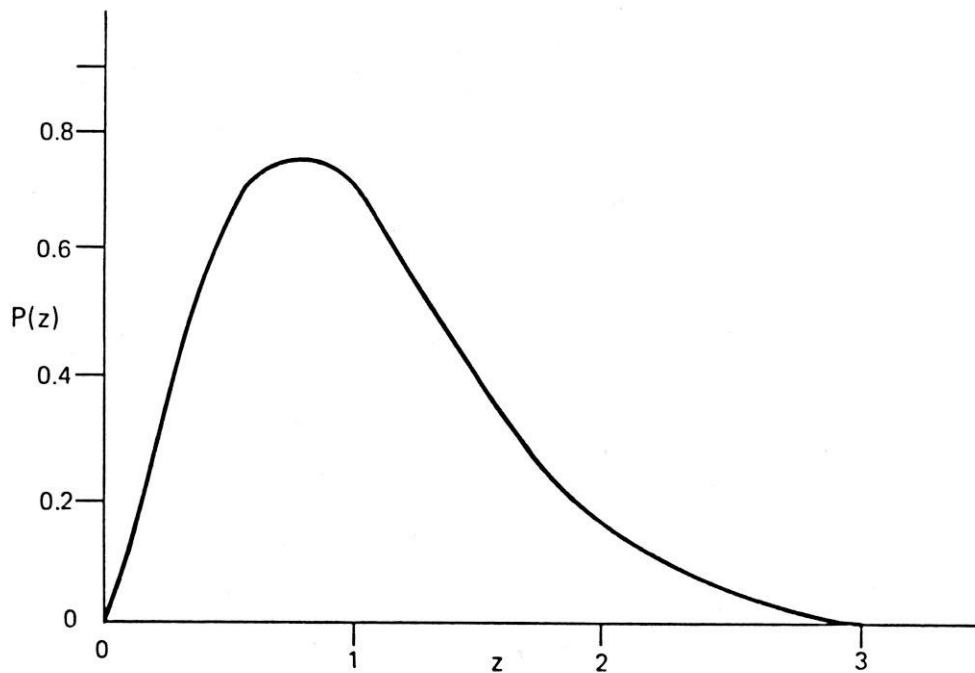
**Fig. 11.14** Porter-Thomas Distribution of Neutron Widths

**Table 11.3**

Statistical Properties for Uranium Resonances

	Uranium-238	Uranium-235
$\Gamma_v$ (mV)	19.0	45.0
$\Gamma_f$ (mV)	-	53.0
$\overline{\Gamma_n^r}$ (mV)	1.9	0.1
$\bar{D}$ (eV)	21.1	1.0

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**Fig. 11.15** Distribution of Level Spacings

The unresolved contribution can be computed by using a Monte Carlo technique. Using random numbers, a resonance scattering width and spacing can be selected from the probability distributions for each unresolved resonance up to a point where the addition of contributions are negligible due to the  $1/E_r$  effect. A number of similar Monte Carlo experiments will generate a series of different possible unresolved structures. From this set, an average total resonance integral and its standard deviation can be derived.

Since the unresolved resonances are treated in the same manner as resolved resonances, Doppler broadening can be included as well. For thermal reactors, the widely spaced resonance approximation is fairly good. However, in fast reactors where considerable absorption occurs at high energy, resonance overlap and interference effects must be included. These will not be treated here.

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### 11.6\* Heterogeneous System Resonance Absorption

Reactor systems are usually made up of repeated arrays of fuel pins, such as  $\text{UO}_2$  pellets loaded in zircaloy cladding tubes, which are mounted together in fuel assemblies. The pins are usually of the order of 0.5 to 1 cm in diameter, with comparable spacing. Since the pins are normally more than 3 meters long, the axial variation is usually negligible.

What we really want to do is solve a spatially-dependent slowing-down problem. We need transport theory because the fuel rod is a very strong absorber near resonance energies and the entire cell is small. The incident flux on a given fuel pin surface varies azimuthally because of the shadowing pattern from adjacent fuel pins. And finally, in modern reactors, the adjacent pin positions are not all alike; some contain control rod pins or burnable poison pins. Even the spacing between pins can change at the interface between fuel assemblies.

The actual problem is far too difficult to solve analytically in a generally useful form. Therefore, a series of simplifying approximations have usually been made in order to make the problem tractable. The usual approximations are:

- 1) Concentrate on a single isolated cell, assuming that there is no net neutron current between adjacent cells;
- 2) Replace the transport flux solution by probabilities that neutrons will escape from one region into the other and vice versa;
- 3) Use an interpolation function to express the energy dependence of the escape probabilities;
- 4) Correct the escape probabilities for the presence of



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the adjacent external pins that are indeed close enough to influence the flux in the isolated cell;

- 5) Interconnect the average flux magnitudes in the isolated cell regions with a concept called reciprocity; and
- 6) Assume an asymptotic flux in both the fuel and moderator regions (this assumption is relaxed in some intermediate resonance (IR) approximations).

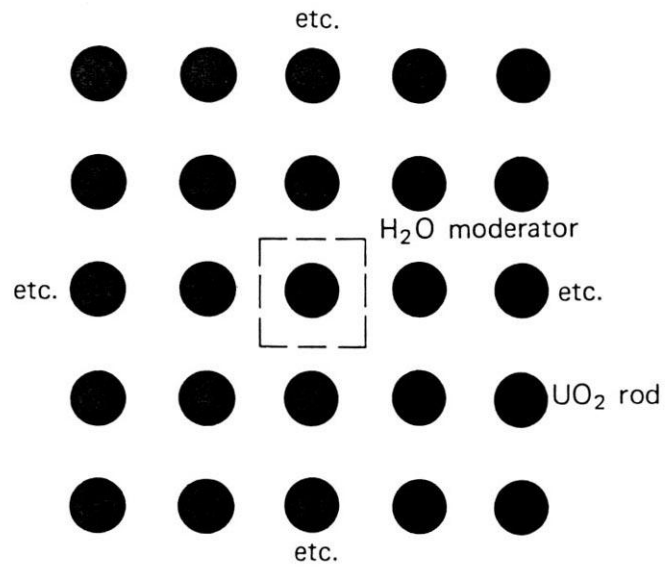
**Heterogeneous Balance Equation.** When we speak of a heterogeneous treatment, we really refer to the analysis of a typical cell within the array such as is shown by the dashed square in Figure 11.16. Hence, we analyze a single rod (or a rod with cladding) surrounded by a moderator region. Let us assign the subscript F to the fuel region and the subscript M to the moderator region, as shown in Figure 11.17. We will use the superscript O for oxygen and the superscript U for uranium in the fuel region. Hence, let

$$\Sigma_{sF} = \Sigma_s^O + \Sigma_s^U,$$

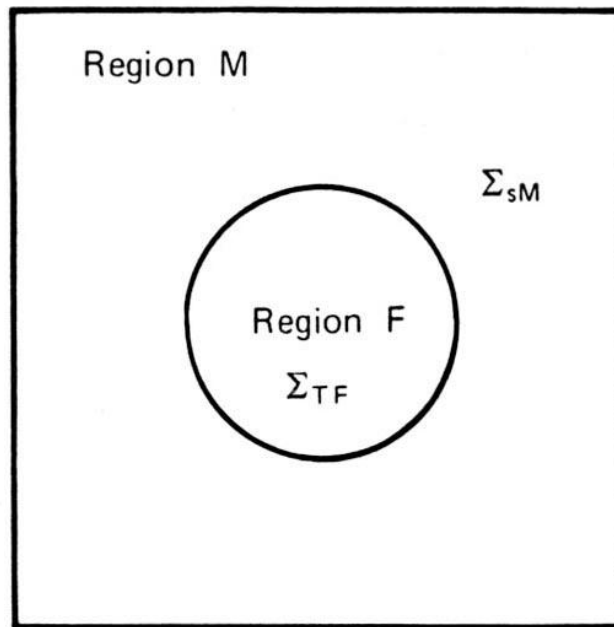
$$\Sigma_{TF} = \Sigma_{sF} + \Sigma_{aF}.$$

Since the fuel region in this example contains both uranium and oxygen, scattering effects from both will have to be treated separately. Let us write a total neutron balance equation for the collision rate in the fuel region, using *volume-averaged fluxes* in both regions. We introduce quantities known as escape probabilities,  $P_M(E)$ , and  $P_F(E)$ , defined as being the probability that a neutron originating in the given region and having energy  $E$  will have its next collision in the other region.

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**Fig. 11.16** Rod-Type Fuel Assembly



**Fig. 11.17** Unit Cell in a Fuel Assembly

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The balance equation is the following,

$$\begin{aligned}
 & \begin{array}{l} \text{collision rate out of} \\ \text{region } F \end{array} & \begin{array}{l} \text{scattering rate into} \\ \text{region } F \text{ due to neutrons} \\ \text{originating in region } M \end{array} \\
 \\
 V_F \Sigma_{TF}(E) \phi_F(E) &= P_M(E) N_M \int_E^{E/\alpha_M} \frac{\Sigma_{SM}(E') \phi_M(E') dE'}{(1 - \alpha_M) E'} \\
 \\
 & \begin{array}{l} \text{scattering rate into region } F \text{ due to} \\ \text{neutrons originating in region } F \end{array} & (11.72) \\
 \\
 + \{1 - P_F(E)\} N_F & \left[ \int_E^{E/\alpha_U} \frac{\Sigma_s^U(E') \phi_F(E') dE'}{(1 - \alpha_U) E'} + \int_E^{E/\alpha_O} \frac{\Sigma_s^O(E') \phi_F(E') dE'}{(1 - \alpha_O) E'} \right].
 \end{aligned}$$

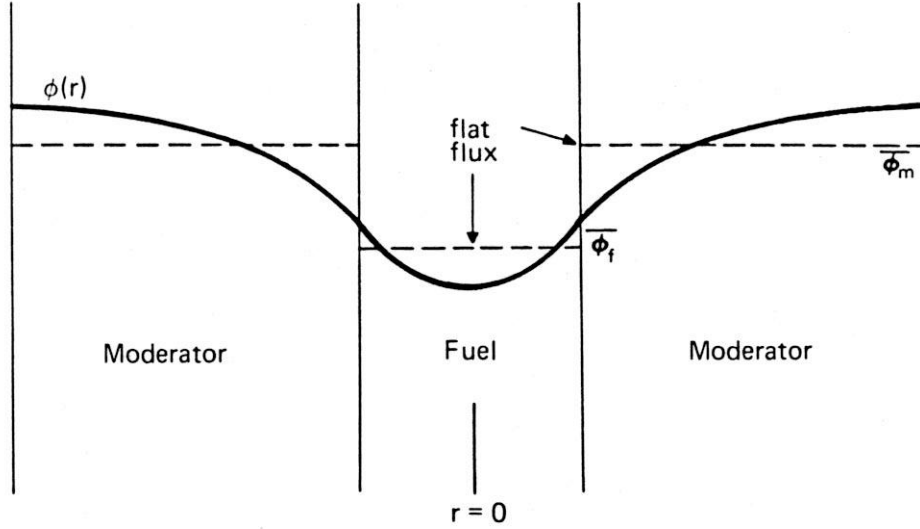
This is the fundamental balance equation for a heterogeneous system, which reduces to the homogeneous balance when only one region is present. Before using this equation, the calculation of escape probabilities will be treated.

Although the balance equation is exact, the escape probabilities are difficult to calculate. However, for most heterogeneous systems, the spatial distribution of neutrons, at least for those energies not too near a resonance peak, is reasonably independent of position, as shown in Figure 11.18. Therefore, one can make an approximation that the flux is spatially flat in each region and use this to derive approximate values for  $P_F$  and  $P_M$ .

In fact, what we will actually do is calculate the escape probability  $P_{\text{esc}}$  for a lump of arbitrary shape embedded in an infinite medium. Next, we will relate  $P_{\text{esc}}$  to  $P_F$  for simple regular bodies such as slabs, cylinders and spheres. Then we

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will correct  $P_F$  for the presence of adjacent cells. Finally, we will obtain  $P_M$  from  $P_F$  using an idea called reciprocity.



**Fig. 11.18** Actual and Approximate Flux Distribution in a Cell

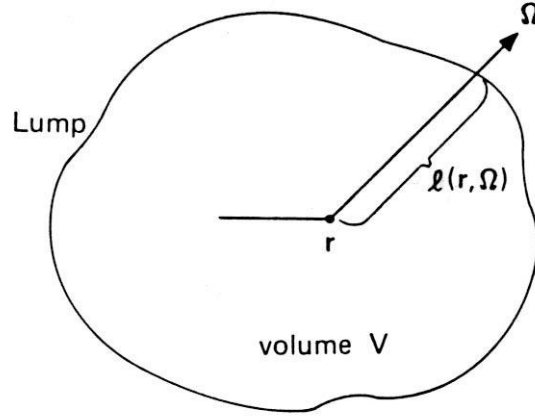
**Calculation of First Collision Escape Probabilities by the Mean Chord Method.** Suppose that neutrons are produced isotropically and uniformly over an isolated region of volume  $V$  that is made of a material with a spatially uniform constant total cross section  $\Sigma_T$ . Consider a neutron generated at position  $\vec{r}$  and traveling in a direction  $\vec{\Omega}$  as shown in Figure 11.19. The probability that the neutron will escape the region is equal to the probability that it will not suffer a collision before reaching the surface of the region. The probability of not having a collision before traveling a distance  $\ell$  and reaching the surface is

$$\left[ \begin{array}{c} \text{Probability of escape} \\ \text{at } \vec{r}, \vec{\Omega} \end{array} \right] = e^{-\Sigma_T \ell(\vec{r}, \vec{\Omega})}. \quad (11.73)$$

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Since the neutrons are produced isotropically and uniformly in the volume, the generation probability is

$$\left[ \begin{array}{c} \text{Generation probability} \\ \text{at } \vec{r}, \vec{\Omega} \end{array} \right] = \frac{d\Omega}{4\pi} \frac{dr}{V}. \quad (11.74)$$



**Fig. 11.19** Chord Length to the Surface of a Lump Along the Direction  $\vec{\Omega}$ .

The escape probability for the entire lump is obtained by taking the product of the above probabilities and integrating over all directions and over the volume of the lump. Formally,

$$P_{esc} = \frac{1}{4\pi V} \iint e^{-\Sigma_T \ell(\vec{r}, \vec{\Omega})} d\Omega dr. \quad (11.75)$$

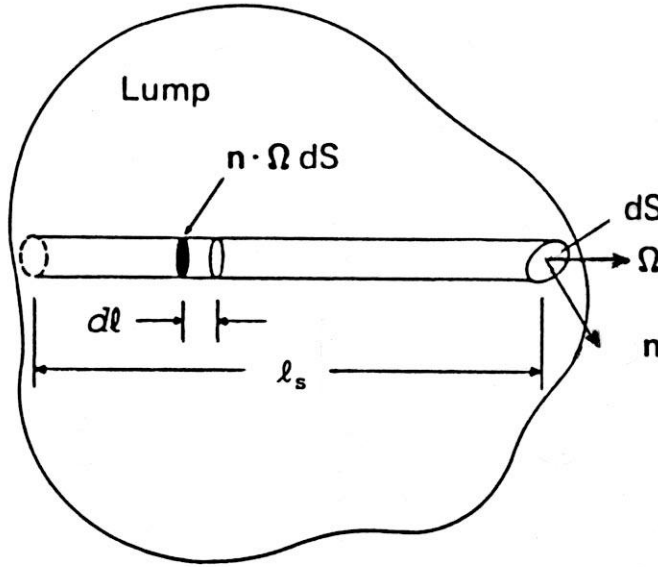
One possible way to perform the integration is to divide the volume up into tubes, all of which are parallel to a given direction  $\vec{\Omega}$ , as illustrated in Figure 11.20. If  $dS$  is the surface area subtended in the outward direction, then the actual projected cross sectional area of the tube is  $\vec{n} \cdot \vec{\Omega} dS$ , where  $\vec{n}$  is the unit normal to the surface.  $\ell_s$  is the length of the tube. Expressing the volume element as

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$$dr = \vec{n} \cdot \vec{\Omega} dS d\ell,$$

we can perform the integral over  $\ell$  from  $\ell = 0$  to  $\ell = \ell_s$  for all outward going neutrons  $\vec{n} \cdot \vec{\Omega} > 0$ . The result, when taken over all allowed directions  $\vec{\Omega}$ , is

$$P_{esc} = \frac{1}{4\pi \Sigma_T V} \int \int_{\vec{n} \cdot \vec{\Omega} > 0} \vec{n} \cdot \vec{\Omega} (1 - e^{-\Sigma_T \ell_s(\vec{r}, \vec{\Omega})}) d\Omega dS. \quad (11.76)$$



**Fig. 11.20** Calculation of  $P_{esc}$  Using Parallel Filaments

We still have a formidable double integral to evaluate, where  $\ell_s$  is a function of both position and direction. However, a useful limiting case presents itself. When  $\Sigma_T \ell_s$  is reasonably large, i.e., for a large lump, the exponential term becomes negligible, and the escape probability approaches the value

$$P_{esc}^{\infty} = \frac{1}{4\pi \Sigma_T V} \int \int_{\vec{n} \cdot \vec{\Omega} > 0} \vec{n} \cdot \vec{\Omega} d\Omega dS = \frac{S}{4\Sigma_T V}. \quad (11.77)$$

The latter result obtains because  $d\Omega = -2\pi d\mu$ ,  $\vec{n} \cdot \vec{\Omega} = \mu = \cos\theta$ , and the condition  $\vec{n} \cdot \vec{\Omega} > 0$  implies an integration over

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the range  $0 > \mu > -1$ , giving

$$\int_{\vec{n} \cdot \vec{\Omega} > 0} \vec{n} \cdot \vec{\Omega} d\Omega = 2\pi \int_0^1 \mu d\mu = \pi. \quad (11.78)$$

On the other hand, the limiting case for a very small lump of material is a situation where essentially all neutrons escape, i.e.,

$$P_{esc}^0 = 1. \quad (11.79)$$

Wigner has proposed a rational (reasonable) interpolation approximation to the general case, applicable to all bodies, which reduces to the correct limits for both large and small lumps, namely,

$$P_{esc}^{RATIONAL} \approx \frac{1}{1 + \frac{4\Sigma_T V}{S}}. \quad (11.80)$$

For any large convex-shaped body, the average chord length  $\bar{\ell}$  can be shown to be equal to the value

$$\bar{\ell} = \frac{4V}{S}, \quad (11.81)$$

which is analogous to the hydraulic diameter used in fluid mechanics. Hence, the Wigner rational approximation also takes the form

$$P_{esc}(E) \approx \frac{1}{1 + \bar{\ell} \Sigma_T(E)}. \quad (11.82)$$

The product  $\bar{\ell} \Sigma_T$  is dimensionless. It is called the optical thickness,  $t$ , and is given in relative mean-free-paths by the expression

$$t = \bar{\ell} \Sigma_T. \quad (11.83)$$

First collision escape probabilities have been calculated exactly

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for a variety of simple geometries. A comparison of these values with the rational approximation is shown in Table 11.4, which shows agreement generally to within 15%. The rational approximation is a convenient analytical form useful in extended derivations, whereas the tabular values can only be used in numerical integrations.

**Table 11.4**

Escape Probabilities for Various Geometries

t	Sphere	Cylinder	Slab	Rational
0.04	0.978	0.974	0.952	0.962
0.1	0.947	0.939	0.902	0.909
0.2	0.896	0.885	0.837	0.823
0.5	0.767	0.753	0.701	0.667
1	0.607	0.596	0.557	0.500
2	0.411	0.407	0.390	0.333
5	0.193	0.193	0.193	0.167
10	0.099	0.099	0.100	0.091

**Dancoff-Ginsberg Correction.** If the fuel rods are separated by moderator regions that are thin in terms of mean-free-paths, then there is a strong probability that a neutron from one fuel rod will have its next collision in one of the other fuel rods of a periodic array, as shown in Figure 11.21. This probability depends upon the chance that the neutron will arrive at the adjacent rod without collision, and also upon the chance that it will collide in that rod when it gets there. The problem is similar to optical shadowing through a translucent medium.

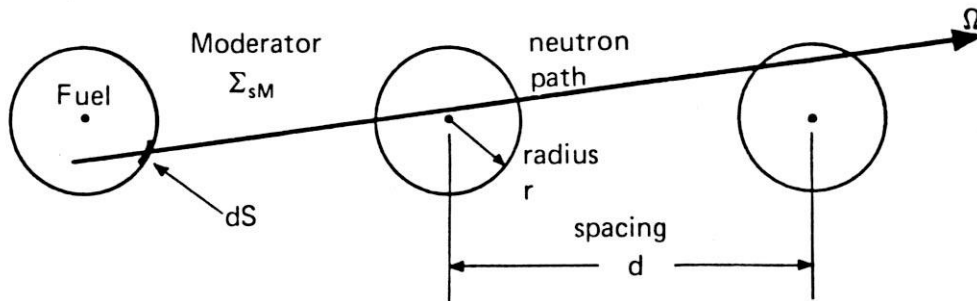
The calculation of this effect for cylindrical rods involves fairly complicated integrals which have been evaluated for perfectly absorbing (black) cylinders by Dancoff in terms of Bickley functions. The result is applied as a correction to the escape probability for a single fuel region. This correction is given in terms of a tabulated factor  $C$ , called the Dancoff



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factor. Bell has shown that the corrected escape probability for a partially absorbing fuel rod is given approximately by the expression

$$P_F \approx P_{esc} \left[ \frac{1 - C}{1 - C(1 - \sum_{TF} \bar{\ell} P_{esc})} \right]. \quad (11.84)$$



**Fig. 11.21** Periodic Array Illustrating the Dancoff Effect

In the limit of strongly absorbing rods,  $P_F$  approaches  $P_{esc}(1 - C)$ , the actual shadowing, while for weakly absorbing rods,  $P_F$  approaches  $P_{esc}$ . One sees that the escape probability for a single rod is slightly reduced as a result of the Dancoff correction.

The Dancoff correction has been calculated for perfectly absorbing cylinders in regular lattice arrays. The parameters of interest are the size of the rod,  $r$ , compared to the center-to-center rod spacing,  $d$ , and also to the effective mean-free-path between fuel rods, which is proportional to the product  $r\Sigma_{sM}$ . The tabulated correction is given for a single adjacent cylinder, so that the total correction must be obtained by summing over all of the nearest cylinders; this summation converges rapidly. Correction factors are tabulated in Table 11.5. Carlvik has tabulated these sums for both square and hexagonal lattices.

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**Table 11.5**

Single Adjacent Cylinder Dancoff Corrections (From ANL-5800)

d/r	$r \Sigma_{sM}$	0	0.25	0.50	1.0	1.5	2.0
2.0		0.182	0.170	0.160	0.144	0.132	0.123
2.5		0.136	0.107	0.0849	0.0550	0.0364	0.0245
4.0		0.081	0.040	0.0205	0.0057	0.0016	0.0005
7.0		0.046	0.0094	0.0021	0.0001	-	
10.0		0.032	0.0028	0.0003	-	-	

**Reciprocity Theorem.** At this point we have a value for the escape probability from the fuel, but we do not have a value for the moderator. To obtain this relationship we need to use a theorem known as reciprocity, which is true in general for the one-speed transport equation and its diffusion theory approximation. The theorem is based upon the fact that the Green's function for the system is symmetric in its arguments.

Consider the diagram given in Figure 11.22. The diffusion equation in the one-speed approximation is

$$-\nabla \cdot D(\vec{r}) \nabla \phi(\vec{r}) + \Sigma_a(\vec{r}) \phi(\vec{r}) = S(\vec{r}). \quad (11.85)$$

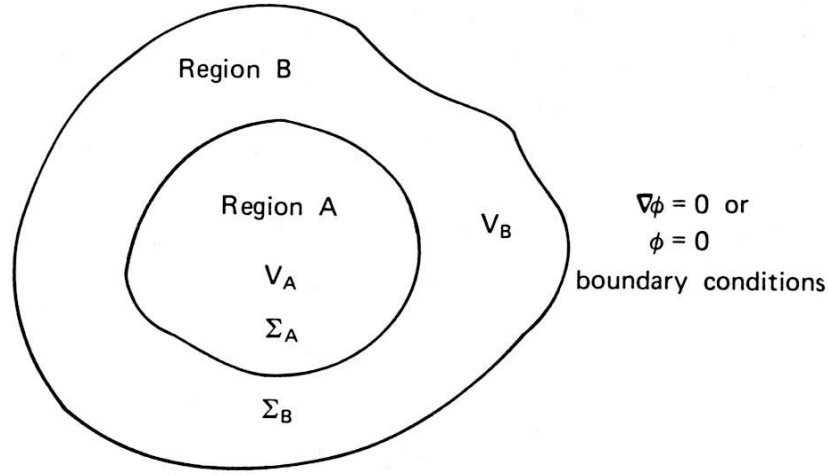
The Green's function is obtained by replacing the source by a delta function at point  $\vec{r}_1$  and then finding the corresponding flux  $G(\vec{r}_1 \rightarrow \vec{r})$ . We do this for two different space points,  $\vec{r}_1$  and  $\vec{r}_2$ . The equations are

$$-\nabla \cdot D(\vec{r}) \nabla G(\vec{r}_1 \rightarrow \vec{r}) + \Sigma_a(\vec{r}) G(\vec{r}_1 \rightarrow \vec{r}) = \delta(\vec{r} - \vec{r}_1)$$

$$\text{and} \quad (11.86)$$

$$-\nabla \cdot D(\vec{r}) \nabla G(\vec{r}_2 \rightarrow \vec{r}) + \Sigma_a(\vec{r}) G(\vec{r}_2 \rightarrow \vec{r}) = \delta(\vec{r} - \vec{r}_2).$$

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**Fig. 11.22** Model for Reciprocity Derivation

As we did in the perturbation theory analysis, we next multiply the first equation by  $G(\vec{r}_2 \rightarrow \vec{r})$ , multiply the second equation by  $G(\vec{r}_1 \rightarrow \vec{r})$ , integrate over the volume of the reactor and subtract the second equation from the first. The result is

$$\begin{aligned} & \int [G(\vec{r}_1 \rightarrow \vec{r}) \nabla \cdot D \nabla G(\vec{r}_2 \rightarrow \vec{r}) - G(\vec{r}_2 \rightarrow \vec{r}) \nabla \cdot D \nabla G(\vec{r}_1 \rightarrow \vec{r})] d\vec{r} \\ & = G(\vec{r}_1 \rightarrow \vec{r}_2) - G(\vec{r}_2 \rightarrow \vec{r}_1). \end{aligned} \quad (11.87)$$

Note that the terms containing  $\Sigma_a$  cancel. Using the second form of Green's theorem, which is equivalent to integrating by parts, the volume integral can be converted to a surface integral with the result that

$$\begin{aligned} & \iint_{\text{outer surface}} D [G(\vec{r}_1 \rightarrow \vec{r}) \nabla G(\vec{r}_2 \rightarrow \vec{r}) - G(\vec{r}_2 \rightarrow \vec{r}) \nabla G(\vec{r}_1 \rightarrow \vec{r})] \cdot \vec{n} dS \\ & = G(\vec{r}_1 \rightarrow \vec{r}_2) - G(\vec{r}_2 \rightarrow \vec{r}_1). \end{aligned} \quad (11.88)$$

But, according to the boundary conditions on the cell, the flux or its gradient must be zero everywhere on the outer surfaces. Hence, the entire surface integral is zero, which leads to the general result that the one-speed Green's function is symmetric,

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i.e.,

$$G(\vec{r}_1 \rightarrow \vec{r}_2) = G(\vec{r}_2 \rightarrow \vec{r}_1). \quad (11.89)$$

The reciprocity theorem can now be proved in a straightforward manner. For a spatially uniform unit source  $S(\vec{r}') = 1$  placed in region B, the integrated production rate is equal to  $V_B$ ; the flux in region A is the volume integral of the Green's function over all source points  $\vec{r}'$ , namely,

$$\phi_A(\vec{r}) = \int_{\text{reg B}} S(\vec{r}') G(\vec{r}' \rightarrow \vec{r}) d\vec{r}'. \quad (11.90)$$

The escape probability  $P_B$  from region B for region-wise constant cross sections is then equal to the number of absorptions occurring in region A divided by the total number of neutrons produced in region B, or

$$P_B = \frac{\int_{\text{reg A}} \sum_{aA} \phi_A(\vec{r}) d\vec{r}}{V_B} = \frac{\sum_{aA}}{V_B} \int_{\text{reg A}} \int_{\text{reg B}} G(\vec{r}' \rightarrow \vec{r}) d\vec{r}' d\vec{r}. \quad (11.91)$$

Likewise, for a spatially uniform unit source  $S(\vec{r}') = 1$  in region A, the escape probability from region A is

$$P_A = \frac{\int_{\text{reg B}} \sum_{aB} \phi_B(\vec{r}) d\vec{r}}{V_A} = \frac{\sum_{aB}}{V_A} \int_{\text{reg B}} \int_{\text{reg A}} G(\vec{r}' \rightarrow \vec{r}) d\vec{r}' d\vec{r}. \quad (11.92)$$

Now, because of the symmetry of  $G(\vec{r}' \rightarrow \vec{r})$ , we can equate the two double integrals and obtain the reciprocity relationship,

$$P_A = P_B \frac{V_B \sum_{aB}}{V_A \sum_{aA}}. \quad (11.93)$$

Since nothing was said about the size or shape of regions A and B, this result can be applied quite generally.

Specifically, for the resonance absorption problem, every scattering event is the equivalent of an absorption event since

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it removes a neutron from the energy interval under consideration. In this case, the relationship for the escape probability from the moderator region can be written in terms of the escape probability from the fuel region as

$$P_M = P_F \frac{V_F}{V_M} \frac{\Sigma_{TF}}{\Sigma_{sM}}. \quad (11.94)$$

### Application of the Reciprocity Theorem to Heterogeneous Systems.

We return to the fundamental neutron balance equation for a heterogeneous system and insert the reciprocity theorem result. After canceling  $V_F$ , we obtain the equation

$$\begin{aligned} \Sigma_{TF}(E)\phi_F(E) = P_F(E)\Sigma_{TF}(E) \int_E^{E/\alpha_M} \frac{\phi_M(E')}{(1 - \alpha_M)} \frac{dE'}{E'} \\ + [1 - P_F(E)] \left\{ \int_E^{E/\alpha_U} \frac{\Sigma_s^U(E')\phi_F(E')}{(1 - \alpha_U)} \frac{dE'}{E'} + \int_E^{E/\alpha_0} \frac{\Sigma_s^O(E')\phi_F(E')}{(1 - \alpha_0)} \frac{dE'}{E'} \right\}. \end{aligned} \quad (11.95)$$

Note that this expression now contains only  $P_F(E)$ , and that  $\Sigma_{TF}$  has come outside of the first integral.

In order to proceed further by analytical means, we must now make use of some additional approximations. Specifically, we assume that just above the resonance energy the flux is asymptotic, and furthermore that for the purpose of evaluating the integral terms it is approximately equal in the two regions. In this case the asymptotic flux is given by the expression

$$\phi_F(E) \approx \phi_M(E) \approx \frac{1}{\xi \Sigma_p E}. \quad (11.96)$$

We volume-average the potential scattering contributions to obtain the term in the denominator, namely

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$$\overline{\xi \Sigma_p} = \frac{(\xi_U \Sigma_p^U + \xi_0 \Sigma_s^O) V_F + \xi_M \Sigma_{sM} V_M}{V_F + V_M}, \quad (11.97)$$

where we use only the background potential scattering term  $\Sigma_p^U$  for the uranium.

We use the asymptotic flux approximation only for the moderator and oxygen terms, allowing the integrals involving those terms to be evaluated easily. The resulting integral equation for the flux is then

$$\begin{aligned} \Sigma_{TF}(E) \phi_F(E) \approx & (1 - P_F(E)) \int_E^{E/\alpha_U} \frac{\Sigma_s^U(E') \phi_F(E') dE'}{(1 - \alpha_U) E'} \\ & + \frac{(1 - P_F(E)) \Sigma_s^O + P_F(E) \Sigma_{TF}(E)}{\overline{\xi \Sigma_p} E}. \end{aligned} \quad (11.98)$$

**NR Approximation.** Assume that the flux entering the resonance in the remaining integral term for uranium is also asymptotic; integrate the remaining integral using only the potential scattering contribution in uranium. Solve for  $\phi_F(E)$  on the left-hand side of the equation. The result is the value

$$\phi_F^{NR}(E) \approx \frac{(1 - P_F) \Sigma_p^U + (1 - P_F) \Sigma_s^O + P_F(E) \Sigma_{TF}(E)}{\Sigma_{TF}(E) \overline{\xi \Sigma_p} E}. \quad (11.99)$$

Note that the functional form is similar to Eq. 11.44 for the homogeneous case. We use this energy-dependent flux in the absorption probability equation to obtain the heterogeneous NR resonance absorption probability. Since the unit slowing down source is for the total cell volume,  $V$ , this expression is

$$\frac{\text{NR Resonance absorption}}{\text{probability}} = \frac{V_F}{V} \int_{\text{resonance}} \Sigma_{aF}(E) \phi_F^{NR}(E) dE. \quad (11.100)$$

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Note that  $\Sigma_{aF} = N_F^U \sigma_{cF}$ . Inserting the flux, and separating out the terms containing  $P_F(E)$ , we obtain

$$\begin{aligned} \frac{NR \text{ Resonance absorption}}{\text{probability}} &= \frac{N_F^U}{\xi \Sigma_p} \left[ \frac{V_F}{V} \int_{\text{resonance}} \frac{\sigma_{cF}(E)(\Sigma_p^U + \Sigma_s^O) dE}{\Sigma_{TF}(E)} \frac{1}{E} \right. \\ &\quad \left. + \frac{V_F}{V} \int_{\text{resonance}} \frac{P_F(E) \sigma_{cF}(E) [\Sigma_{TF}(E) - \Sigma_p^U - \Sigma_s^O] dE}{\Sigma_{TF}(E)} \frac{1}{E} \right] \end{aligned} \quad (11.101)$$

Note that this expression is in the same general form obtained previously for a homogeneous system, but it contains an effective resonance integral having two *separate* contributions. Since the escape of neutrons must occur over the surface of the fuel lump while the main absorption occurs in the fuel volume, it is natural to define these contributions accordingly. Therefore, we write the equivalent expression

$$\frac{NR \text{ Resonance absorption}}{\text{probability}} = \frac{N_F^U}{\xi \Sigma_p} \left[ I_r^{VNR} + I_r^{SNR} \right] \quad (11.102)$$

where the volume term is

$$I_r^{VNR} \equiv \frac{V_F}{V} \int_{\text{resonance}} \frac{\sigma_{cF}(E)(\Sigma_p^U + \Sigma_s^O) dE}{\Sigma_{TF}(E)} \frac{1}{E}, \quad (11.103)$$

and the surface term, which contains the probability of escape over the fuel surface, is

$$I_r^{SNR} \equiv \frac{V_F}{V} \int_{\text{resonance}} \frac{P_F(E) \sigma_{cF}(E) [\Sigma_{TF}(E) - \Sigma_p^U - \Sigma_s^O] dE}{\Sigma_{TF}(E)} \frac{1}{E}. \quad (11.104)$$

These effective resonance integrals are similar in form to the integrals that we have evaluated previously.

If one inserts the Breit-Wigner form for the absorption cross section, and makes the following definition,

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$$\beta^{NR} \equiv \frac{\Sigma_p^U + \Sigma_s^O}{N_F^U \sigma_r}, \quad (11.105)$$

then the Doppler-broadened form of the volume term is

$$I_r^{VNR} = \frac{\Sigma_{pF}^{NR} \Gamma_\gamma V_F}{N_F^U E_r V} J(\zeta, \beta^{NR}), \quad (11.106)$$

where  $\Sigma_{pF}^{NR} = \Sigma_p^U + \Sigma_s^O$ . Recognizing that  $P_F(E)$  is a function of the optical thickness  $t$  through the mean chord length  $\bar{\ell}$ , the surface term can be put into a similar form, namely,

$$\begin{aligned} I_r^{SNR} &= \frac{\sigma_r \Gamma_\gamma V_F}{E_r V} \int_0^\infty P_F(\bar{\ell}, \zeta, \beta^{NR}) \left[ \frac{\psi^2}{\psi + \beta^{NR}} \right] dx \\ &\equiv \frac{\sigma_r \Gamma_\gamma V_F}{E_r V} L(\bar{\ell}, \zeta, \beta^{NR}). \end{aligned} \quad (11.107)$$

The function  $L(\bar{\ell}, \zeta, \beta^{NR})$  has been computed by Adler and Nordheim and is also a tabulated function.

**NRIM Approximation.** Similar results are obtained using the NRIM approximation. The major differences are a redefinition of parameters to exclude the potential and resonance scattering in the uranium in Eq. (11.98), and the addition of a first-order correction of the escape probabilities.

**Discussion.** The above methodology depends on the validity of a number of assumptions. The foremost assumption is that the slowing down transient in the collision density can be ignored, so that an asymptotic flux exists at each single energy. This justifies the use of the reciprocity theorem to connect the escape probabilities between regions, giving a functional form that can be interpreted in terms of volume absorption and surface



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absorption. A second assumption is that the Dancoff correction for a black cylinder can be used for all energies, and it can be combined with the Wigner rational approximation interpolation function to represent the energy-dependent escape probability from the fuel pin. Finally, we restrict ourselves to the use of the Doppler-broadened single level Breit Wigner form for the resonance, without a cross term, and make an assumption of the validity of either the NR or NRIM approximations.

It is surprising that this methodology works as well as it does. In fact, for hydrogen, deuterium and beryllium moderators, the assumption of asymptotic slowing down is fairly good, but for carbon it is not completely valid, and an intermediate resonance treatment is needed to avoid errors of the order of 20%. In the wings of a resonance, the absorption cross section is low, and neutrons penetrate deep into the fuel pin; this is the source of most of the volume absorption. Near the peak of the resonance, the absorption cross section is high and spatial self-shielding is strong; this is the source of most of the surface absorption, which justifies and limits the range over which the rational approximation needs to be valid.

To do significantly better requires more sophisticated cross section representations, greater spatial detail, and the inclusion of slowing down calculations for moderators that do not obey the NR conditions. This requires computationally intensive methods that are not well suited to routine design calculations.

It should be pointed out that the standard treatments used in some computer codes can usually be replaced with more sophisticated treatments where necessary. Some of the modern "Modular" computer code systems, which are in operation at a number of laboratories, are designed to allow ready substitution of nonstandard special calculations at arbitrary positions in the flow "path" of a reactor design study.

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### 11.7 Reactor Design Implications of Heterogeneous Lumping

The appearance of surface and volume terms is physically plausible in the heterogeneous case. But the overall effect on the reactor is obtained as a function of the relative spatial effects on the thermal flux and the resonance energy fluxes. Specifically, for a given cell composition (moderator/fuel ratio) the fission rate and the resonance absorption rates have the following forms:

$$\text{Fission rate} = \int_{\text{volume}}^{\text{cell}} N_{25}(\vec{r}) \sigma_{25} \phi_{\text{th}}(\vec{r}) d\vec{r},$$

$$\left[ \begin{array}{c} \text{Resonance absorption} \\ \text{rate in a typical} \\ \text{resonance} \end{array} \right] = \int_{\text{volume}}^{\text{cell}} N_{28}(\vec{r}) \sigma_{c28} \phi_{\text{epi}}(\vec{r}) d\vec{r}.$$

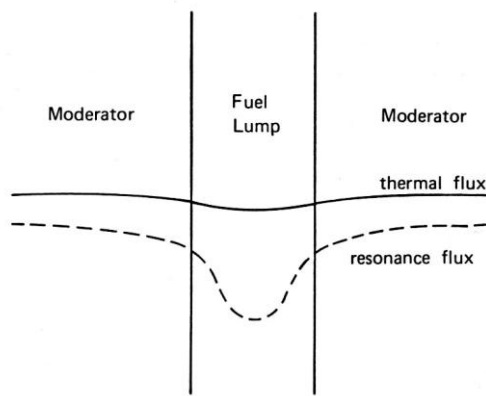
Postulate three cases: (1) homogeneous cell; (2) small lump of fuel; and (3) large lump of fuel. We have the following results.

Case 1. For a homogeneous mixture, the flux is spatially uniform and all  $^{235}\text{U}$  and  $^{238}\text{U}$  atoms are equally effective regardless of spatial position.

Case 2. For a small lump, the thermal flux will decrease slightly in the lump, while the resonance flux will decrease strongly just inside the surface of the lump as shown in Figure 11.23. Hence, the  $^{235}\text{U}$  atoms are approximately equally effective no matter where they are, while a large fraction of the  $^{238}\text{U}$  atoms become ineffective in absorbing resonance neutrons due to spatial self-shielding. The relative resonance-absorption-to-fission ratio decreases.

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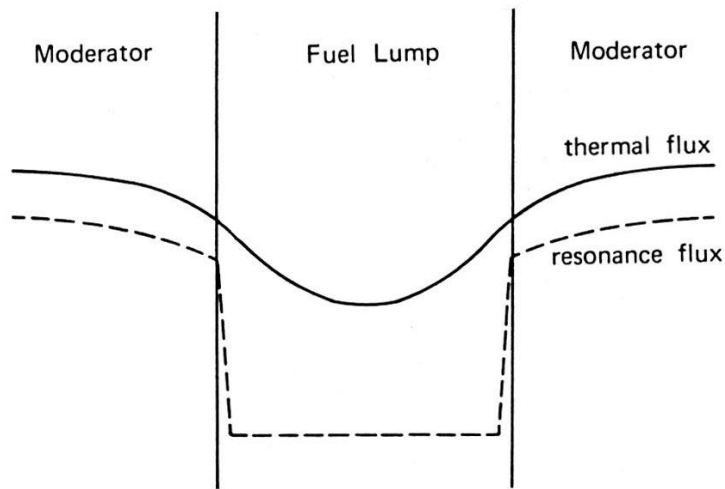
Case 3. In a large lump the thermal flux also decreases significantly in the fuel as shown in Figure 11.24, and the effectiveness of the  $^{235}\text{U}$  decreases. The  $^{238}\text{U}$  atoms are already strongly self-shielded approaching an asymptotic value, so that the relative change in resonance absorption is small. Hence, the primary effect is a decrease in the fission rate.



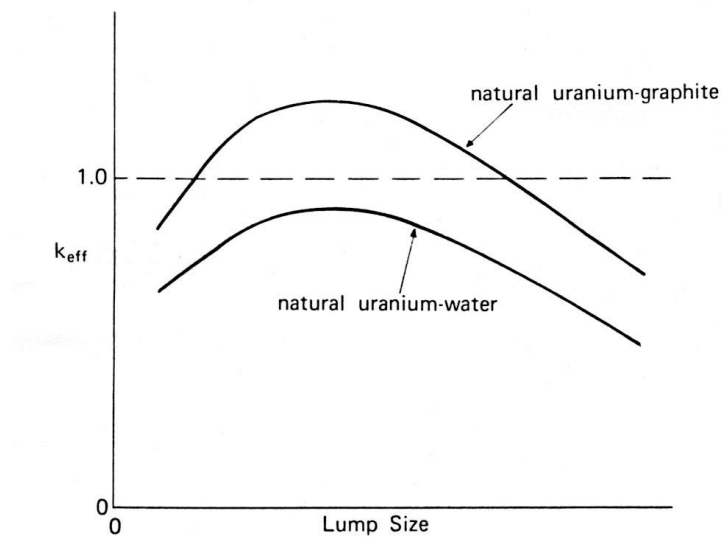
**Fig. 11.23** Small-Lump Flux Distributions, Schematic Variations

Comparing the three cases, one sees that in going from the homogeneous case to the small lump case the relative fission/resonance absorption ratio increases, thus raising  $k_{\infty}$ . As the lump gets bigger, the absolute fission rate decreases, causing  $k_{\infty}$  to drop. One sees a maximum in the  $k_{\infty}$  vs. lump size curve for a given fuel/moderator ratio in a given size reactor. Since one needs  $k_{\text{eff}} = 1$  to obtain a critical configuration, the reactor will sustain a chain reaction only if the maximum of the  $k_{\infty}$  curve exceeds unity as shown in Figure 11.25. Natural uranium-water assemblies will never achieve criticality under the above considerations, while natural uranium-graphite systems will go critical when the fuel is lumped sufficiently.

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**Fig. 11.24** Large-Lump Flux Distributions, Schematic Variations



**Fig. 11.25**  $k_{\infty}$  vs. Fuel Lump Size, Schematic Variation for Fixed Fuel/Moderator

A similarly shaped curve is obtained when one first picks the lump size and then varies the fuel-to-moderator ratio. When

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the fuel-to-moderator ratio is large, there is not enough moderator to effectively slow the neutrons down before they are captured. When this ratio is small, there is not enough fuel to produce a sufficient number of fission neutrons relative to those captured. The peak of the  $k_{\infty}$  curve occurs for comparable amounts of fuel and moderator. Reactors are designed to be on the under-moderated side of the  $k_{\infty}$  peak, so that if for some reason the moderator is lost or its density is reduced accidentally, the reactivity effect will be negative.

Total effective resonance integrals have been experimentally correlated to expressions involving the surface/mass ratio,  $S/M$ , of the lump. These expressions are of the form

$$I = a + b \left( \frac{S}{M} \right) \quad (11.108)$$

or

$$I = a' + b' \sqrt{\frac{S}{M}}. \quad (11.109)$$

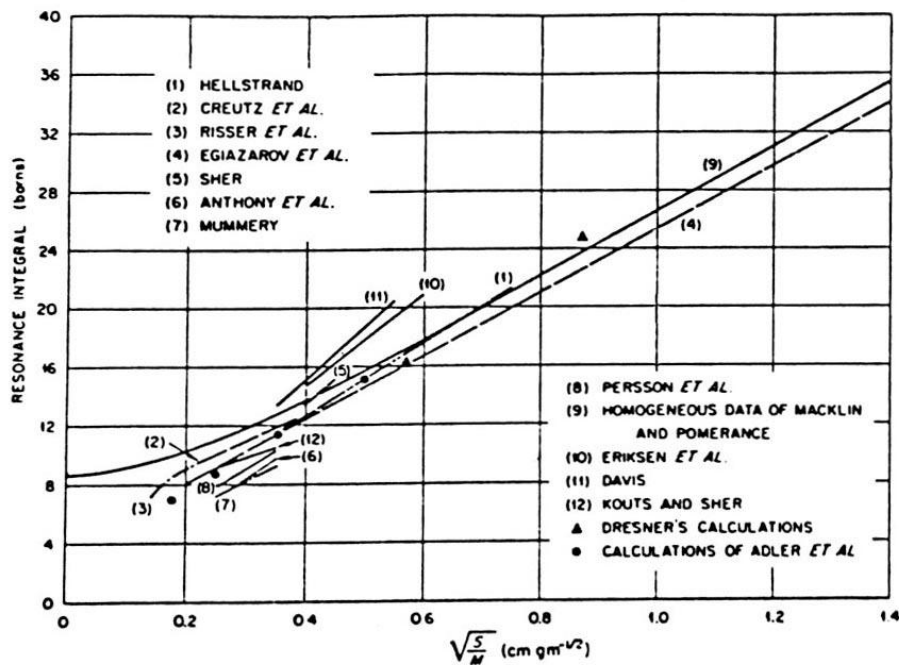
The latter correlation is shown in Figure 11.26 for  $^{238}\text{U}$ , and demonstrates the validity of the theoretical prediction of separate volume and surface resonance neutron absorption effects.

**General Comments.** At this point it is useful to look back upon the heterogeneous treatment to examine its accuracy. The treatment presented here dates back to the early 1960's, and has been used fairly successfully in thermal reactor design. It is the basis of various commonly used reactor design codes such as GAM, in which the energy range from 10 MeV down to 0.4 eV is divided into 68 groups having a uniform lethargy spacing of  $\Delta u = 1/4$ . With a lethargy spacing of this magnitude, several resonances typically fall entirely within a single energy group, and resonance capture must be approached from the standpoint of

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effective resonance integrals.

The above treatment is not entirely adequate if one considers fast reactors, where the entire reaction rate occurs typically above 10 keV. In a fast reactor one has scattering resonances in materials such as sodium, which requires a detailed numerical treatment with many energy intervals taken to cover a single resonance. Fortunately, the problem is primarily one of energy self-shielding and not of spatial self-shielding. It is treatable, for example, by the Bondarenko method, which has been automated using cross section fits in the Los Alamos-developed MXS code. Codes such as MC<sup>2</sup>, which allow one to treat the slowing down problem using as many as 2000 energy groups, have also been developed. Hence, one solves the integral balance equation directly using numerical techniques.



**Fig. 11.26** Experimental Effective Resonance Integral Correlation for  $^{238}\text{U}$

(From *Resonance Absorption in Nuclear Reactors* by L. Dresner, 1960, Pergamon Press)

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At the highest level of sophistication, one attempts to solve the complete cell space-energy problem numerically, thus avoiding the use of escape probabilities completely. It has been attacked by such techniques as "synthesis" or "factorization," in which the solution at any space point is constrained to be made up of linear combinations of energy-dependent trial functions. The object is to find the "best" linear combination of solutions (say from several MC<sup>2</sup> runs), valid over specific energy ranges, at each position within the cell. Another approach involves doing detailed Monte Carlo spatial transport solutions in a lattice at several discrete energies, with the object of fitting the energy-dependent flux in the pin to a rational approximation form for use with modified J-functions in the calculation of resonance integrals. This is an alternative to running coupled MC<sup>2</sup>-Monte Carlo models. Such methods are usually too costly for routine design applications.

### 11.8 The GAM Multigroup Slowing Down Equations

The GAM computer code solves the space-independent slowing down equations using the  $P_1$  approximation to the Boltzmann transport equation. The effect of spatial leakage is included in a gross fashion by means of an energy-dependent buckling term. Since thermal neutrons are not included, the effect of fission is obtained by separately inserting an isotropic energy-dependent fast neutron source, which can have the shape of a fission spectrum.

The spatially-dependent Boltzmann equation is the starting point in the derivation. It is written as

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leakage

absorption and outscatter

$$\vec{\Omega} \cdot \nabla \Phi(\vec{r}, E, \vec{\Omega}) + \Sigma_T(E) \Phi(\vec{r}, E, \vec{\Omega}) = \frac{S_0(\vec{r}, E)}{4\pi} + \int_{4\pi} \int_E^\infty \Sigma_s(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(\vec{r}, E', \vec{\Omega}') dE' d\Omega'. \quad (11.110)$$

isotropic source

in scatter

$$= \frac{S_0(\vec{r}, E)}{4\pi} + \int_{4\pi} \int_E^\infty \Sigma_s(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \Phi(\vec{r}, E', \vec{\Omega}') dE' d\Omega'.$$

Recall that, for elastic scattering, the energy  $E$  of the scattered neutron of initial energy  $E'$  is uniquely determined by the cosine of the angle through which the neutron scatters in the CM system, namely,  $\cos\Theta$ . This relationship can be written as

$$(E - E') = \frac{-2A'E}{(A+1)^2} (1 - \cos\Theta). \quad (11.111)$$

We replace the cross-section term  $\Sigma_s(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})$ , which in this treatment contains both an isotropic and a linearly anisotropic component, by an equivalent scattering cross section at energy  $E'$  and angle  $\vec{\Omega}'$  times a delta function that contains the energy-angle relationship given above; the equation is

$$\Sigma_s(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) = \Sigma_s(\vec{\Omega}', E' \rightarrow E) \delta \left[ E' - E - \frac{2A'E}{(A+1)^2} (1 - \cos\Theta) \right]. \quad (11.112)$$

The basic procedure at this point, as shown in Chapter 4, is to expand both the unknown flux and the known scattering cross section in a series of Legendre polynomials, and then successively weight the Boltzmann equation by each Legendre polynomial in turn and integrate over the angular variable. The result is a set of coupled first order energy-dependent equations called the  $P_n$  equations, where  $n$  is the highest order term kept in the series expansion. In this case we stop with  $n = 1$ , which



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gives the  $P_1$  equations. The first moment of angular flux is the total flux  $\phi$  and the second moment of the angular flux is the current  $\vec{J}$ , i.e.,

$$\phi(\vec{r}, E) = \int_{4\pi} \Phi(\vec{r}, E, \vec{\Omega}) d\Omega$$

and

$$\vec{J}(\vec{r}, E) = \int_{4\pi} \Phi(\vec{r}, E, \vec{\Omega}) \vec{\Omega} d\Omega \quad (11.113)$$

Similarly, the scattering cross section has components

$\Sigma_{s0}(E' \rightarrow E)$ , which is the isotropic part, and

$\Sigma_{s1}(E' \rightarrow E)$ , which is the linearly anisotropic part.

The actual derivation is somewhat complicated and only the result will be given here, which is the pair of equations,

$$\text{scalar } \nabla \bullet \vec{J}(\vec{r}, E) + \Sigma_T(E)\phi(\vec{r}, E) = \int_E^\infty \Sigma_{s0}(E' \rightarrow E)\phi(\vec{r}, E') dE' + S_0(\vec{r}, E), \quad (11.114)$$

and

$$\text{vector } \nabla \phi(\vec{r}, E) + 3\Sigma_T(E)\vec{J}(\vec{r}, E) = 3 \int_E^\infty \Sigma_{s1}(E' \rightarrow E)\vec{J}(\vec{r}, E') dE'. \quad (11.115)$$

In our previous work on slowing down, we have only treated the first of these equations, omitting leakage.

Now, the spatial dependence is averaged out. The first equation is integrated over space directly, while the divergence of the second equation is integrated over space. The results are the two scalar equations,

$$J(E) + \Sigma_T(E)\phi(E) = \int_E^\infty \Sigma_{s0}(E' \rightarrow E)\phi(E') dE' + S(E) \quad (11.116)$$

and

$$-B^2(E)\phi(E) + 3\Sigma_T(E)J(E) = 3 \int_E^\infty \Sigma_{s1}(E' \rightarrow E)J(E') dE', \quad (11.117)$$

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where the following definitions have been used:

$$-B^2(E) \equiv \frac{\int \nabla^2 \phi(\vec{r}, E) d\vec{r}}{\int \phi(\vec{r}, E) d\vec{r}} = \frac{\text{Average buckling for}}{\text{spatial leakage}};$$

$$\phi(E) \equiv \frac{\int \phi(\vec{r}, E) d\vec{r}}{\int d\vec{r}} = \text{Space averaged flux};$$

$$S(E) \equiv \frac{\int S_0(\vec{r}, E) d\vec{r}}{\int d\vec{r}} = \text{Space averaged source spectrum}$$

$$J(E) \equiv \frac{\int \nabla \cdot \vec{J}(\vec{r}, E) d\vec{r}}{\int d\vec{r}} = \frac{\text{Net average out - leakage}}{\text{from the reactor surface}}.$$

Note the distinction between  $J(E)$  and  $B^2(E)$ . The former is the leakage actually crossing the surface of the reactor while the latter is the proportionally factor between the flux and the curvature of the flux.  $J(E)$  is unknown, while  $B^2(E)$  is an *input* quantity.

In order to solve the coupled first-order equations we must discretize them over lethargy by integrating from  $u_{g-1}$  to  $u_g$  for  $g = 1$  to  $G$ . Let the lethargy interval for the  $g$ th group be defined as

$$\Delta u_g \equiv \int_{u_{g-1}}^{u_g} du = u_g - u_{g-1}.$$

Then, the discretization process gives us the following form for the first equation,

# NUCLEAR REACTOR THEORY AND DESIGN

$$\begin{aligned}
 & \int_{u_{g-1}}^{u_g} J(u) du + \int_{u_{g-1}}^{u_g} \sum_T(u) \phi(u) du \\
 & = \int_{u_{g-1}}^{u_g} \left[ \sum_{g'=1}^g \int_{u_{g'-1}}^{u_{g'}} \sum_{s0}(u' \rightarrow u) \phi(u') du' \right] du + \int_{u_{g-1}}^{u_g} S(u) du.
 \end{aligned}
 \tag{11.118}$$

In a similar fashion, the second equation gives

$$\begin{aligned}
 & \int_{u_{g-1}}^{u_g} -B^2(u) \phi(u) du + 3 \int_{u_{g-1}}^{u_g} \sum_T(u) J(u) du \\
 & = 3 \int_{u_{g-1}}^{u_g} \left[ \sum_{g'=1}^g \int_{u_{g'-1}}^{u_{g'}} \sum_{s1}(u' \rightarrow u) \phi(u') du' \right] du.
 \end{aligned}
 \tag{11.119}$$

Now, we make some additional definitions for each group term:

$$\begin{aligned}
 S_g & \equiv \frac{\int_{u_{g-1}}^{u_g} S(u) du}{\Delta u_g} = \text{Group source;} \\
 \phi_g & \equiv \frac{\int_{u_{g-1}}^{u_g} \phi(u) du}{\Delta u_g} = \text{Group flux;} \\
 J_g & \equiv \frac{\int_{u_{g-1}}^{u_g} J(u) du}{\Delta u_g} = \text{Group current} \\
 \sum_{Tog} & \equiv \frac{\int_{u_{g-1}}^{u_g} \sum_T(u) \phi(u) du}{\int_{u_{g-1}}^{u_g} \phi(u) du} = \begin{array}{l} \text{Flux-averaged} \\ \text{total cross section;} \end{array} \\
 \sum_{Tlg} & \equiv \frac{\int_{u_{g-1}}^{u_g} \sum_T(u) J(u) du}{\int_{u_{g-1}}^{u_g} J(u) du} = \begin{array}{l} \text{Current-averaged} \\ \text{total cross section;} \end{array}
 \end{aligned}$$

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$$\begin{aligned}\Sigma_{s'og \rightarrow g} &\equiv \frac{\int_{u_{g-1}}^{u_g} \int_{u_{g'-1}}^{u_{g'}} \Sigma_{so}(u' \rightarrow u) \phi(u') du' du}{\int_{u_{g'-1}}^{u_{g'}} \phi(u') du'} \\ &= \frac{\text{Isotropic group transfer}}{\text{cross section;}}\end{aligned}$$

and

$$\begin{aligned}\Sigma_{s'lg \rightarrow g} &\equiv \frac{\int_{u_{g-1}}^{u_g} \int_{u_{g'-1}}^{u_{g'}} \Sigma_{sl}(u' \rightarrow u) J(u') du' du}{\int_{u_{g'-1}}^{u_{g'}} J(u') du'} \\ &= \frac{\text{Linearly anisotropic}}{\text{group transfer}} \\ &\quad \text{cross section.}\end{aligned}$$

Note that we have not yet faced the problem of treating the allowed scattering intervals of the various scattering isotopes, in relation to the integration ranges given above. This decidedly nontrivial problem will be considered later.

When the group width  $\Delta u_g$  is very large with respect to the width of a resonance, the resonance effect can be included by using the effective resonance integral. If there are a total of  $K$  resonances in the given group, then the effective resonance portion of the macroscopic absorption cross section for the group for a homogeneous medium would be given by the expression

$$\Sigma_{ag} = \left[ \sum_{r=1}^K \frac{N_F I_r}{\Delta u_g} \right]_{in g}. \quad (11.120)$$

This term would be added to the group absorption from isotopes with slowly varying absorption cross sections.

In the case of a heterogeneous lattice, the number density of the fuel region is used along with the surface and volume

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resonance integrals that have already been smeared over the whole cell volume.

In multi-group slowing down codes such as GAMTEC, the  $J(\zeta, \beta)$  and  $L(\bar{\ell}, \zeta, \beta)$  functions are built in as tabulations over a range of values of  $\bar{\ell}$ ,  $\zeta$ , and  $\beta$ ; a means is provided for interpolating to obtain intermediate values. The appropriate approximation, NR or NRIM, is automatically made for each resonance and for each resonance absorber included in the code library. Furthermore, the codes contain tabulations of the Dancoff correction factor or a provision for inserting this factor externally; hence the Dancoff correction is applied to modify the escape probability. The mean chord length is also obtained internally using the surface area and size of the fuel lump. Thus, all of the resonance effects with Doppler broadening are properly included in the detailed zero-dimensional slowing down calculation, from which is derived the appropriate few-group absorption cross sections for reactor design calculations.

With the above definitions, the two equations for a typical group are the following:

$$J_g \Delta u_g + \sum_{\text{To}g} \phi_g \Delta u_g = \sum_{g'=1}^g \mathbf{E}_{s'og \rightarrow g} \phi_{g'} \Delta u_{g'} + S_g \Delta u_g \quad (11.121)$$

and

$$-B_g^2 \phi_g \Delta u_g + 3 \sum_{\text{To}g} J_g \Delta u_g = 3 \sum_{g'=1}^g \mathbf{E}_{slg' \rightarrow g} J_{g'} \Delta u_{g'} \quad (11.122)$$

We have a similar pair of equations for each of the  $G$  fast groups, for a total of  $2G$  equations, all of which are coupled. We supply the cross sections and the values of  $B_g^2$  and solve for  $\phi_g$  and  $J_g$  for all groups.

The definitions of our group cross sections involve averaging the detailed microscopic cross sections over flux and current spectra. Actually, we do not know the values for either

## NUCLEAR REACTOR THEORY AND DESIGN

of these quantities beforehand. Therefore, we must guess spectra, such as an asymptotic  $1/E$  distribution, or use a detailed spectrum from another problem to perform this task; an iterative process may be needed in order to obtain consistency. To simplify our task, and since we have to guess the spectra in any event, we shall use the flux averaged definitions throughout; thus we make the approximation that

$$\Sigma_{Tog} \approx \Sigma_{Tlg}. \quad (11.123)$$

Furthermore, since we have down-scatter only, the sum in the group transfer term goes only from the fastest group (group 1) down to group  $g$ . If we look specifically at the fastest group, we find that the only term included is within-group scattering. In this case the first two equations are

$$J_1 + \Sigma_{T01}\phi_1 = \Sigma_{s01 \rightarrow 1} + S_1 \quad (11.124)$$

and

$$-B_1^2\phi_1 + 3\Sigma_{T01}J_1 = 3\Sigma_{s11 \rightarrow 1}J_1 \quad (11.125)$$

At this point it is convenient to combine some of the cross section terms. We define a new total group removal cross section which excludes the within-group scattering, namely,

$$\Sigma_{Tg} \equiv \Sigma_{Tog} - \Sigma_{sog \rightarrow g}. \quad (11.126)$$

Applying this definition, the pair of equations for group 1 can be put into the vector-matrix form,

$$\begin{bmatrix} \Sigma_{T1} & I \\ -B_1^2 & 3(\Sigma_{T1} + \Sigma_{s01 \rightarrow 1} - \Sigma_{s11 \rightarrow 1}) \end{bmatrix} \begin{bmatrix} \phi_1 \\ J_1 \end{bmatrix} = \begin{bmatrix} S_1 \\ 0 \end{bmatrix}. \quad (11.127)$$

The flux and current in the first group can be obtained by inverting the matrix giving

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$$\phi_l = \frac{3(\sum_{Tl} + \sum_{sol \rightarrow l} - \sum_{sl \rightarrow l})S_l}{3\sum_{Tl}(\sum_{Tl} + \sum_{sol \rightarrow l} - \sum_{sl \rightarrow l}) + B_l^2} \quad (11.128)$$

and

$$J_l = \frac{B_l^2 \phi_l}{3(\sum_{Tl} + \sum_{sol \rightarrow l} - \sum_{sl \rightarrow l})}. \quad (11.129)$$

Note the similarity of the latter equation to the Fick's law equation, namely,

$$J_l = -D_l \nabla^2 \phi_l = D_l B_l^2 \phi_l. \quad (11.130)$$

Here the group diffusion coefficient is defined as

$$D_l \equiv \frac{1}{3(\sum_{Tl} + \sum_{sol \rightarrow l} - \sum_{sl \rightarrow l})}, \quad (11.131)$$

so that Eq. (11.128) reduces to the balance

$$S_l = \sum_{Tl} \phi_l + D_l B_l^2 \phi_l.$$

The equations for the next energy group contain a sum of group transfers from higher energy groups, which are all known at the time that the equation is to be solved. If we denote the group transfer sums as

$$S_g^0 \equiv \sum_{g'=l}^{g-1} \sum_{s'og \rightarrow g} \phi_{g'} \Delta u_{g'} \quad (11.132)$$

and

$$S_g^l \equiv \sum_{g'=l}^{g-1} \sum_{slg' \rightarrow g} J_{g'} \Delta u_{g'}, \quad (11.133)$$

then the solutions in general are the following:

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$$\phi_g = \frac{3(\sum_{Tg} + \sum_{sog \rightarrow g} - \sum_{slg \rightarrow g})(S_g \Delta u_g + S_g^0) - S_g^I}{[3 \sum_{Tg} (\sum_{Tg} + \sum_{sog \rightarrow g} - \sum_{slg \rightarrow g}) + B_g^2] \Delta u_g} \quad (11.134)$$

and

$$J_g = \frac{S_g^I + B_g^2 \phi_g \Delta u_g}{[3(\sum_{Tg} + \sum_{sog \rightarrow g} - \sum_{slg \rightarrow g})] \Delta u_g}. \quad (11.135)$$

These equations can be solved, two at a time, from the highest energy group down because we have down-scatter only.

**Scattering Transfer Cross Sections.** The total cross-section terms are not difficult to treat, except when there are resonances. For a group containing a resonance, the Doppler-broadened resonance integral is used, which includes appropriate heterogeneous effects such as rod size, Dancoff correction, etc.

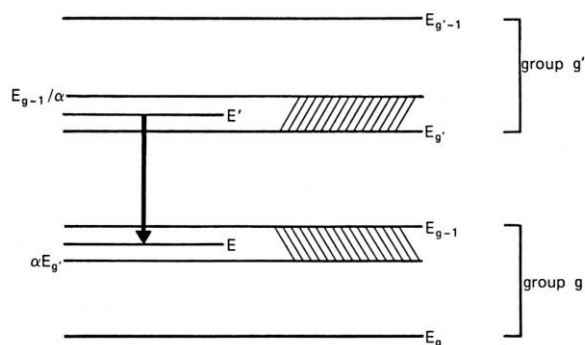
The scattering transfer cross sections, on the other hand, are reasonably complicated. The main question is, how does the range of the scattering integral compare to the group structure chosen for each isotope in the library? If we draw a plot of  $E'$  vs.  $E$ , we can superimpose the group structure and find the allowable integration ranges.

For example, consider the energy diagram given in Figure 11.27. For the given value of  $\alpha$ , the minimum energy that a neutron coming from group  $g'$  can have is  $E = \alpha E_{g'}$ , while the maximum starting energy is  $E' = E_{g-1}/\alpha$  if the neutron is to end up in group  $g$ .

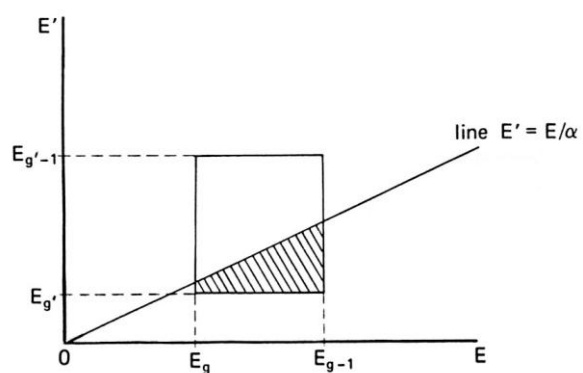
Actually, there are six possible cases, as shown in Figures 11.28 and 11.29. Figure 11.27 corresponds to case number 2.



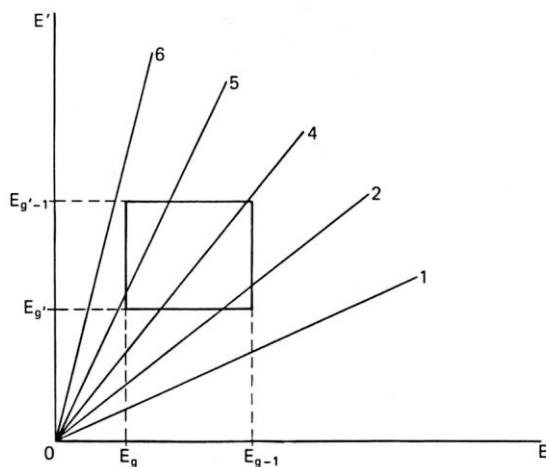
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**Fig. 11.27** Energy Diagram for Transfer of Neutrons from Group  $g'$  to  $g$



**Fig. 11.28** Orientation of the Group  $g'$  and Group  $g$  Limits with Respect to the Line  $E' = E/\alpha$ .



**Fig. 11.29** Additional Orientations of the Group  $g'$  and Group  $g$  Limits with Respect to the Line  $E' = E/\alpha$

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On the  $E'$  vs.  $E$  diagram the double integral is taken over the cross-hatched area below the line  $E' = E/\alpha$ . For case number 3, the limits of integration are obtained by inspection to be  $E_{g'} < E' < E/\alpha$  and  $E_g < E < E_{g-1}$ . Hence, for this particular isotope and group structure, the integral would be of the form

$$\Sigma_{s'og \rightarrow g} = \frac{\int_{E_g}^{E_{g-1}} \int_{E_{g'}}^{E/\alpha} \Sigma_{so}(E' \rightarrow E) \phi(E') dE' dE}{\int_{E_{g'}}^{E_{g-1}} \phi(E') dE'}. \quad (11.136)$$

The corresponding limits for the other cases will not be derived here, but all integrals can be evaluated analytically or numerically to give the appropriate group transfer cross sections for each isotope present in the cross section library.

**Fast Fission.** As indicated in Chapter 3, a number of different transuranic isotopes are fissionable if enough kinetic energy is supplied by the incident neutron to overcome the critical energy needed for fission. These reactions are threshold reactions, which usually have microscopic cross sections that are of the order of barns for neutron energies greater than approximately 1 MeV. Fast neutrons from fission have energies in this range, so that fast fission can be significant and must be considered. In fact, in some cases fast fission can be as much as 10% of the total fission rate.

For homogeneous mixtures of materials, the effect of fast fission can be included in the GAM equations by simply supplying the appropriate fission cross sections in the high-energy groups. No special treatment is necessary. On the other hand, for heterogeneous systems, a complicated treatment is necessary. Fast neutrons can traverse several lattice cells before they suffer a sufficient number of scattering collisions to lower

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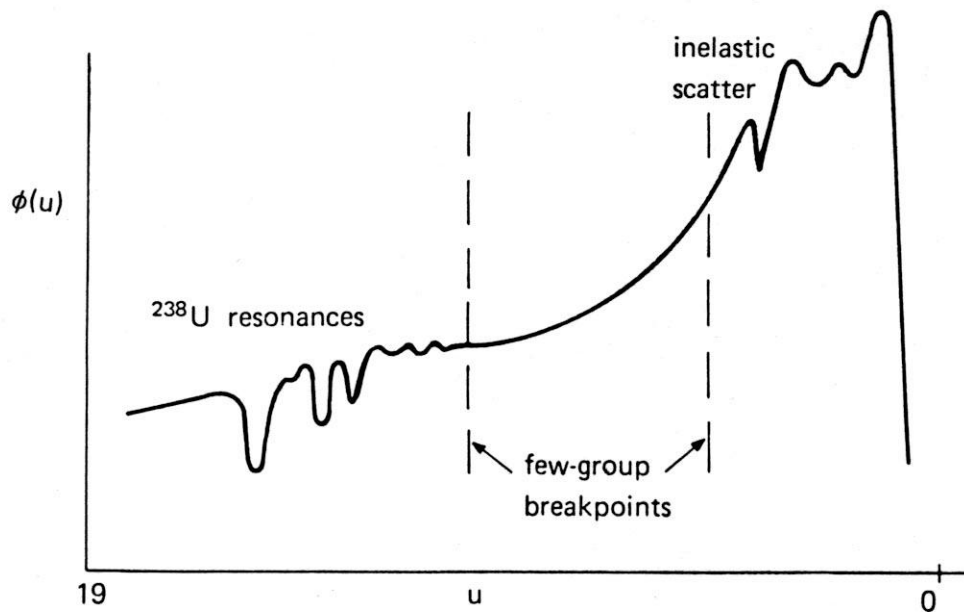
their energies below the fission threshold. Hence, not only first collision escape probabilities must be considered, but also multiple collision escape probabilities. The detailed treatment of the heterogeneous fast fission effect is beyond the scope of this book. One such treatment is Bonalumi's method.

Heterogeneous fast fission is included in computer codes such as GAMTEC by computing correction factors by which all of the fast group fission cross sections are appropriately modified.

The slowing down calculation then proceeds as if the medium was homogeneous. In any event, the few-group average cross sections produced by the code implicitly contain the effects of fast fission.

**Typical Numerical Results.** A typical fast neutron and slowing down spectrum is shown in Figure 11.30. The high-energy peak represents the fission spectrum source, and the dips around 2 MeV are caused primarily by inelastic scattering in oxygen. At the low-energy end of the spectrum, one also observes the smoothed-out absorption in the  $^{238}\text{U}$  resonances and the resulting drop in the slowing down density with net absorption.

Cross-section averages over broad groups are obtained by choosing energy breakpoints and averaging the cross sections over the flux in each range. In Figure 11.30, the fast spectrum is divided into three broad groups. When the thermal group average cross sections are added, the result is a set of few-group cross sections suitable for one region of a 4-group reactor criticality problem.



**Fig. 11.30** Typical Fast Neutron Spectrum vs. Lethargy

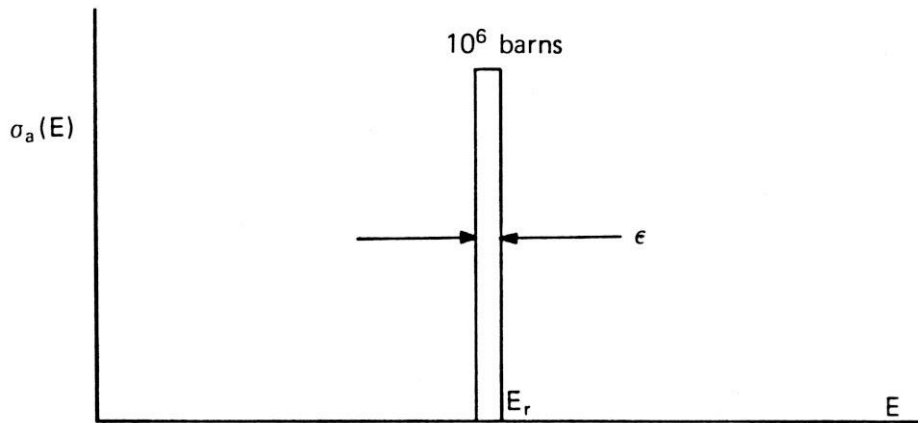
### Problems

**11.1** Fast neutrons of energy  $E_0$  are uniformly produced in an infinite homogeneous scattering medium having a constant  $\Sigma_s$ . They slow down without absorption to a lower energy  $E_1$ , where  $E_1 \ll \alpha E_0$ . At  $E_1$  there is a strong resonance that extends down to  $E_2$ .

- a) Assuming that all the neutrons in the interval  $E_1 - E_2$  are absorbed, calculate the resonance escape (non-absorption) probability if  $\alpha E_1 < E_2 < E_1$ . Use fundamental slowing down theory to obtain the answer.
- b) What should the result be for  $E_2 < \alpha E_1$ ? Show that your answer to part (a) reduces to this result at  $E_2 = \alpha E_1$ .

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- 11.2** Consider a material whose resonance absorption cross section can be approximated by a narrow rectangle at energy  $E_r$  which is  $\epsilon$  eV wide and  $10^6$  barns high as shown in the figure below. The material does not scatter neutrons. The moderator is non-absorbing with a constant scattering cross section of  $\sigma_{SM} = 1$  barn. The ratio of moderator to absorber is  $N_M/N_A = 1.0$ . Write an approximate expression for the resonance absorption probability in an asymptotic energy region where the narrow resonance approximation (NR) is valid. State your assumptions.



- 11.3** You are given a pure scattering medium ( $A > 1$ ) with a constant scattering cross section  $\Sigma_s$ . Consider an energy region far below the source energy. Between  $E_1$  and  $E_2$  there is a resonance whose absorption cross section is  $\Sigma_a = 9\Sigma_s$ . Above  $E_1$ , the flux is asymptotic,  $\phi(E) = \frac{I}{\xi \Sigma_s E}$ . Also,  $\alpha E_1 < E_2$ . Make an assumption that in the resonance region the flux varies as  $\phi(E) = \frac{I}{\xi \Sigma_s E}$ . Neglect the Doppler effect.

- a) Derive an expression for the approximate value of the slowing down density  $q(E_2)$ .
- b) Evaluate this expression if  $A = 12$ ,  $\Sigma_s = 0.1 \text{ cm}^{-1}$

## NUCLEAR REACTOR THEORY AND DESIGN

and  $E_2 = 0.9E_1$ .

- c) Find the non-absorption probability using  $q(E_1)$  and  $q(E_2)$ .
- d) Find the non-absorption probability by directly evaluating the absorption.
- e) Explain the difference seen in parts c) and d).

**11.4** What is the Doppler effect? Explain what happens when a resonance absorber is heated. What type of feedback is obtained in the following situations:

- a) a thermal reactor fueled with natural uranium?;
- b) a thermal reactor fueled with highly enriched  $^{235}\text{U}$ ?
- c) a fast reactor fueled with highly enriched  $^{235}\text{U}$ ?

**11.5** Prove that  $\chi(\zeta, x)$  is given by the differential equation

$$\chi(\zeta, x) = 2x\psi(\zeta, x) + \frac{4}{\zeta^2} \frac{d\psi(\zeta, x)}{dx},$$

where  $\psi(\zeta, x)$  is the ordinary Doppler function.

**11.6** Show that the integral of the Gaussian function  $N(V_x)$  is unity, i.e.,

$$\int_{-\infty}^{\infty} \left[ \frac{M}{2\pi kT} \right]^{1/2} \exp\left( -\frac{MV_x^2}{2kT} \right) dV_x = 1.0.$$

**11.7\*** The radiation widths and neutron widths of two of the lowest energy resonances in  $^{238}\text{U}$  are given below. Complete the table.

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$E_r$ (eV)	$\Gamma_\gamma$ (mV)	$\Gamma_n^r$ (mV)	$\sigma_r$ (b)
6.67	26	1.52	?
21.0	26	8.5	?

Calculate the resonance absorption probabilities for these two resonances for a one-to-one atom mixture of uranium and hydrogen at the following temperatures:

- a)  $T = 0^\circ\text{K}$  ;
- b)  $T = 300^\circ\text{K}$  ;
- c)  $T = 600^\circ\text{K}$  ;

**11.8** You are the head of the Reactor Physics Design Group at Xenon Nuclear Industries, one of the commercial suppliers of thermal reactors that is competing with Westinghouse, etc., for a share of the market. As a result of regulatory decision, the maximum fuel pellet temperature must be lowered, and the company's Thermal-Hydraulics group recommends meeting this criterion by making the fuel rods 10% smaller in diameter than the present design. Discuss the impact of this decision on your design group. Specifically, list the jobs that must be done and estimate the time and amount of manpower needed to accomplish this task. Make an estimate of the cost to the company of this seemingly minor design change.

**11.9** What is reciprocity? Prove reciprocity for the one-speed slab geometry system that obeys the equation

$$-\frac{d}{dx}D(x)\frac{d\phi}{dx} + \sum_a(x)\phi(x) = S(x),$$

where  $\phi(x)|_{\text{outer surfaces}} = 0$ .

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Hint: Consider using a Green's function for this problem.

**11.10** Compute the flux-weighted scattering transfer cross section (a number) from Group 5 to Group 10 for hydrogen with  $\sigma_s = 20$  barns where Group 5 lethargy is from 1.00 to 1.25 and Group 10 lethargy is from 2.25 to 2.50.

**11.11** For cases 4 and 5 shown in Figure 11.29,

- a) derive the limits for the scattering transfer integral. Draw the corresponding energy diagrams, similar to the one shown in Figure 11.27, for each case.
- b) Given that the scattering transfer cross section has linear energy dependence,  

$$\Sigma_s(E' \rightarrow E) = \Sigma_{s0}(1 + E')\left(\frac{1}{(1 - \alpha)E'}\right)$$
 where  $\Sigma_{s0}$  is a constant, and assuming  $\phi(E') = \frac{1}{E'}$ , evaluate the integral for case 4 in terms of  $E_g, E_{g-1}, E_{g'}, E_{g'-1}$ , and  $\alpha$ .

Note: For computer-based resonance and slowing down problems, refer to the problem set given in Chapter 12.

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## THERMALIZATION

It is well known that the atoms of a material at a temperature  $T$  have a Maxwellian-like distribution of kinetic energies that peaks around the value  $E = kT$ , where  $k$  is Boltzmann's constant and  $T$  is in degrees Kelvin. At a typical room temperature of  $293^\circ\text{K}$ , the corresponding energy is  $0.025\text{ eV}$ . The atoms in this distribution have a wide range of energies, but relatively few are found with energies below  $0.0001\text{ eV}$  or above  $1\text{ eV}$ . The temperature of the water in a typical operating PWR is about  $580^\circ\text{K}$ , corresponding to an energy of about  $0.05\text{ eV}$ . The temperature of the  $\text{UO}_2$  in the fuel rods may average as high as  $1800^\circ\text{K}$  under full power operation.

Thermal neutrons are neutrons that are in thermal equilibrium or semi-equilibrium with the atoms of the materials in which they are found. This state comes about as a result of elastic and inelastic collisions with those atoms. Fission neutrons suffer moderating collisions, slow down and enter the thermal neutron distribution from energies above  $1\text{ eV}$ . Thermal neutrons are removed both by leakage and by absorption. Thermal neutron absorption produces the bulk of the fission in a thermal reactor as well as most of the conversion of fertile atoms to fissionable ones. This process is very important to the overall neutron balance and to the spatial power profile in a reactor. It must therefore be treated in a careful and realistic manner.

The bulk of the operational design of modern thermal reactors is accomplished using 2- and 3-dimensional few-group computer codes. Typically, 3 or 4 groups are used, with all of

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the thermal neutrons lumped together into a single average thermal neutron group. The spatial diffusion of these neutrons is calculated over the entire core, which consists of reflector regions, fuel elements of varying enrichments and states of depletion, water gaps, control blades or pins, and lumped poison regions. Thermal group cross section libraries must be prepared for each different region, necessitating a detailed calculation of the thermal neutron spectrum in each region for use in the averaging process. Most of the spectra are obtained by treating the regions as infinite media. However, in some cases, a spectrum is "borrowed" from an adjacent region to do the averaging.

In this chapter we treat the formulation of the neutron balance equation over the thermal neutron range. The energy-dependent cross sections that appear in the balance are *not* simply the values taken from the BNL-325 "barn book", but instead must be suitably averaged over the actual thermal distribution of atom velocities.

Once the cross section expressions have been obtained, the energy-dependent thermal neutron flux can be found for the given mixture of materials. For the special case of an infinite medium containing a moderator that has no chemical binding effects, a first-order nonlinear differential equation must be solved numerically, or a semi-analytic series solution must be evaluated. For the more general case, the neutron balance equation must be discretized in energy and solved numerically. Graphical comparisons of the spectral solutions are given.

For the case of a small heterogeneous cell, such as a fuel pin in water, a spatial averaging process is also required. This can be done in one of two ways. The first method uses the assumption that space and energy are separable. The problem is broken into two steps, homogenization over space, by finding a spatial flux "disadvantage factor", followed by the solution of

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the homogeneous thermalization problem. In the second method, the space-energy problem is solved simultaneously using numerical techniques. Both methods are outlined.

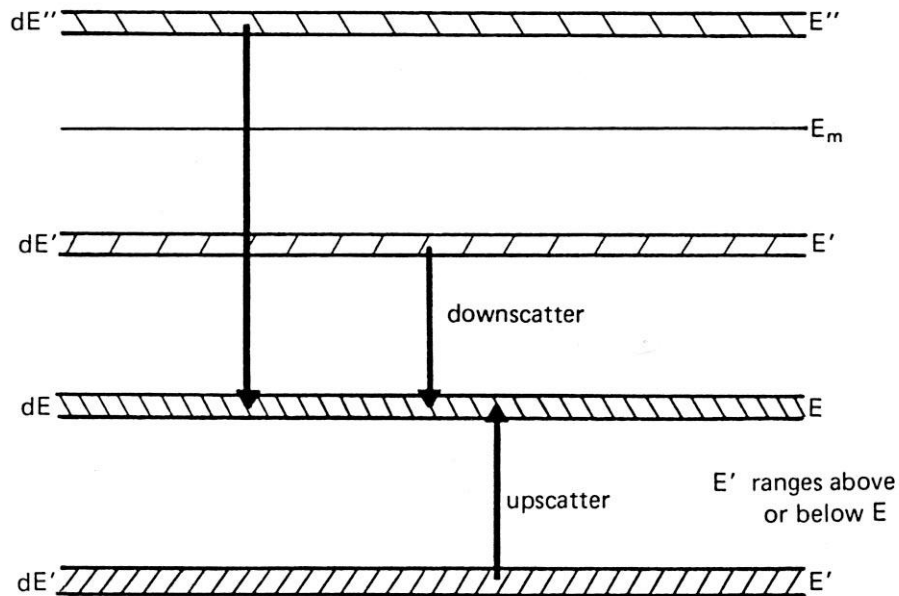
### 12.1 Neutron Balance Equation

The basic governing equation for the steady-state thermalization problem is the Boltzmann transport equation. The general form of this equation is identical to that used to solve the slowing down problem, but we make a small distinction between the two. For the thermalization case, we consider the source term to be the result of neutron slowing down from energies above a value that we shall call  $E_m$ , which is defined as that energy above which there is negligible neutron up-scatter. Furthermore, in the in-scatter integral, we must consider both up-scatter and down-scatter, since some neutrons gain energy upon collision with an atom in the assembly. The Boltzmann equation for this situation is written as,

$$\begin{aligned}
 & \begin{array}{ccc} \text{leakage} & \text{absorption} & \text{outscatter} \\ \bar{\Omega} \cdot \nabla \Phi(\bar{r}, E, \bar{\Omega}) & + \sum_a \Phi(\bar{r}, E, \bar{\Omega}) & + \sum_s \Phi(\bar{r}, E, \bar{\Omega}) \end{array} \\
 & \hspace{20em} (12.1) \\
 & \begin{array}{cc} \text{inscatter} & \text{source} \\ = \int_{4\pi} \int_0^{E_m} \sum_s (\bar{r}, E' \rightarrow E, \bar{\Omega}' \rightarrow \bar{\Omega}) \Phi(\bar{r}, E', \bar{\Omega}') d\bar{\Omega}' dE' & + S(\bar{r}, E, \bar{\Omega}). \end{array}
 \end{aligned}$$

In effect, above the energy  $E_m$ , we consider that we have obtained a solution to the slowing down problem by means already discussed. We seek the solution for energies below  $E_m$ . The energy diagram is given in Figure 12.1.

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**Fig. 12.1** Energy Diagram for Neutron Thermalization

The thermalization problem is among the most difficult found in reactor physics, and its complete treatment generally involves quantum solid state physics. Among the reasons for the difficulty are the following:

1. The scattering nuclei are all in thermal motion, so that their velocity distribution is a complicated function of temperature;
2. Chemical binding effects cannot be ignored, since the kinetic energy of the neutron is less than the binding energy of the scattering molecules;
3. Any collision of a neutron with a nucleus that changes the vibrational or rotational state of the molecule is an inelastic collision;
4. If the nuclei are bound in a crystal lattice, such as graphite, the scattering event involves the entire lattice and energy quanta called phonons are absorbed

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or emitted in the process;

5. Coherent (Bragg) scattering and incoherent scattering are possible;
6. Heterogeneous lattices, such as fuel rods arranged in periodic arrays, generally have dimensions that are too small to be adequately treated in the Diffusion Theory approximation.

The general case is well beyond the scope of this text, and will not be treated here. However, there is one quite useful case that gives a considerable amount of insight into the problem and which can be treated without great difficulty. This is the case of a monatomic moderator gas.

### 12.2\* Monatomic Gas Moderator Cross Sections

A monatomic or "free" gas moderator can be treated easily because there are no inelastic scattering collisions to be considered. Chemical binding and crystal lattice effects are absent, so that one needs only to consider the thermal distribution of the atoms in computing the neutron reaction rates. The solution was first derived in 1944 by Wigner and Wilkins, who treated the case where spatial and directional effects were unimportant by assuming an infinite medium at steady state. They were not only able to simplify the form of the equation but were also able to solve the resulting differential equation semi-analytically. The form of the Boltzmann equation treated is the angle-independent form:

$$\begin{array}{cccc} \text{absorption} & \text{outscatter} & \text{inscatter} & \text{source} \\ \Sigma_a(E)\phi(E) + \Sigma_s(E)\phi(E) & = & \int_0^\infty \Sigma_s(E' \rightarrow E)\phi(E')dE' & + S(E). \end{array} \quad (12.2)$$

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The solution procedure is to first find the analytic forms of the energy-dependent free gas scattering and absorption cross sections, and then to use these results to actually solve the integral equation to determine the flux  $\phi(E)$ . We consider the following points in our derivation:

1. The absorption cross section varies as  $1/v$ ;
2. The neutron scattering cross section is constant and is isotropic in the CM system. We will designate this cross section as  $\sigma_{s0}$ ;
3. For thermal equilibrium, the moderator gas atoms are assumed to have a Maxwellian velocity distribution in polar three-dimensional velocity space of the form

$$N(\vec{V})d\vec{V} = N_0 \left( \frac{M}{2\pi kT} \right)^{3/2} e^{-MV^2/2kT} V^2 d\psi d\mu dV. \quad (12.3)$$

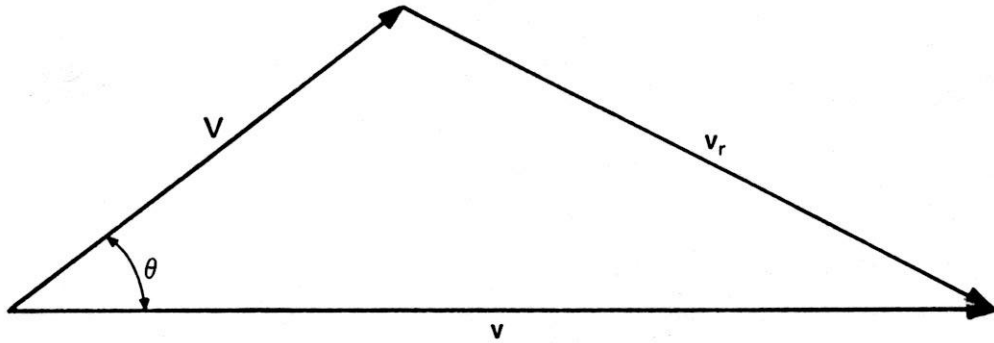
Here  $\vartheta$  is the polar angle,  $\mu \equiv \cos\vartheta = (\vec{v} \cdot \vec{V})/vV$ , and  $\psi$  is the rotational angle, both referred to the direction of the neutron  $\vec{v}$  which is taken along the polar axis of the spherical coordinate system;

4. The reaction rate is governed by the *relative* speed between the neutron and the moderator atom, which is obtained by taking the vector difference between the velocity of the neutron and the velocity of the atom, i.e.,

$$v_r = |\vec{v} - \vec{V}| = \sqrt{v^2 + V^2 - 2vV\mu}, \quad (12.4)$$

as shown in Figure 12.2. This is similar to the Doppler-broadening derivation given in Chapter 10, but here we do not neglect the quantity  $V^2$ . Furthermore, the resulting integrals are two dimensional instead of one dimensional.





**Fig. 12.2** Vector Diagram Relating the Relative Velocity to the Velocity of the Neutron and the Atom

**Absorption Cross Section  $\Sigma_a(E)$ .** The effective absorption cross section is the easiest term to handle, because most materials have an absorption cross section that varies inversely proportional to the velocity between the atom and the neutron. You will recall that  $1/v$  behavior is the low energy limiting case of the Breit-Wigner resonance equation. Hence, one can define the effective cross section for an atom at rest that is struck by a neutron of velocity  $v$  by the equation

$$\begin{array}{l} \text{effective absorption} \quad \text{actual absorption} \\ \text{probability per second} \quad \text{probability per second} \end{array} \quad (12.5)$$

$$v \sigma_a(v) N_0 \quad \equiv \quad \int_0^\infty v_r \frac{\sigma_{a0} v_0}{v_r} N(\vec{V}) d\vec{V},$$

where  $\sigma_{a0}$  is the value from the BNL-325 barn book at the velocity  $v_0$ . Since the  $v_r$  terms cancel, and  $\sigma_{a0} v_0$  is a constant, we have left  $\int_0^\infty N(\vec{V}) d\vec{V} = N_0$ . Hence, the effective absorption cross section is still  $1/v$ , namely,

$$\Sigma_a(v) = \frac{\Sigma_{a0} v_0}{v}. \quad (12.6)$$

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**Total Scattering Cross Section  $\Sigma_s(\mathbf{E})$ .** In the same manner that we followed in computing the Doppler broadening of resonances, we define an effective average scattering cross section for a scattering nucleus at rest which gives the same

$$\frac{\text{averagescattering}}{\text{probability per second}} = \frac{\text{integraloveractual}}{\text{scattering probability per second}} \quad (12.7)$$

$$v \sigma_s(v) N_0 \equiv \int_0^\infty v_r \sigma_{s0} N(\vec{V}) d\vec{V}.$$

scattering rate as is observed in the actual case, namely, Since  $\sigma_{s0}$  is a constant, and we know  $v_r$  and  $N(\vec{V})$ , the integral can be evaluated. Assuming rotational symmetry, the result is of the form

$$\Sigma_s(v) = \frac{2\pi \Sigma_{s0}}{v} \int_{-1}^1 \int_0^\infty v_r \left( \frac{M}{2\pi kT} \right)^{3/2} e^{-MV^2/2kT} V^2 dV d\mu. \quad (12.8)$$

The easiest way to do the double integral is to first convert from the variable  $\mu$  to the variable  $v_r$  and do this integral first. The integral over  $V$  must then be broken into two ranges because of the form of the lower limit on the  $v_r$  integral, one from 0 to  $v$  and the other from  $v$  to  $\infty$ . The resulting solution contains probability-type functions. In terms of energy, the result is

$$\Sigma_s(E) = \frac{\Sigma_{s0}}{\beta^2} \left[ \left( \beta^2 + \frac{1}{2} \right) \text{erf } \beta + \frac{1}{\sqrt{\pi}} \beta e^{-\beta^2} \right], \quad (12.9)$$

where  $\beta^2 \equiv AE/kT$  and  $A$  is the mass number of the scattering nucleus. We have the following definitions for the error function

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt,$$

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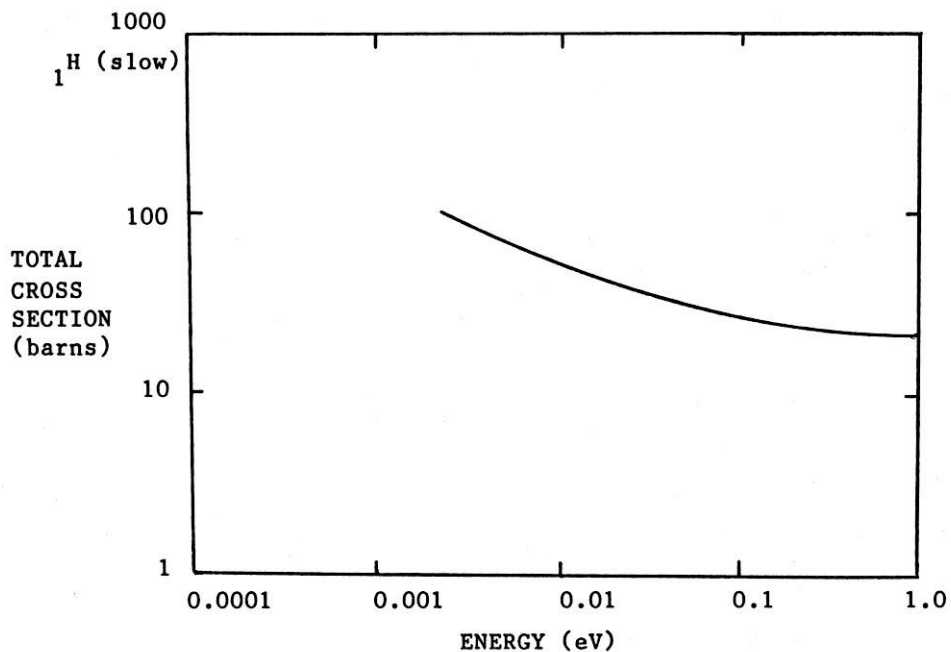
and its integral,

$$\int \text{erf}(x) dx = x \text{erf}(x) + \frac{1}{\sqrt{\pi}} e^{-x^2}.$$

Although the expression given by Eq. (12.9) looks complicated, its functional dependence is not greatly different than the measured curve for hydrogen shown in Figure 12.3. A better agreement can be obtained by using the Brown-St. John assumption that

$$\Sigma_s(v_r) = A + B \exp(-\kappa v_r^2),$$

where A, B and  $\kappa$  are chosen to fit the data. The exponential form is easily handled in the derivation.



**Fig 12.3** Total Cross Section for Hydrogen at Low Energy

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**Energy Transfer Cross Section**  $\Sigma_s(E' \rightarrow E)$ . As we did in the case of the total scattering cross section, we must also define an effective energy transfer cross section that gives the same scattering rate for stationary atoms as one observes when both the atom and the neutron are in motion. In this case, we must not only consider the relative motion between the atom and the neutron *before* the collision, but also consider the relative motion *after* the collision. The scattering process is isotropic in the CM system, with a constant total cross section  $\sigma_{s0}$ , but we must convert back to the LAB system to obtain the initial and final neutron velocities. Considering  $P(v' \rightarrow v)$  as the probability of having a neutron scatter from velocity  $v'$  to  $v$ , the effective cross section is defined by the relationship,

$$\begin{array}{ll} \text{effective transfer} & \text{actual transfer probability} \\ \text{probability per second} & \text{per second} \end{array} \quad (12.10)$$

$$v' \sigma_s(v' \rightarrow v) N_0 \quad \equiv \quad \int_0^\infty v_r \sigma_{s0} P(v' \rightarrow v) N(\vec{V}) d\vec{V}.$$

In order to evaluate this integral, we must find an expression for  $P(v' \rightarrow v)$ . We proceed by first defining the collision mechanics in both the LAB and CM systems, and then make use of the fact that the scattering is isotropic in the CM system.

When both the atom and the neutron are in motion, the center of mass moves with the vector velocity

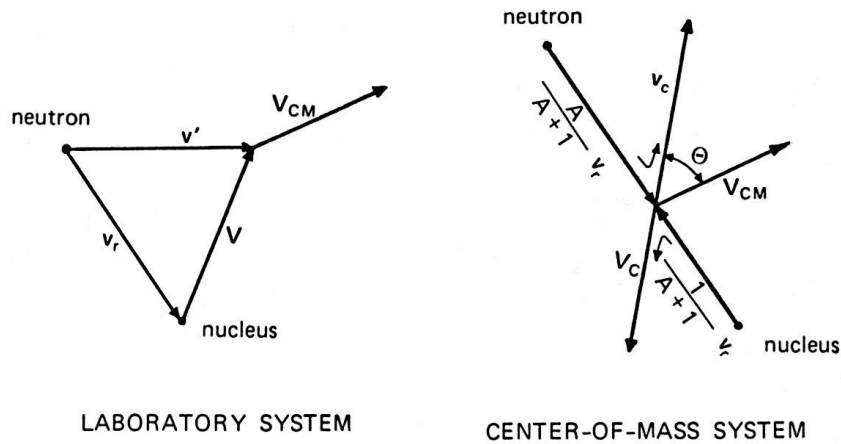
$$\vec{V}_{\text{CM}} = \frac{\vec{v}' + A\vec{V}}{A + 1}, \quad (12.11)$$

which is not collinear with the motion of either particle but is coplanar. The vector diagrams, in both the LAB and CM systems, are given in Figure 12.4. In the laboratory, the particles approach each other with a relative velocity equal to the vector difference between their actual velocities,

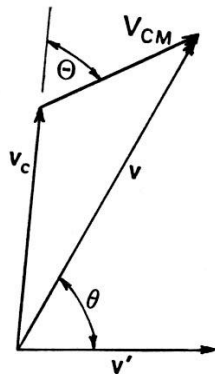
$$\vec{v}_r = \vec{v}' - \vec{V}.$$

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In the CM system, the two particles approach each other along the direction of the relative velocity with zero net momentum. After scattering through an angle  $\Theta$  relative to the direction of motion of the center of mass, both particles recede from one another with their original speeds. By conservation of momentum, the neutron has the speed  $v'_c = v_c = Av_r/(A + 1)$ , while the atom has the speed  $V'_c = V_c = v_r/(A + 1)$ . One constructs the laboratory velocity  $\vec{v}$  of the scattered neutron by adding the velocity of the center of mass  $\vec{V}_{CM}$  to the vector velocity  $\vec{v}_c$  of the scattered neutron in the CM system, as shown in Figure 12.5.



**Fig. 12.4** Scattering Mechanics in the Laboratory and Center of Mass Systems



**Fig. 12.5** Diagram to Calculate the Velocity of the Scattered Neutron in the Laboratory

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The only difference between this vector diagram and that used in the slowing down derivation is the fact that  $\vec{v}'$  and  $\vec{V}_{CM}$  are not collinear because the atom is not at rest. Using trigonometric identities, one can write an expression for the speed of the scattered neutron in terms of the speed of the center of mass and the relative speed between the incident neutron and atom. This expression is

$$v = \sqrt{V_{CM}^2 + \left(\frac{Av_r}{A+I}\right)^2 + \frac{2V_{CM}Av_r}{A+I}\cos\Theta}. \quad (12.12)$$

Obviously,  $v$  is a minimum for  $\Theta = 180^\circ$ , and is a maximum for  $\Theta = 0^\circ$ . These limits are

$$v_{\max} = V_{CM} + \frac{Av_r}{A+I}$$

and

$$v_{\min} = \left| V_{CM} - \frac{Av_r}{A+I} \right|. \quad (12.13)$$

Forming the difference of the squares of these velocities, we obtain

$$\frac{v_{\max}^2 - v_{\min}^2}{4} = \frac{Av_r V_{CM}}{A+I}, \quad (12.14)$$

which will be used shortly.

Now we turn to the scattering probabilities. For isotropic scattering in the CM system, the probability of scattering into angle  $d\Theta$  about  $\Theta$  is

$$P(\Theta)d\Theta = \frac{I}{2}\sin\Theta d\Theta. \quad (12.15)$$

This happens to be the same as the probability for scattering from a speed  $v'$  into a speed interval  $dv$  about  $v$ . Hence,

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$$P(v' \rightarrow v) dv = -P(\Theta) d\Theta = -\frac{I}{2} \sin \Theta d\Theta. \quad (12.16)$$

We can find  $d\Theta/dv$  by squaring the expression for  $v$  as a function of  $\Theta$  given in Eq. (12.12), and differentiating. The result is

$$v dv = -\left(\frac{Av_r V_{CM}}{A + I}\right) \sin \Theta d\Theta. \quad (12.17)$$

By combining the terms from Eqs. (12.14), (12.16), and (12.17), the energy transfer probability can be written as

$$P(v' \rightarrow v) = \begin{cases} 0 & \text{for } v < v_{\min}, \\ \frac{2v}{v_{\max}^2 - v_{\min}^2} & \text{for } v_{\min} < v < v_{\max}, \\ 0 & \text{for } v > v_{\max}. \end{cases} \quad (12.18)$$

The important point to notice is that the allowed scattering range is *limited* on both the high- and the low-energy ends. Furthermore,  $V_{CM}$  and  $v_r$  are known in terms of  $v'$  and  $V$  so that the integral for the effective cross section can be evaluated. Converting to energy using the equation

$$\Sigma_s(E' \rightarrow E) dE = \Sigma_s(v' \rightarrow v) dv, \quad (12.19)$$

where

$$dE = mv dv,$$

we can now (non-trivially) integrate Eq.(12.10) analytically assuming a Maxwellian distribution for the atom speeds. We obtain the effective energy transfer cross section

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$$\begin{aligned} \Sigma_{s \text{ free}}(E' \rightarrow E) = \frac{\Sigma_{so}}{E'} \frac{\eta^2}{2} \left\{ \exp\left(\frac{E'-E}{kT}\right) \left[ \operatorname{erf}\left(\eta\sqrt{\frac{E'}{kT}} - \rho\sqrt{\frac{E}{kT}}\right) \right. \right. \\ \left. \pm \operatorname{erf}\left(\eta\sqrt{\frac{E'}{kT}} + \rho\sqrt{\frac{E}{kT}}\right) \right] + \operatorname{erf}\left(\eta\sqrt{\frac{E}{kT}} - \rho\sqrt{\frac{E'}{kT}}\right) \\ \left. \mp \operatorname{erf}\left(\eta\sqrt{\frac{E}{kT}} + \rho\sqrt{\frac{E'}{kT}}\right) \right\}, \end{aligned} \quad (12.20)$$

where  $\eta$  and  $\rho$  are defined as

$$\eta \equiv \frac{A+1}{2\sqrt{A}} \quad \text{and} \quad \rho \equiv \frac{A-1}{2\sqrt{A}}.$$

The upper signs are used if  $E' < E$  while the lower signs are used if  $E' > E$ . Note that the expressions are *not* symmetric about  $E = E'$ .

For the special case of monatomic hydrogen gas,  $A = 1$  and  $\rho = 0$ , the formula simplifies to

$$\begin{aligned} \Sigma_{s \text{ free}}^{\text{hydrogen}}(E' \rightarrow E) &= \frac{\Sigma_{so}}{E'} \exp\left(\frac{E'-E}{kT}\right) \operatorname{erf}\sqrt{\frac{E'}{kT}} \quad \text{for } E' < E \\ \Sigma_{s \text{ free}}^{\text{hydrogen}}(E' \rightarrow E) &= \frac{\Sigma_{so}}{E'} \operatorname{erf}\sqrt{\frac{E}{kT}} \quad \text{for } E' > E \end{aligned} \quad (12.21)$$

By definition, the total scattering cross section is the integral of the differential cross section,

$$\Sigma_s(E') = \int_0^\infty \Sigma_s(E' \rightarrow E) dE. \quad (12.22)$$

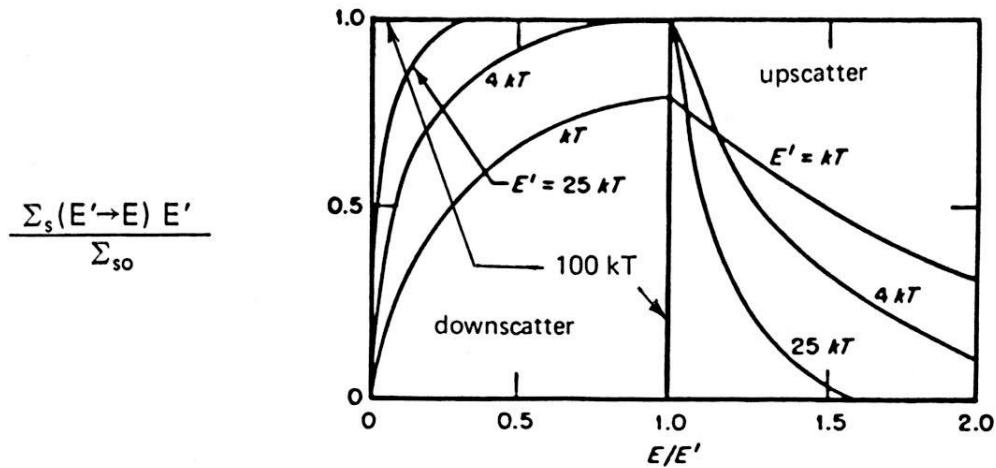
When Eq. (12.21) is integrated over all values of  $E$ , it gives the total scattering cross section derived previously, namely, the expression given in Eq. (12.9).

The plots of the energy transfer cross section are quite interesting as shown in Figures 12.6 and 12.7. One sees that for



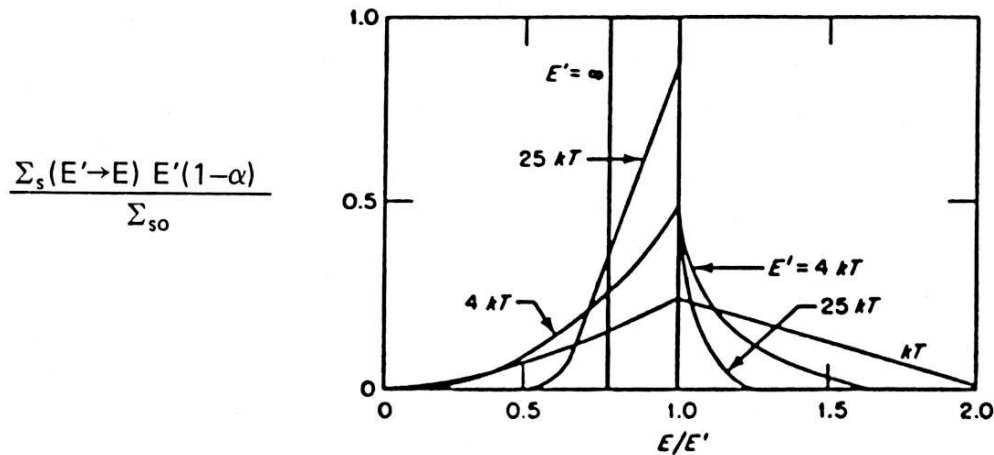
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high-energy neutrons, down-scattering is the only process possible, while for low-energy neutrons up-scattering begins to be very important. The curves for  $A > 1$  are more discontinuous looking than the curve for hydrogen.



**Fig. 12.6** Energy Transfer Function for Hydrogen Monatomic Free Gas

(From *Neutron Physics*, by K.H. Beckurts and K. Wirtz, 1964, Springer Verlag)



**Fig. 12.7** Energy Transfer Function for Oxygen Monatomic Gas

(From *Neutron Physics*, by K.H. Beckurts and K. Wirtz, 1964, Springer Verlag)

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### 12.3 Solution to the Monatomic Gas Thermalization Problem

Since the effective cross sections are all known and mathematically related analytic functions of energy, and the scattering integral is taken over the energy range of 0 to  $\infty$ , there exists a possibility of obtaining an analytic solution for the energy-dependent flux  $\phi(E)$ . As a matter of fact, by making a series of variable changes on both the independent and dependent variables, the integral equation can be reduced to a nonlinear first-order differential equation, known as the Ricatti equation, which has been studied extensively.

The Ricatti equation is of the form

$$\frac{dJ}{dE} = A(E) + B(E)J(E) + C(E)J^2(E), \quad (12.23)$$

where the coefficients A, B and C are functions of the cross sections and the source, and the initial condition is  $J(0) = 0$ . Once  $J(E)$  has been evaluated, the flux is then constructed by solving a definite integral of the form

$$\phi(E) = D(E) \exp \left[ \int_0^E f\{J(E')\} \frac{dE'}{E'} \right], \quad (12.24)$$

where  $D(E)$  contains error functions and exponentials, and  $f$  is a function of  $J$  containing similar terms.

By postulating a series-type solution, the differential equation can be integrated analytically and then evaluated numerically. This is, in fact, the procedure developed by Wigner and Wilkins, which is used in the GAMTEC computer code and the parent TEMPEST code. The results are often labeled as the "free

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gas" solution. In other more recent codes, the equations are integrated numerically.

The energy transfer cross section for  $A > 1$ , e.g., the one shown in Figure 12.7, exhibits a considerably more discontinuous behavior than that exhibited for free hydrogen gas. Eq. (12.20) can be approximated to first order in  $1/A$  to obtain a simplified scattering kernel known as the *heavy gas model*,

$$\begin{aligned} \Sigma_{s\text{ heavy}}(E' \rightarrow E) \approx \Sigma_{so} \sqrt{\frac{E}{E'}} \left\{ \delta(E - E') \right. \\ \left. + \frac{(E + E')}{A} \left[ \delta'(E - E') + kT \delta''(E - E') \right] \right\}, \end{aligned} \quad (12.25)$$

where  $\delta'$  and  $\delta''$  are the first and second derivatives of the Dirac  $\delta$ -function, i.e., they are singularity functions. The corresponding total scattering cross section is

$$\Sigma_{s\text{ heavy}}(E) = \Sigma_{so} \left( 1 + \frac{kT}{2AE} \right). \quad (12.26)$$

When the heavy gas cross sections are substituted into the integral balance equation, it can be shown that the balance reduces to a second-order differential equation with non-constant coefficients, which is known as the *heavy gas equation*,

$$\Sigma_a(E) \phi(E) = \xi \Sigma_{so} \left[ EkT \frac{d^2 \phi}{dE^2} + E \frac{d\phi}{dE} + \phi(E) \right], \quad (12.27)$$

where  $\xi$  is the average logarithmic energy decrement. The boundary conditions are  $\phi(0) = 0$  and  $\phi(\infty) = \text{asymptotic } 1/E$ . The heavy gas equation is also a solution option in the GAMTEC code for cases where hydrogen is not present in the model, i.e., for beryllium or graphite-moderated systems.

In the limit of very small absorption, at thermal equilibrium, and with no sources present, the neutron flux distribution approaches a Maxwellian shape that has the analytic

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form

$$\phi_M(E) = \frac{2\pi m}{(\pi kT)^{3/2}} \left(\frac{2}{m}\right)^{1/2} E e^{-E/kT}. \quad (12.28)$$

Here  $n$  is the total neutron density integrated over all energy. The maximum value of the flux occurs at an energy of

$$E/\phi_{\max} = kT, \quad (12.29)$$

which can be verified by taking the derivative of Eq. (12.28) and setting the result equal to zero.

In the limit of no absorption, the following neutron balance must be valid, regardless of the form of the scattering kernel,

$$\sum_s(E)\phi_M(E) = \int_0^\infty \sum_s(E' \rightarrow E)\phi_M(E')dE. \quad (12.30)$$

This implies what is known as the *principle of detailed balance*, which states that

$$\sum_s(E' \rightarrow E)\phi_M(E') = \sum_s(E \rightarrow E')\phi_M(E), \quad (12.31)$$

i.e., neutrons scattered from  $E'$  to  $E$  must be exactly balanced by neutrons scattered from  $E$  to  $E'$  for all values of  $E$  and  $E'$  at the equilibrium temperature  $T$ . This constraint applies to the scattering kernels discussed thus far, and it *must* also apply to any approximate or synthetic kernels that are developed for real materials.

One requirement for any such kernel is that it must match the measured total scattering cross section as a function of energy. As seen in Figure 12.8 for heavy water ice, some so-called "cold neutron" moderators exhibit a cross section behavior at different temperatures that varies considerably from the simple functional dependence shown in Figure 12.3 for hydrogen. Of course, detailed balance must also apply. Fortunately, the actual details are not extremely important for reactor design

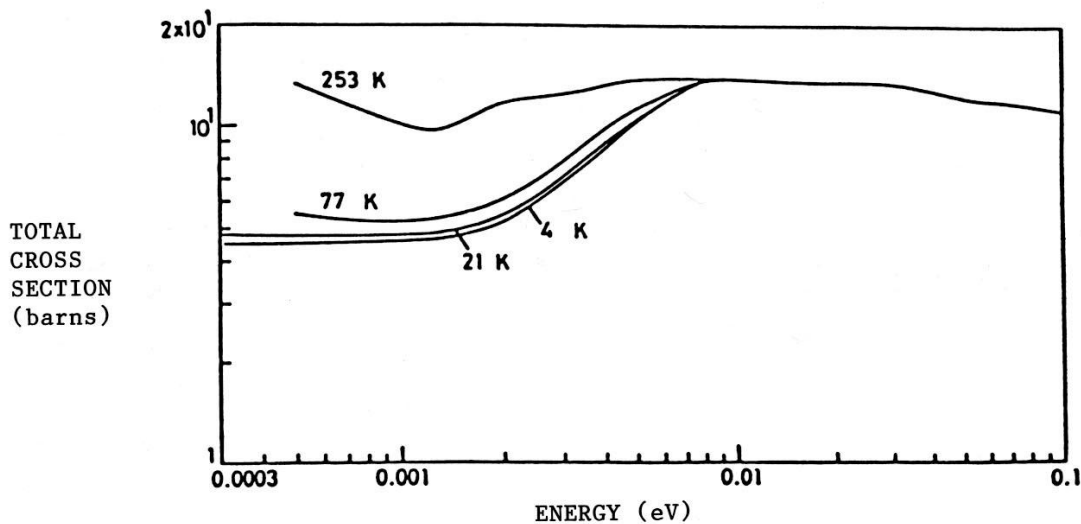
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applications, since scattering does not remove neutrons. Thermal flux distributions are usually Maxwellian-like, regardless of the scattering materials present in the system.

When absorption is present, the lower-energy neutrons are preferentially absorbed because the absorption cross section varies as  $1/v$ . The net effect is to harden the spectrum and shift the neutron distribution to a slightly higher energy. One sometimes defines a *neutron temperature*  $T_n$  to correspond to the energy at the maximum value of the flux when absorption is present, that is to say, we let

$$kT_n \equiv E/\phi_{\max}. \quad (12.32)$$

In older work, an approximate method was used to predict the effective neutron temperature of the system depending on the amount of absorption present, and the spectrum was then assumed to be a Maxwellian at this temperature.



**Fig. 12.8** Total Scattering Cross Section vs. Energy for Heavy Water Ice

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### 12.4 General Case Solution

For molecules or crystals, the energy-dependent thermal neutron scattering properties must be described quantum-mechanically. Scattering kernels are not easy to derive for real materials. Theoretically based scattering kernels are usually produced using what is known as the *scattering law*,  $S(\alpha, \beta)$ , where  $\alpha$  and  $\beta$  are related to the momentum and energy change in a collision, and where the necessary phonon frequency distribution parameters are fit to theoretical or experimental data. The scattering kernel is generated using codes such as GASKET and FLANGE.

There exist water kernels for  $H_2O$  and  $D_2O$  that treat the molecule assuming certain allowed and hindered rotational and vibrational states. There is also a polyethylene kernel, and kernels for crystalline graphite and beryllium that include such effects as Bragg scattering. With any of these kernels, an analytic solution is no longer possible and one must use the finite-range in-scattering integral plus a slowing-down source, and solve the neutron balance equation after discretization into thermal energy groups by direct numerical inversion. The process is illustrated below.

We start with the neutron balance equation

$$\sum_a(E)\phi(E) + \sum_s(E)\phi(E) = \int_0^{E_m} \sum_s(E' \rightarrow E)\phi(E')dE' + S(E), \quad (12.33)$$

and integrate the equation over an energy group  $g$  to obtain the expression

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$$\int_{E_g}^{E_{g-1}} [\Sigma_a(E) + \Sigma_s(E)] \phi(E) dE$$

$$(12.34)$$

$$= \int_{E_g}^{E_{g-1}} \sum_{g'=1}^G \left\{ \int_{E_{g'}}^{E_{g'-1}} \Sigma_s(E' \rightarrow E) \phi(E') dE' dE \right\} \int_{E_g}^{E_{g-1}} S(E) dE.$$

Now, define the following group averages:

$$S_g \equiv \int_{E_g}^{E_{g-1}} S(E) dE, \text{ group source};$$

$$\phi_g \equiv \int_{E_g}^{E_{g-1}} \phi(E) dE, \text{ group flux};$$

$$\Sigma_{ag} \equiv \frac{\int_{E_g}^{E_{g-1}} \Sigma_a(E) \phi(E) dE}{\int_{E_g}^{E_{g-1}} \phi(E) dE}, \text{ group absorption};$$

$$\Sigma_{sg} \equiv \frac{\int_{E_g}^{E_{g-1}} \Sigma_s(E) \phi(E) dE}{\int_{E_g}^{E_{g-1}} \phi(E) dE}, \text{ group scattering};$$

and

$$\Sigma_{sg' \rightarrow g} \equiv \frac{\int_{E_g}^{E_{g-1}} \int_{E_{g'}}^{E_{g'-1}} \Sigma_s(E' \rightarrow E) \phi(E') dE' dE}{\int_{E_{g'}}^{E_{g'-1}} \phi(E') dE'}, \text{ group transfer}.$$

The group  $\Sigma$  values must be supplied as a cross section library. Note that we need a separate library at each physical temperature because the cross sections change with temperature and the approximate spectrum  $\phi(E)$  used in the averaging process also changes with temperature. When these group averages are used, the resulting equation for thermal group  $g$  is

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$$\sum_{ag} \phi_g + \sum_{sg} \phi_g = \sum_{g'=1}^G \sum_{sg \rightarrow g} \phi_{g'} + S_g. \quad (12.35)$$

Now, by defining appropriate vectors and matrices, the problem can be put into the form

$$\underline{\underline{H}} \underline{\phi} = \underline{Q} \quad (12.36)$$

where

$$\underline{\phi} \equiv \begin{bmatrix} \phi_1 \\ \phi_2 \\ \cdot \\ \cdot \\ \cdot \\ \phi_G \end{bmatrix}, \quad \underline{Q} \equiv \begin{bmatrix} S_1 \\ S_2 \\ \cdot \\ \cdot \\ \cdot \\ S_G \end{bmatrix},$$

and

$$\underline{\underline{H}} \equiv \begin{bmatrix} (\sum_{a1} + \sum_{s1} - \sum_{s1 \rightarrow 1}) & -\sum_{s2 \rightarrow 1} & \cdots & -\sum_{sG \rightarrow 1} \\ -\sum_{s1 \rightarrow 2} & (\sum_{a2} + \sum_{s2} - \sum_{s2 \rightarrow 2}) & \cdots & \cdots \\ -\sum_{s1 \rightarrow 3} & -\sum_{s2 \rightarrow 3} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & (\sum_{aG} + \sum_{sG} - \sum_{sG \rightarrow G}) \end{bmatrix}.$$

Note that  $\underline{\underline{H}}$  is a full matrix for the thermalization problem.

A unique solution can be obtained by inverting the  $\underline{\underline{H}}$  matrix, namely,

$$\underline{\phi} = \underline{\underline{H}}^{-1} \underline{Q}. \quad (12.37)$$

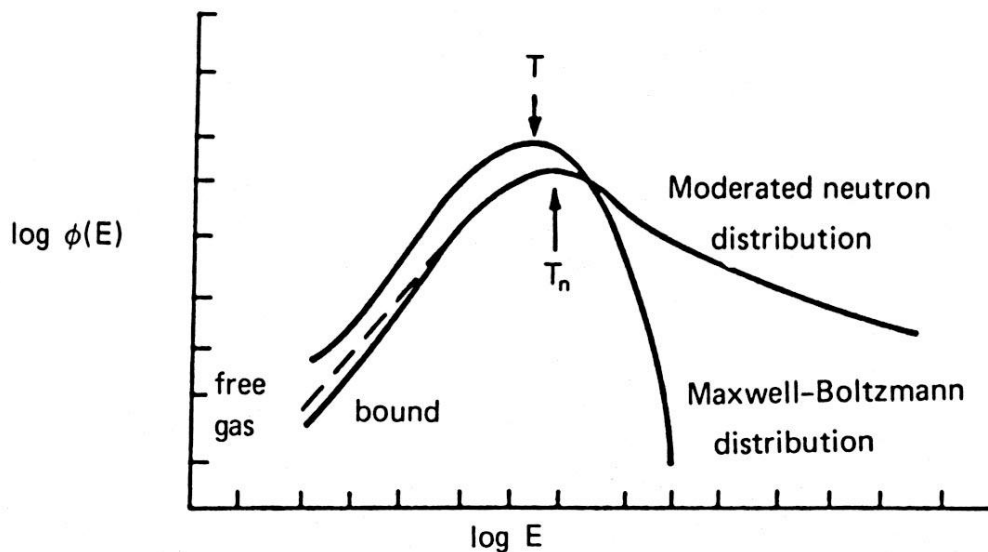
The source can be chosen, for example, to be a  $1/E$  asymptotic slowing-down source in the highest-energy groups. For a typical 30-group formulation, direct inversion of the matrix by Gaussian



## NUCLEAR REACTOR THEORY AND DESIGN

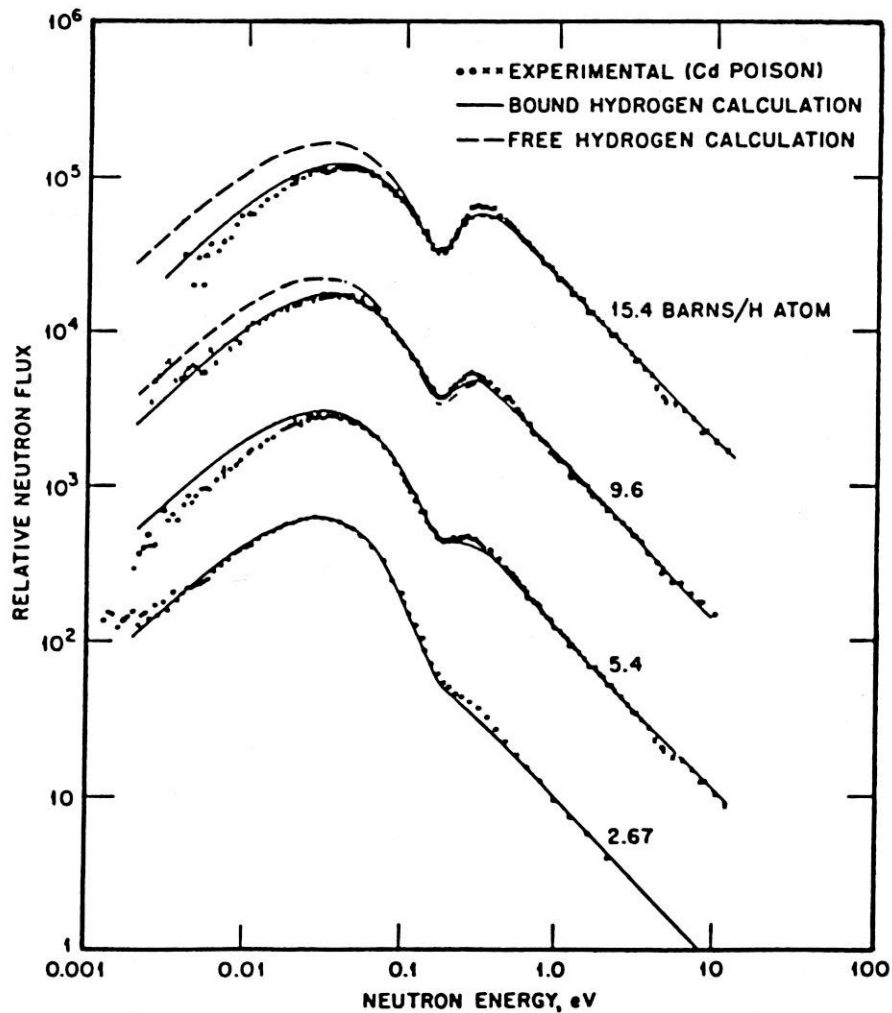
elimination is quite straightforward.

Since the molecular or crystal binding effects tend to come into play at low energy, one would expect to see the major deviations between different formulations in this energy region. A typical neutron spectrum for water is shown in Figure 12.9, where the difference between the results obtained using the free gas kernel and the water kernel is illustrated. Note that there is a significant difference between *either* thermalization calculation and a pure Maxwellian distribution at the same physical temperature. In particular, the neutron temperature  $T_n$  is higher than  $T$ . A comparison of the spectra calculated for cases of strong absorption (hardening) and weak absorption is shown in Figure 12.10. Selective absorption of low energy neutrons shifts the neutron temperature upwards and significantly alters the spectral shape. The dip at 0.14 eV is caused by an absorption resonance in cadmium.



**Fig. 12.9** Comparison of Free Gas and Water Kernel Thermalization Calculations

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**Fig. 12.10** Illustration of Spectral Hardening

(From J.R. Beyster, J.L. Wood, M.W. Lopez and R.B. Walton, *Nucl. Sci. Eng.* 9, 168, 1961)

Once the detailed thermal spectrum is known, the thermal group cross-section averages for a few-group code such as EXTERMINATOR can be determined. These averages are defined as follows, where  $G$  denotes the single thermal group in the few-group notation;  $\phi(E)$  represents the solution vector from Eq. (12.37), and the macroscopic cross sections are taken from the code library. We obtain:

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$$\Sigma_{aG} = \frac{\int_0^{E_m} \Sigma_a(E) \phi(E) dE}{\int_0^{E_m} \phi(E) dE},$$

$$\Sigma_{fG} = \frac{\int_0^{E_m} \Sigma_f(E) \phi(E) dE}{\int_0^{E_m} \phi(E) dE},$$

and

$$D_G = \frac{\int_0^{E_m} \frac{1}{3\Sigma_{tr}} \phi(E) dE}{\int_0^{E_m} \phi(E) dE}.$$

Since there is no up-scatter from the thermal group, an average scattering cross section is not needed. Note also that these cross sections are only valid at the physical temperature at which they were calculated.

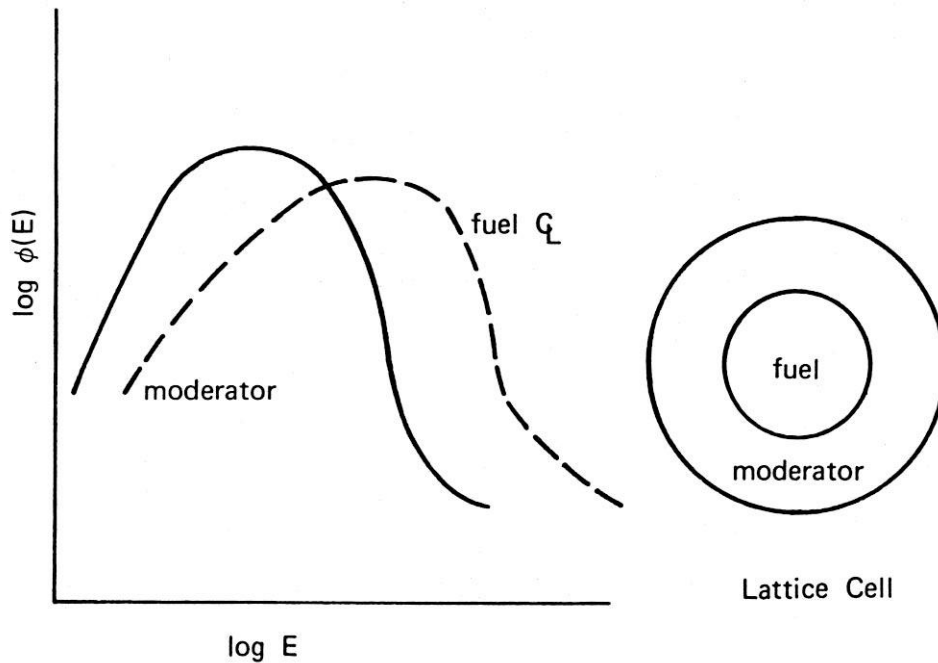
### 12.5 Spatial Effects in the Thermalization Problem

Now that we have examined the solution to the space-independent thermalization problem, we shall consider in a qualitative manner several ways of taking the spatial flux distribution into account. Specifically, we shall consider a lattice cell and examine the general requirements for a satisfactory solution. Two factors are immediately apparent: (1) the cell dimensions are usually sufficiently small so that diffusion theory is inadequate and a transport approximation must be used; and (2) the spectrum in the fuel region will be harder than that in the moderator region because the absorption is greater there and the physical temperature may also be higher.

Of course, the actual spectral distribution varies spatially across the cell, but to a good approximation the spectrum at an

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interior point is a linear combination of the spectra given in Figure 12.11. The general spatial shape of the flux is shown in Figure 12.12. The flux is relatively flat in the moderator region but begins to dip near the fuel surface indicating a net current flow into the fuel. The spatial flux then drops considerably as the fuel centerline is approached because of the relatively high absorption cross section of the fuel.



**Fig. 12.11** Thermal Spectra at Selected Points in a Heterogeneous Cell

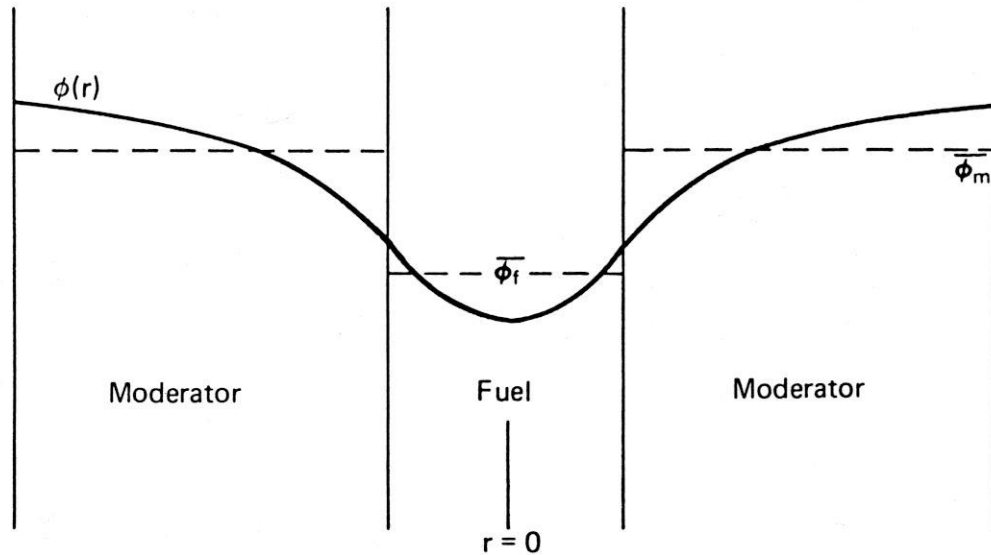
**Assumption of Separability.** The approach used in the GAMTEC code is to assume that space and energy are separable, i.e., let

$$\Phi(\vec{r}, \vec{\Omega}, E) \approx \Phi(\vec{r}, \vec{\Omega})f(E). \quad (12.38)$$

With this assumption, one first solves a spatial one-speed

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transport theory cell problem and then uses the results to homogenize the various materials in the cell in order to next do an infinite-medium spectrum problem. The assumption is that the spectrum thus obtained is a reasonable average for the whole cell.

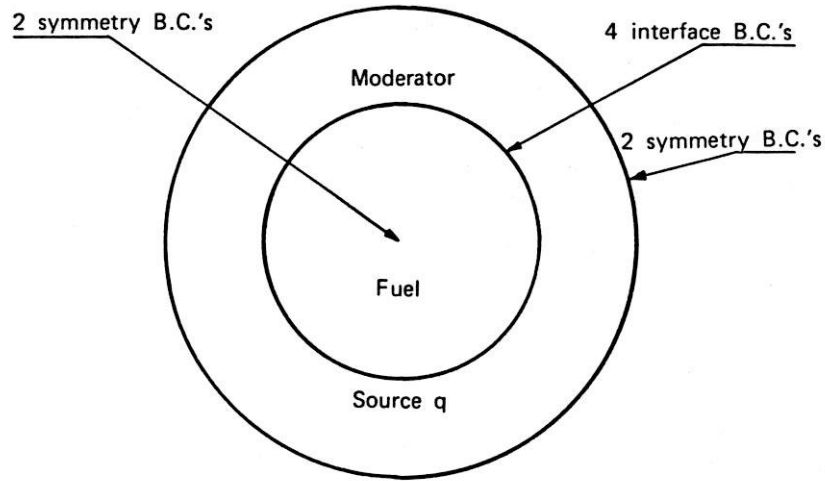


**Fig. 12.12** Spatial Thermal Flux in a Cell

Recall that the  $P_1$  approximation to the one-speed transport equation gives a second-order differential equation in the spatial variable,  $r$ , which for a long cylindrical cell corresponds to the one-dimensional radius  $r$ . For the  $P_3$  approximation, which treats two additional angular flux moments, the result is a fourth-order ordinary differential equation in  $r$ . If one assumes that the fission neutrons slow down entirely in the moderator region, and in fact form a spatially uniform source over this region, one can proceed to solve for the spatial flux distribution in the entire cell. We have a fourth-order differential equation in each region, with a uniform source in the moderator and no source in the fuel. We have four boundary

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conditions at the fuel-moderator interface, two symmetry conditions at the cell centerline and two symmetry boundary conditions at the outer boundary of the cell as shown in Figure 12.11. Hence a unique solution can be obtained.



**Fig. 12.13** P<sub>3</sub> Cell Problem

One must use a set of approximate spectrum-averaged one speed cross sections, which correspond to an assumed thermal neutron spectrum, in order to solve the spatial flux distribution problem. The solution is in fact a linear combination of the modified Bessel functions  $I_n$  and  $K_n$  for  $n = 0$  to 3, whose arguments depend upon the absorption and scattering cross sections of the two regions.

Once the spatial flux solution is obtained, it is then used to average the region number densities into an equivalent homogeneous cell according to the prescription

$$N_{cell}V_{cell}\bar{\phi}_{cell} = N_{region}V_{region}\bar{\phi}_{region}. \quad (12.39)$$

This procedure is used for each isotope in each region in the cell. The number densities thus obtained are used in the Wigner-

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Wilkins infinite-medium calculation or in a multi-group solution, and the resulting one-thermal group averaged cross sections from the spectrum calculation are used to represent the entire homogenized cell.

**Integral Transport Method.** A second approach, which is considerably more accurate, is the approach used in the THERMOS code. In this treatment the transport equation is first converted using an integrating factor into a special form known as the integral transport equation, which resembles a Green's function formulation. In effect, one must evaluate a kernel that describes the flux at any point  $\vec{r}$  and energy  $E$  due to a unit source at point  $\vec{r}'$ . Once the kernel is known, the spatial flux in each energy group is found numerically by an iterative scheme. The result is a complete thermal neutron spectrum at each mesh point in the cell.

The kernel is the most difficult part of the problem. Fortunately, this term can be reasonably well approximated using escape probabilities that are evaluated for various regions in the cell using a technique such as Monte Carlo simulation.

The form of the equation that is solved in THERMOS for the case of isotropic scattering is

$$\phi(\vec{r}, E) = \int_{cell} K(\vec{r}, \vec{r}', E) \sum_s (\vec{r}', E' \rightarrow E) \phi(\vec{r}', E') dE' + q(\vec{r}', E) \quad (12.40)$$

*kernel      inscattering      source from  
   slowing down*

The Green's function-type first-flight kernel is defined as

$$K(\vec{r}, \vec{r}', E) \equiv \frac{\exp[-\tau(E, \vec{r}' \rightarrow \vec{r})]}{4\pi |\vec{r} - \vec{r}'|^2}, \quad (12.41)$$

where  $\tau$  is the optical path length (dimensionless) in mean free

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paths between  $\vec{r}$  and  $\vec{r}'$ , which is dependent upon the macroscopic scattering and absorption cross sections. The factor  $4\pi/|\vec{r} - \vec{r}'|^2$  in the denominator is the isotropic geometrical attenuation at  $\vec{r}$  from a point source at  $\vec{r}'$ .

Since the flux appears on both sides of the equation, the solution procedure is to discretize over both space and energy to form the source problem

$$\underline{\psi} = \underline{\underline{H}}\underline{\psi} + \underline{S}, \quad (12.42)$$

where  $\underline{\psi}$  is a vector containing the flux at each space point in each energy group and  $\underline{\underline{H}}$  and  $\underline{S}$  contain the Green's function kernel which has been discretized into group-wise region transfer coefficients,  $\underline{T}_{g,i \rightarrow j}$ . The order of the matrix is the product of the number of energy groups times the number of space points. Therefore, the solution must be obtained by iteration rather than by direct matrix inversion. The THERMOS code uses various acceleration techniques to speed convergence of the solution.

Cross sections for one effective thermal group are properly space-and spectrum averaged after the THERMOS calculation is completed. These results are again used to represent the complete cell as a single homogenized entity in a two- or three-dimensional few-group criticality calculation. Comparisons between GAMTEC and THERMOS indicate that the solutions agree remarkably well as long as the fuel pin diameter is not excessively large.

**Synthesis Method.** Finally, we should mention the synthesis approach that is sometimes known as the "overlapping thermal group calculation." In the synthesis approach, one calculates two or more trial spectra using infinite media calculations (for example, those shown in Figure 12.11) and then attempts to calculate the spatially-dependent spectrum in a cell or other heterogeneous medium as a linear combination of the trial



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functions. The primary advantage is that the result is a full spectrum at each spatial point, but the calculation is few group (i.e., one calculates the combining coefficients rather than the group fluxes) instead of multi-group, which makes the computation considerably less expensive to run. The disadvantage, of course, is that the result is an approximation rather than an exact calculation, and its accuracy depends upon having a good set of trial functions for the problem being solved.

### Problems

- 12.1** The principle of detailed balance states that, for thermal equilibrium, the number of neutrons that scatter from energy  $E'$  to  $E$  is exactly balanced by the number that scatter from  $E$  to  $E'$ . Hence,

$$\Sigma_s(E' \rightarrow E)\phi(E') = \Sigma_s(E \rightarrow E')\phi(E).$$

Show that the Wigner-Wilkins expression for the scattering transfer cross section for hydrogen, given by Eq. (12.21), satisfies the condition of detailed balance, when  $\phi(E)$  is a Maxwellian.

- 12.2** Using the expression for  $\Sigma_s(E' \rightarrow E)$  given by Eq. (12.21) show that the total scattering cross section,

$$\Sigma_s(E') = \int_0^\infty \Sigma_s(E' \rightarrow E)dE,$$

is equal to the expression given by Eq. (12.9).

- 12.3** The Maxwellian flux distribution is given by Eq. (12.28).

- a) Since  $\phi(E) = n(E)v(E)$ , find the corresponding neutron density distribution function.

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- b) Show that the average energy of the neutron density distribution function is  $\bar{E} = 3/2 \text{ kT}$ , while the most probable energy is  $E/n_{\text{max}} = 1/2 \text{ kT}$ .

Note that these values are different from the corresponding values for the flux distribution.

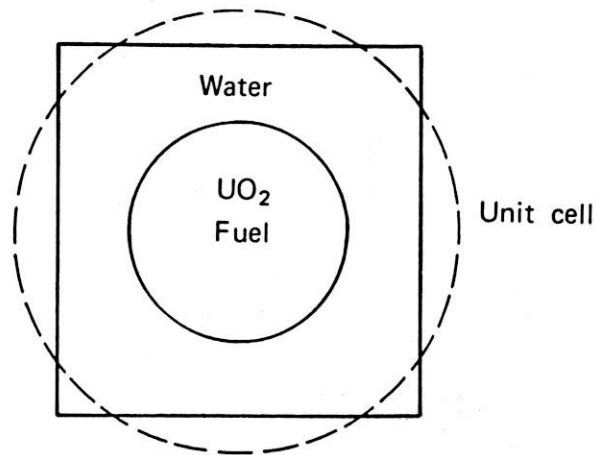
**12.4\*** Derive Eq. (12.9) for  $\Sigma_s(E)$  starting from Eqs. (12.4) and (12.8).

**12.5\*** The fuel elements for the Pebble Bed High Temperature Reactor (HTR) are spherical balls, about the size of tennis balls, that contain an inner core of pyrolytic-coated fuel particles of  $^{233}\text{U}$ ,  $^{235}\text{U}$  or  $^{232}\text{Th}$  in a graphite matrix. Assume that, as a first approximation, the fuel region is a homogeneous 5 cm diameter sphere surrounded by a 1 cm thick graphite shell. Assume that the slowing down source is stepwise constant in the two regions, and that one speed diffusion theory is valid. Refer to Figure 12.12, and calculate the spatial flux, the cell average flux and the region average fluxes in the ball in terms of the source,  $S_m = 2S_f = S_0$  neutrons/cm<sup>3</sup>-s and the region properties which are  $D_f = 1.5 \text{ cm}$ ,  $D_m = 1.3 \text{ cm}$ ,  $\Sigma_{af} = 10 \text{ cm}^{-1}$  and  $\Sigma_{am} = 0.0012 \text{ cm}^{-1}$ .

**Note:** The following problems depend upon the availability of suitable slowing down and thermalization computer codes. These problems are primarily intended for a code such as GAMTEC which solves both the  $P_1$  slowing down problem and the Wigner-Wilkins thermalization problem for heterogeneous cells. Comparisons can be made for the thermalization calculation using THERMOS. The following fixed parameters will be used for the cell calculations:

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1. The enrichment will be 3%  $^{235}\text{U}$  by weight.
2. The water/ $\text{UO}_2$  ratio will be equal to 2 by volume.
3. We will use three broad groups with breakpoints at 0.6 eV and 10 KeV.



#### 12.6 Temperature survey, $\text{H}_2\text{O}$ - $\text{UO}_2$ Cell

For a fuel rod diameter of 0.8 cm and  $B^2 = 0$  for all energy groups, do cell calculations for the following cases:

- a) the entire cell is at 300° K;
- b) the water is at 550° K and the fuel temperature varies from 600° K to 2000° K. Use compressed water tables at 2000 psia to obtain the appropriate water density. Use  $\rho\text{-UO}_2 = 10 \text{ gm/cm}^3$ . Compute the average moderator temperature coefficient and the average Doppler temperature coefficient from the  $k_\infty$  edits.

#### 12.7 Buckling survey, $\text{H}_2\text{O}$ - $\text{UO}_2$ Cell.

For a fuel rod diameter of 0.8 cm and  $T = 300^\circ \text{ K}$  in both regions, do cell calculations for the following cases:

- a) The value of  $B^2$  is the same in all groups and takes values from 0 to  $0.1 \text{ cm}^{-2}$ ;
- b) The value of  $B^2$  varies from  $0.1 \text{ cm}^{-2}$  in the fastest

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group down to 0 in the thermal group.

Use  $\rho\text{-UO}_2 = 10 \text{ gm/cm}^3$  and  $\rho\text{-H}_2\text{O} = 1 \text{ gm/cm}^3$ .

Comment on the sensitivity of the calculation to  $B^2$ .

### 12.8 Lattice size survey, $\text{H}_2\text{O-UO}_2$ Cell.

For a temperature of  $300^\circ \text{ K}$  in both regions and  $B^2 = 0$ , do cell calculations for fuel rod diameters varying from 0 (homogeneous mixture) to 2 cm. Use  $\rho\text{-UO}_2 = 10 \text{ gm/cm}^3$  and  $\rho\text{-H}_2\text{O} = 1 \text{ gm/cm}^3$ . Comment on the trends of  $k_\infty$ ,  $p$ , etc., as the fuel rod size varies.

### 12.9 Spectral Shift Reactor, $\text{H}_2\text{O/D}_2\text{O-UO}_2$ .

For a temperature of  $300^\circ \text{ K}$  in both regions, a fuel rod diameter of 0.8 cm, and  $B^2 = 0$ , do cell calculations for  $\text{D}_2\text{O-H}_2\text{O}$  mixtures varying from almost pure heavy water (0.5%  $\text{H}_2\text{O}$ ) to dilute heavy water (50%  $\text{H}_2\text{O}$ ). Use  $\rho\text{-UO}_2 = 10 \text{ gm/cm}^3$ , and  $\rho\text{-water}$  equals an appropriate average between  $\rho\text{-D}_2\text{O} = 1.1 \text{ gm/cm}^3$  and  $\rho\text{-H}_2\text{O} = 1.0 \text{ gm/cm}^3$ . Comment on the trends of  $k_\infty$ ,  $p$ , etc., as the heavy water is diluted with light water.

### 12.10 Moderator Survey

Do a homogeneous cell calculation for the following cases:

- a)  $\text{H}_2\text{O}$  at  $300^\circ \text{ K}$  and  $600^\circ \text{ K}$  - Use the compressed water tables at 2000 psia to find the water density. At  $600^\circ \text{ K}$  also find the Maxwellian spectrum averages;
- b)  $\text{D}_2\text{O}$  at  $300^\circ \text{ K}$  and  $600^\circ \text{ K}$  - Compute the Wigner-Wilkins spectrum only. Scale the  $\text{H}_2\text{O}$  density by a factor of 1.1 to simulate  $\text{D}_2\text{O}$ ;
- c) Graphite at  $300^\circ \text{ K}$  and  $600^\circ \text{ K}$  - Compute the Wigner-Wilkins spectrum only.

Put in a trace (say  $10^{-10}$ ) of  $^{235}\text{U}$  to obtain spectrum-averaged

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edits for these materials. Compare the resulting cross sections.

- 12.11** Repeat the thermalization part of Problem 12.8 using an integral transport code such as THERMOS. Comment upon the separability of space and energy based upon the calculated results. Compare the spatial flux distribution to that computed by the  $P_3$  method in GAMTEC.

### References

- J.R. Lamarsh**, op. cit., Chapter 9.  
**G.I. Bell** and **S. Glasstone**, op. cit., Chapter 11.  
**L.L. Carter**, **C.R. Richey** and **C.E. Hughey**, op. cit.  
**H.C. Honeck**, *THERMOS, A Thermalization Code for Reactor Lattice Calculations*, (Brookhaven National Laboratory, Upton, NY, 1961) BNL-5826.  
**J.J. Duderstadt** and **L.J. Hamilton**, *Nuclear Reactor Analysis*, John Wiley and Sons, New York, 1976, Chapter 9.

## NUCLEAR REACTOR THEORY AND DESIGN

## THE SINGULARITY FUNCTIONS

The Dirac delta function is a member of a class of singularity functions that is widely used, for example, in the time-domain analysis of dynamic systems. The common names of some of the more useful singularity functions are the unit step, the unit ramp and the unit impulse. The unit step function is also called the Heaviside function, while the Dirac delta function or, more properly, the Dirac delta distribution, is identified with the unit impulse. We shall examine some of the properties of these functions and their interrelationships here.

Perhaps the most familiar singularity function is the unit step function, which is denoted by  $U_{-1}$  and is shown in Figure A.1a. This function has the properties

$$U_{-1}(t) = \begin{cases} 0 & \text{for } t < 0 \\ 1 & \text{for } t > 0 \end{cases}, \quad (\text{A.1})$$

where the function is commonly left undefined at  $t = 0$ , although it can be assigned the value  $1/2$ . It is called a unit function because its value is either zero or unity depending upon whether its argument is negative or positive.

If one displaces the unit step function a units to the right by making the variable change  $\tau = t - a$ , then the discontinuity occurs when the argument  $\tau = 0$ , and the displaced unit step function has the properties

$$U_{-1}(t - a) = \begin{cases} 0 & \text{for } t < a \\ 1 & \text{for } t > a \end{cases}, \quad (\text{A.2})$$

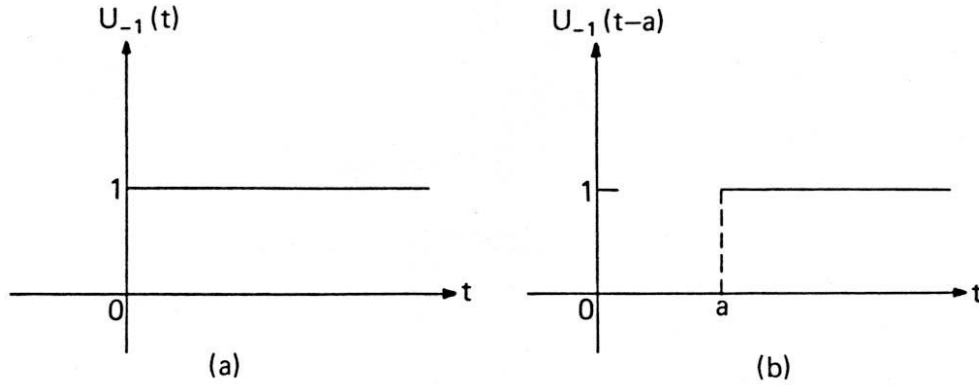
## NUCLEAR REACTOR THEORY AND DESIGN

This function is shown in Figure A.1b.

If the unit step function is integrated successively, then other singularity functions are obtained. Using a consistent notation, we can define the unit ramp function  $U_{-2}$  as the integral of the unit step function  $U_{-1}$ , i.e.,

$$U_{-2}(t) = \int_{-\infty}^t U_{-1}(\tau) d\tau = \begin{cases} 0 & \text{for } t < 0 \\ 1 & \text{for } t > 0 \end{cases}, \quad (\text{A.3})$$

We see that the unit ramp function is simply a straight line with a slope of unity, which begins at  $t = 0$ . In a similar manner, the higher-order function  $U_{-n}$  can be obtained recursively.



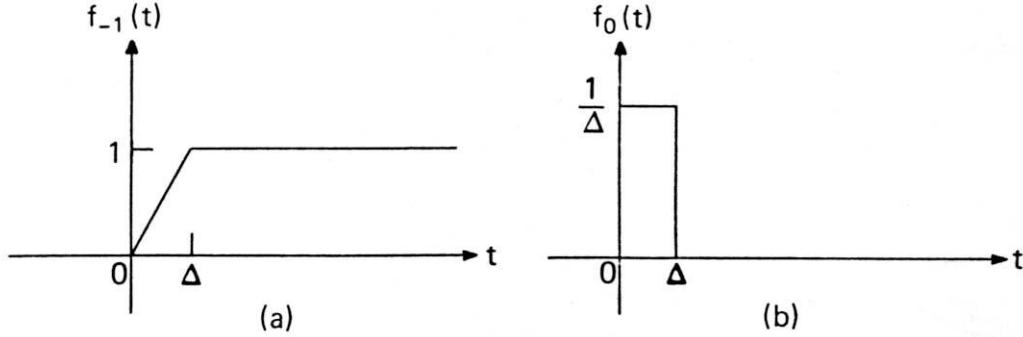
**Fig. A.1** Unit Step Functions

Since successive integration of the unit step function leads to new singularity functions, it is logical to inquire into the result of successive differentiation of the unit step function. However, the derivative of  $U_{-1}$  is zero for  $t \neq 0$ , and it does not exist for  $t = 0$ . Therefore, useful results can only be obtained by the employment of a limiting process. Consider the piecewise-linear function  $f_{-1}(t)$ , shown in Figure A.2a, which approximates  $U_{-1}(t)$  as the value of  $\Delta$  approaches zero. As shown in Figure A.2b, the function  $f_{-1}$  does indeed possess a well-defined derivative,  $f_0 = df_{-1}/dt$ , which is given by the expression



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$$f_0(t) = \begin{cases} 0 & \text{for } t < 0 \\ 1/\Delta & \text{for } 0 < t < \Delta, \\ 0 & \text{for } t > \Delta \end{cases} \quad (\text{A.4})$$



**Fig A.2.** An Approximation to the Unit Step Function and Its Derivative

Also note that the area under the  $f_0$  curve is unity, i.e.,

$$\int_{-\infty}^{+\infty} f_0(\tau) d\tau = \int_0^{\Delta} \frac{1}{\Delta} d\tau = 1. \quad (\text{A.5})$$

Since, in the limit as  $\Delta$  approaches zero,

$$\lim_{\Delta \rightarrow 0} f_{-1}(t) = U_{-1}(t), \quad (\text{A.6})$$

we can also define the corresponding value of  $U_0$  as

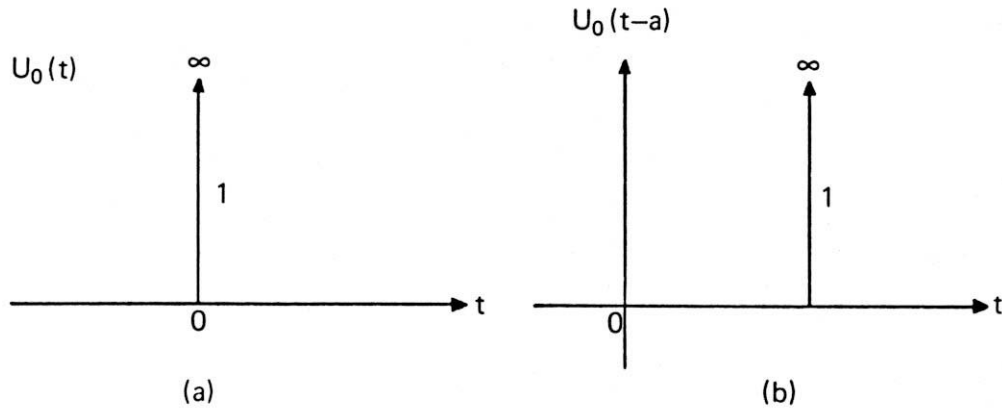
$$U_0(t) \equiv \lim_{\Delta \rightarrow 0} f_0(t) = \begin{cases} 0 & \text{for } t \neq 0 \\ \infty & \text{for } t = 0 \end{cases}, \quad (\text{A.7})$$

$U_0(t)$  is called the unit impulse function. But it is also known as the Dirac delta distribution,  $\delta(t)$ . Hence,

$$\delta(t) = U_0(t). \quad (\text{A.8})$$

This function is shown in Figure A.3a as an arrow with a value of infinity above it, while the number 1 placed alongside the arrow serves to remind us that the area under the curve is unity.

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**Fig. A.3** The Unit Impulse Function

The unit impulse function can also be displaced along the axis by setting  $\tau = t - a$ . In terms of  $\tau$ , the most useful properties of the unit impulse function can then be summarized as follows:

1. Its value is

$$U_0(t - a) = 0 \text{ for } t \neq a; \quad (\text{A.9})$$

2. Its integral, consistent with Eq. (A.3), is

$$\int_{-\infty}^t U_0(t - a) dt = U_{-1}(t - a), \quad (\text{A.10})$$

but only in the sense of Stieltjes and Lebesgue integration, because a limiting process was employed in the definition of  $U_0$ ; and

3. Its integral with respect to the continuous function  $f(t)$  is

$$\int_{-\infty}^{+\infty} f(t) U_0(t - a) dt = f(a) \lim_{\epsilon \rightarrow 0} \int_{a-\epsilon}^{a+\epsilon} U_0(t - a) dt = f(a), \quad (\text{A.11})$$

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where use has been made of the mean-value theorem to derive the final result.

The property given by Eq. (A.11) is extremely useful, and is sometimes called the sampling property of the impulse function.

Successive differentiation of the unit impulse function leads to other singularity distributions such as the unit doublet, etc. These will not be discussed here.

### Reference

**P.M. DeRusso, R.J. Roy and C.M. Close,** *State Variables for Engineers*, (John Wiley and Sons, New York, New York, 1967), Chapter 1.

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## THE LAPLACE TRANSFORM

A transform is, in effect, a type of mapping of one function into another. The transformation is accomplished by performing a definite integral of the original function, weighted by a suitable factor that contains the transform variable, over the range of the original independent variable. In the case of the Laplace Transform, the original independent variable is  $t$ ; the transform variable is the complex quantity  $s$ , the weighting function is  $e^{-st}$  and the integral is taken over the range of  $t = 0$  to  $t = \infty$ . Hence, the Laplace Transform,  $\bar{F}(s)$ , of a function,  $f(t)$ , is defined as

$$\bar{F}(s) = \int_0^{\infty} f(t)e^{-st} dt \equiv L[f(t)], \quad (\text{B.1})$$

if the integral exists.

The primary utility of a transformation of this type is that it can be used to simplify the solution of a differential equation. A linear differential equation in  $f(t)$  can be converted into a much simpler equation in  $\bar{F}(s)$ , often an algebraic equation, and the initial conditions are automatically included. The resulting equation is usually considerably easier to solve than the original differential equation. Of course, one never gets something for nothing. In this case, the ease obtained in solving the transformed equation must be paid for by the difficulty met in converting the solution back to the original variable. For the Laplace Transform, the inverse transform is a line integral in the complex  $s$ -plane that lies parallel to the imaginary axis. The inverse transform is of the form

$$f(t) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \bar{F}(s)e^{st} ds \equiv L^{-1}[\bar{F}(s)] \quad (\text{B.2})$$

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where  $\sigma$  is a small real number which is employed to assure convergence of the result. Fortunately, in most practical cases, the contour can be closed by an infinite semicircle, and then use can be made of Cauchy's theorem to evaluate the contour integral in terms of the residues of the enclosed singularities. In fact, extensive tabulations of inverse transforms exist, so that the primary work involved in obtaining the inverse of a particular transform is the algebra required to manipulate the transformed solution into a sum of recognizable pieces. This will be illustrated shortly.

Some of the most important properties of Laplace Transforms, which assist in solving differential equations, are the following:

1. *Additivity or linearity property*

$$L[Af(t) + Bg(t)] = A\bar{F}(s) + B\bar{G}(s). \quad (\text{B.3})$$

2. *Differentiation property*

$$L\left[\frac{df}{dt}\right] = s\bar{F}(s) - f(0+), \quad (\text{B.4})$$

where  $f(0+)$  is the initial condition of the function  $f(t)$ , and, in general,

$$L\left[\frac{d^n f}{dt^n}\right] = s^n \bar{F}(s) - s^{n-1} f(0+) - s^{n-2} \frac{df}{dt}\bigg|_{t=0+} - \dots - \frac{d^{n-1} f}{dt^{n-1}}\bigg|_{t=0+}, \quad (\text{B.5})$$

where  $\frac{d^{n-1} f}{dt^{n-1}}\bigg|_{t=0+}$  is the initial value of the (n-1)th derivative of  $f(t)$ .

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### 3. *Integration property*

$$L\left[\int_0^t f(\tau) d\tau\right] = \frac{\bar{F}(s)}{s}, \quad (\text{B.6})$$

and

$$L\left[\int_{-\infty}^t f(\tau) d\tau\right] = \frac{\bar{F}(s)}{s} + \frac{f^{-1}(0+)}{s}, \quad (\text{B.7})$$

where the initial condition is the integral

$$f^{-1}(0+) = \lim_{t \rightarrow 0+} \int_{-\infty}^t f(\tau) d\tau. \quad (\text{B.8})$$

### 4. *Linear transformation property*

$$L[e^{-at} f(t)] = \bar{F}(s + a). \quad (\text{B.9})$$

### 5. *Treatment of non-constant coefficients*

$$L[tf(t)] = -\frac{d\bar{F}(s)}{ds}, \quad (\text{B.10})$$

and

$$L\left[\frac{f(t)}{t}\right] = \int_s^\infty \bar{F}(\sigma) d\sigma, \quad (\text{B.11})$$

etc. Note that equations with non-constant coefficients in the original variable are not algebraic in the transform variable.

### 6. *Translation property*

$$L[f(t - a)U_{-1}(t - a)] = e^{-as} \bar{F}(s). \quad (\text{B.12})$$

### 7. *Convolution property*

$$L\left[\int_0^t f(t - \tau)g(\tau) d\tau\right] = \bar{F}(s)\bar{G}(s). \quad (\text{B.13})$$

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Note that the convolution integral of two functions is converted into the product of two transforms. This simple result is one of the key features that allows dynamic systems to be analyzed in terms of their transfer functions.

### 8. *Initial value*

$$\lim_{t \rightarrow 0} f(t) = \lim_{s \rightarrow \infty} s\bar{F}(s), \quad (\text{B.14})$$

if the limits exist.

### 9. *Final value*

$$\lim_{t \rightarrow \infty} f(t) = \lim_{s \rightarrow 0} s\bar{F}(s). \quad (\text{B.15})$$

Consider the problem of solving an  $n$ th order, inhomogeneous, ordinary differential equation with constant coefficients. When the differentiation property given by Eq. (B.5) is applied successively to each derivative term, the result is the transform of the function multiplied by a suitable power of  $s$  plus terms corresponding to the initial conditions. These terms can be summed by virtue of the additivity property given by Eq. (B.3). The inhomogeneous term must also be transformed. The resulting expression can then be manipulated algebraically into the solution form

$$\bar{F}(s) = \frac{P(s)}{Q(s)}, \quad (\text{B.16})$$

where  $P(s)$  contains terms proportional to the initial conditions and to the inhomogeneous part of the differential equation, and  $Q(s)$  is a polynomial in  $s$ . Eq. (B.16) must now be inverted to find  $f(t)$ . We first obtain the characteristic equation of the system by setting  $Q(s)$  equal to zero. This polynomial can be factored into a product of the type



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$$Q(s) = (s - s_1)^r (s - s_2) \dots (s - s_n) = 0, \quad (\text{B.17})$$

where for the sake of generality the root  $s_1$  is shown repeated  $r = 2$  times, while the other roots  $s_2, \dots, s_n$  are distinct. In the case where  $P(s)$  is a polynomial of order less than  $Q(s)$ , the method of partial fractions can then be used to put the solution into the form

$$\bar{F}(s) = \frac{K_1}{(s - s_1)} + \dots + \frac{K_r}{(s - s_1)^r} + \frac{K_{r+1}}{(s - s_{r+1})} + \dots + \frac{K_n}{(s - s_n)}. \quad (\text{B.18})$$

The coefficients of each of the terms are found as follows: for the simple roots,

$$K_i = \left[ (s - s_i) \bar{F}(s) \right]_{s=s_i}, \quad \text{for } i = r + 1, \dots, n; \quad (\text{B.19})$$

while for the repeated roots,

$$K_{r-k} = \frac{1}{k!} \left[ \frac{d^k}{ds^k} (s - s_1)^r \bar{F}(s) \right]_{s=s_1}, \quad \text{for } k = 0, 1, 2, \dots, r - 1. \quad (\text{B.20})$$

When  $P(s)$  is not a polynomial, but contains roots of its own, then Eq. (B.16) must be rewritten as a sum of the form

$$\bar{F}(s) = \bar{F}_1(s) + \bar{F}_2(s) + \dots = \frac{P_1(s)}{Q_1(s)} + \frac{P_2(s)}{Q_2(s)} + \dots \quad (\text{B.21})$$

The  $P_1(s)$ , etc. are polynomials, and the  $Q_1(s)$ , etc. are obtained by augmenting the characteristic equation, Eq. (B.17), with the roots of the corresponding terms from  $P(s)$ . The partial fraction expansion is then applied separately to each of the terms in Eq. (B.21). The reason for putting the solution for  $\bar{F}(s)$  into the form of Eq. (B.18) is that the inverse transform of contributions of the type  $1/(s - s_1)^r$  are tabulated, and therefore they are easily evaluated. Hence, the final solution in terms of the

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original variable is

$$f(t) = L^{-1}(\overline{F}(s)), \quad (\text{B.22})$$

which becomes nothing more than a sum of the coefficients  $K_i$  times the corresponding tabulated inverses. A short tabulation of some of the more useful transform pairs appears in Table B.1.

**Table B.1** Laplace Transform Pairs

$f(t)$ for $t > 0$	$\overline{F}(s)$
$U_0(t) = \delta(t)$	1
$U_{-1}(t) = 1$	$\frac{1}{s}$
$U_{-2}(t) = t$	$\frac{1}{s^2}$
$e^{-at}$	$\frac{1}{s + a}$
$te^{-at}$	$\frac{1}{(s + a)^2}$
$\frac{t^{n-1} e^{-at}}{(n-1)!}$	$\frac{1}{(s + a)^n}$
$\sin \omega t$	$\frac{\omega}{s^2 + \omega^2}$
$\cos \omega t$	$\frac{s}{s^2 + \omega^2}$

As an example of the procedure to be followed, consider the following inhomogeneous, second-order, ordinary differential equation with constant coefficients:

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$$\frac{d^2 x}{dt^2} + 2 \frac{dx}{dt} = 1, \quad (\text{B.23})$$

where the initial values are

$$x(0+) = 2 \quad \text{and} \quad \frac{dx}{dt}\bigg|_{t=0+} = 0.$$

By taking Laplace Transforms, this equation is reduced to the algebraic form

$$s^2 \bar{X}(s) - 2s + 0 + 2[s\bar{X}(s) - 2] = \frac{1}{s}.$$

We solve for  $\bar{X}(s)$ , obtaining

$$\bar{X}(s) = \frac{2s + 4 + \frac{1}{s}}{s^2 + 2s}.$$

Now we must find  $x(t)$ .

The characteristic equation is simply

$$Q(s) = s^2 + 2s = 0,$$

which can be factored into the form

$$Q(s) = s(s + 2).$$

Hence,  $s_1 = 0$  and  $s_2 = -2$ . The transformed solution,  $\bar{X}(s)$ , is

$$\bar{X}(s) = \frac{P_1(s)}{Q_1(s)} + \frac{P_2(s)}{Q_2(s)} = \frac{2s + 4}{s(s + 2)} + \frac{1}{s^2(s + 2)}.$$

Now, the partial fraction expansion of the first term is simply

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$$\begin{aligned}\frac{P_1(s)}{Q_1(s)} &= \frac{K_1}{s} + \frac{K_2}{s+2} \\ &= \frac{s \left[ \frac{2s+4}{s(s+2)} \right]_{s=0}}{s} + \frac{(s+2) \left[ \frac{2s+4}{s(s+2)} \right]_{s=-2}}{s+2} \\ &= \frac{2}{s},\end{aligned}$$

which could have been found by inspection. The partial fraction expansion of the second term, which contains a repeated root, is

$$\begin{aligned}\frac{P_2(s)}{Q_2(s)} &= \frac{K_1'}{s} + \frac{K_2'}{s^2} + \frac{K_3'}{s+2} \\ &= \frac{\frac{1}{1!} \frac{d}{ds} s^2 \left[ \frac{1}{s^2(s+2)} \right]_{s=0}}{s} + \frac{s^2 \left[ \frac{1}{s^2(s+2)} \right]_{s=0}}{s^2} + \frac{(s+2) \left[ \frac{1}{s^2(s+2)} \right]_{s=-2}}{s+2} \\ &= \frac{-\frac{1}{(s+2)^2} \Big|_{s=0}}{s} + \frac{\frac{1}{s+2} \Big|_{s=0}}{s^2} + \frac{\frac{1}{s^2} \Big|_{s=-2}}{s+2} \\ &= -\frac{1}{4s} + \frac{1}{2s^2} + \frac{1}{4(s+2)}.\end{aligned}$$

Hence, the final solution can easily be obtained with the aid of Table B.1. This solution is

$$x(t) = 2 - \frac{1}{4} + \frac{t}{2} + \frac{1}{4}e^{-2t},$$

where the first term corresponds to the general solution and the last three terms correspond to the particular or forced solution of the differential equation. It is a simple matter to show that this solution indeed corresponds to the differential equation and the given initial conditions.

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### References

- P.M. DeRusso, R.J. Roy, and C.M. Close**, *State Variables for Engineers*, (John Wiley and Sons, New York, New York, 1967), Chapter 3.
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## Matrix Relationships

It is assumed that the reader has a working knowledge of vectors and matrices. Therefore, only some of the more useful properties of matrices and matrix relationships will be presented here, without proof. The discussion will be limited to square matrices with real components.

A system of linear equations can be written compactly in summation form as

$$\sum_{j=1}^n a_{ij} x_j = k_i, \quad \text{for } i = 1, 2, \dots, n. \quad (\text{C.1})$$

It is convenient to rewrite these equations in the shorthand matrix form

$$\underline{\underline{A}} \underline{x} = \underline{k}. \quad (\text{C.2})$$

When  $\underline{\underline{A}}$  is a square matrix, the solution is simply

$$\underline{x} = \underline{\underline{A}}^{-1} \underline{k}, \quad (\text{C.3})$$

if the inverse of  $\underline{\underline{A}}$  exists. This condition is met when the determinant of  $\underline{\underline{A}}$  is nonzero, i.e., we obtain a solution when

$$\det \underline{\underline{A}} = |\underline{\underline{A}}| \neq 0. \quad (\text{C.4})$$

A number of computer programs exist which can be used to compute the determinant and the inverse of a matrix. These programs are available at most computer installations.

The primary reason for working with the matrix form of the equations is the fact that the set of equations can be manipulated by simply manipulating the vectors and matrices. Moreover, a considerable amount of information about the nature

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of the solution can be obtained by examining the properties of the matrices. Of special interest are the eigenvalues of the matrix and the norms of the matrix and its eigenvectors. We will discuss these later.

A few of the useful matrix manipulation properties are summarized below. For example, we know that the product of a matrix and its inverse is equal to the identity matrix  $\underline{\underline{I}}$ , which has ones on the diagonal and zeros elsewhere. Hence,

$$\underline{\underline{A}}\underline{\underline{A}}^{-1} = \underline{\underline{A}}^{-1}\underline{\underline{A}} = \underline{\underline{I}}. \quad (\text{C.5})$$

The transpose of the product of two matrices is the product of the transposes in reverse order, i.e.,

$$[\underline{\underline{AB}}]^T = \underline{\underline{B}}^T \underline{\underline{A}}^T. \quad (\text{C.6})$$

In general, matrix manipulation is not commutative. A similar expression holds for inverses, namely

$$[\underline{\underline{AB}}]^{-1} = \underline{\underline{B}}^{-1} \underline{\underline{A}}^{-1}. \quad (\text{C.7})$$

But since determinants are simply numbers, the order is irrelevant, and

$$|\underline{\underline{AB}}| = |\underline{\underline{A}}||\underline{\underline{B}}| = |\underline{\underline{B}}||\underline{\underline{A}}|. \quad (\text{C.8})$$

The characteristic equation of a square matrix  $\underline{\underline{A}}$  is given the expression

$$\det(\underline{\underline{A}} - \lambda \underline{\underline{I}}) = 0. \quad (\text{C.9})$$

The determinant is a polynomial in  $\lambda$  of degree equal to the order of the matrix  $\underline{\underline{A}}$ , which is  $n$  in this case. If  $\underline{\underline{A}}$  represents the system matrix in a matrix differential equation, then this is the same characteristic equation as is obtained using Laplace Transforms. The polynomial can also be factored into a product of terms of the form



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$$\det(\underline{\underline{A}} - \lambda \mathbf{I}) = P_n(\lambda) = \prod_{i=1}^n (\lambda_i - \lambda). \quad (\text{C.10})$$

The numbers,  $\lambda_i$ , are the eigenvalues of the matrix  $\underline{\underline{A}}$ . The spectral radius of the matrix  $\underline{\underline{A}}$  is defined as the magnitude of its largest eigenvalue, i.e.,

$$\mu(\underline{\underline{A}}) \equiv \max_{i=1}^n |\lambda_i(\underline{\underline{A}})|. \quad (\text{C.11})$$

In many cases, such as the reactor balance equation and the poisoning and depletion equations, all of the  $\lambda_i$  are distinct. We shall restrict ourselves to this case. Then, for each  $\lambda_i$  there is at least one right eigenvector  $\underline{u}_i$ , which corresponds to the equation

$$\underline{\underline{A}} \underline{u}_i = \lambda_i \underline{u}_i. \quad (\text{C.12})$$

There is also at least one left (adjoint) eigenvalue  $\underline{v}_i^T$  which corresponds to the equation

$$\underline{v}_i^T \underline{\underline{A}} = \lambda_i \underline{v}_i^T. \quad (\text{C.13})$$

Using Eq. (C.7), this can be rewritten as

$$\underline{\underline{A}}^T \underline{v}_i = \lambda_i \underline{v}_i. \quad (\text{C.14})$$

The Cayley-Hamilton theorem states that a matrix satisfies its own characteristic equation, i.e.,

$$P_n(\underline{\underline{A}}) = 0. \quad (\text{C.15})$$

This important result implies that matrix functions can be expressed in terms of the same functional form which operates on the eigenvalues of the matrix. For distinct eigenvalues, Sylvester's theorem states that the arbitrary matrix function  $N(\underline{\underline{A}})$  is given by the expression

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$$N(\underline{\underline{A}}) = \sum_{i=1}^n N(\lambda_i) \frac{\prod_{\substack{j=1 \\ j \neq i}}^n (\underline{\underline{A}} - \lambda_j \underline{\underline{I}})}{\prod_{\substack{j=1 \\ j \neq i}}^n (\lambda_i - \lambda_j)}. \quad (\text{C.16})$$

For example, consider the inhomogeneous, first-order, matrix differential equation,

$$\dot{\underline{\underline{X}}} - \underline{\underline{A}}\underline{\underline{X}} = \underline{\underline{k}}, \quad (\text{C.17})$$

where the initial conditions are  $\underline{\underline{X}}(0) = \underline{\underline{X}}_0$ . If  $\underline{\underline{A}}$  is constant with respect to time, then this equation has the formal solution

$$\underline{\underline{X}}(t) = \exp(\underline{\underline{A}}t)\underline{\underline{X}}_0 + \int_0^t \exp[\underline{\underline{A}}(t - \tau)]\underline{\underline{k}}(\tau) d\tau. \quad (\text{C.18})$$

Note that this is not the correct solution when  $\underline{\underline{A}}$  is not a constant because matrix operations do not generally commute. The exponential function of a matrix is itself a matrix, which can be evaluated with the aid of Sylvester's theorem. While the procedure appears to be tedious, it is readily found that alternate methods are even more time consuming when the order of the system of equations is  $n = 4$  or larger.

A norm of a vector  $\underline{\underline{u}}$  is a means of describing its magnitude in some sense. The  $l_p$  norm, denoted by the expression  $\| \underline{\underline{u}} \|_p$  is defined for a positive values of  $p$  by the expression

$$\| \underline{\underline{u}} \|_p \equiv \left( \sum_{i=1}^n |\underline{\underline{u}}_i|^p \right)^{1/p}. \quad (\text{C.19})$$

The commonly used vector norms are the following:

1. The  $l_1$  norm is the sum of the lengths of the vector components,

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$$\|\underline{u}\|_1 = \sum_{i=1}^n |\underline{u}_i|; \quad (\text{C.20})$$

2. The  $l_2$ , or Euclidean, norm is the length of the vector,

$$\|\underline{u}\|_2 = (\underline{u}, \underline{u})^{1/2}; \quad (\text{C.21})$$

3. The  $l_\infty$  norm is the length of the largest vector component,

$$\|\underline{u}\|_\infty = \max_{i=1}^n |\underline{u}_i|. \quad (\text{C.22})$$

The matrix norm which is subordinate to the  $l_p$  vector norm is denoted by the symbol  $\|\cdot\|_p$ . The spectral norm of a matrix is defined by the expression

$$\|\underline{A}\|_2 = \max_{\underline{u} \neq 0} \left[ \frac{(\underline{A}\underline{u}, \underline{A}\underline{u})}{(\underline{u}, \underline{u})} \right]^{1/2}. \quad (\text{C.23})$$

When  $\underline{A}$  is real,  $\|\underline{A}\|_2$  is equal to the square root of the spectral radius  $\mu(\underline{A}^T \underline{A})$ . The spectral radius is, in turn, related to the convergence properties of various matrix iterative schemes, etc.

### References

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## Spherical Harmonics

When the Helmholtz equation,  $\nabla^2 \psi + B^2 \psi = 0$ , is written in spherical coordinates, it has the form

$$\left[ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \psi + B^2 \psi = 0. \quad (\text{D.1})$$

If one assumes that a separation of variables of the form  $\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$  is valid, then the angular portion of the separated equation becomes

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} + \alpha^2 Y = 0, \quad (\text{D.2})$$

where  $\alpha^2$  is the separation constant. Solutions of Eq. (D.2) exist only when  $\alpha^2$  takes on the discrete values

$$\alpha^2 = l(l+1), \quad \text{for } l = 0, 1, 2, \dots \quad (\text{D.3})$$

Equation (D.2) can again be separated into a product solution  $Y(\theta, \phi) = P(\theta)F(\phi)$ . The equation in  $\phi$  is of the form

$$\frac{d^2 F}{d\phi^2} + m^2 F = 0, \quad (\text{D.4})$$

where  $m$  is an integer. This equation has periodic solutions that are proportional to  $e^{im\phi}$ . The remaining portion in the variable  $\theta$  obeys the differential equation

$$(1 - x^2) \frac{d^2 P_l^m}{dx^2} - 2x \frac{dP_l^m}{dx} + \left[ l(l+1) - \frac{m^2}{1 - x^2} \right] P_l^m = 0, \quad (\text{D.5})$$

where  $m = 0, \pm 1, \dots, \pm l$ , for  $l = 0, 1, \dots$ , where  $x \equiv \cos \theta$ . The

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solutions of Eq. (D.5) are the associated Legendre functions  $P_l^m$ .

When  $m = 0$ , Eq. (D.5) reduces the Legendre equation, whose solutions are the Legendre polynomials  $P_l$ . These polynomials are defined by the relationships

$$P_0(x) = 1$$

and

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n \quad \text{for } n = 1, 2, \dots \quad (\text{D.6})$$

They obey the recursion relationships

$$xP_n(x) = \frac{1}{2n+1} [(n+1)P_{n+1}(x) + nP_{n-1}(x)] \quad (\text{D.7})$$

and

$$(x^2 - 1) \frac{dP_n}{dx} = n(xP_n - P_{n-1}). \quad (\text{D.8})$$

When  $m \neq 0$ , the general definition for the associated Legendre functions is given in terms of the Legendre polynomials by the equation

$$P_l^m(x) = (-1)^m (1 - x^2)^{m/2} \frac{d^m P_l(x)}{dx^m}. \quad (\text{D.9})$$

The corresponding recursion relations are

$$xP_l^m(x) = \frac{1}{2l+1} [(l-m+1)P_{l+1}^m(x) + (l+m)P_{l-1}^m(x)] \quad (\text{D.10})$$

and

$$(x^2 - 1) \frac{dP_l^m(x)}{dx} = lxP_l^m(x) - (l+m)P_{l-1}^m(x). \quad (\text{D.11})$$

For negative values of  $m$ ,

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$$P_l^m(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x). \quad (\text{D.12})$$

The associated Legendre functions also satisfy an orthogonality relationship of the form

$$\int_{-1}^1 P_l^m P_r^m(x) dx = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{lr}. \quad (\text{D.13})$$

When the  $\theta$  and  $\phi$  portions of the solution are combined to form the angular solution  $Y(\theta, \phi)$ , and the normalization coefficient from Eq. (D.13) is included, then the results are the  $2l+1$  spherical harmonics defined by the equations

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi}. \quad (\text{D.14})$$

and

$$Y_{l,-m}(\theta, \phi) = (-1)^m Y_{lm}^*(\theta, \phi), \quad (\text{D.15})$$

where  $Y_{lm}^*$  is the complex conjugate of  $Y_{lm}$ .

The spherical harmonics are orthonormal in the sense that

$$\int_0^{2\pi} \int_{-1}^1 Y_{lm}(\theta, \phi) Y_{l'm'}^*(\theta, \phi) d\cos\theta d\phi = \delta_{ll'} \delta_{mm'}. \quad (\text{D.16})$$

Hence, they can be used for the purpose of expanding any function of  $\theta$  and  $\phi$  in a Fourier series. The coefficients of the expansion can easily be obtained using the orthogonality property of the spherical harmonics.

An important application of spherical harmonics is to the problem of neutron scattering, wherein a neutron which is originally traveling in the direction  $\vec{\Omega}(\theta, \phi)$  is scattered into the direction  $\vec{\Omega}'(\theta', \phi')$ . The angle of scattering is the dot, or vector, product of the two unit direction vectors, namely

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$$\vec{\Omega}(\theta, \phi) \cdot \vec{\Omega}'(\theta', \phi') = \cos\gamma. \quad (\text{D.17})$$

But,

$$\vec{\Omega} = \vec{i} \sin\theta \cos\phi + \vec{j} \sin\theta \sin\phi + \vec{k} \cos\theta, \quad (\text{D.18})$$

so that upon substitution into Eq. (D.17) we obtain

$$\cos\gamma = \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\phi - \phi'). \quad (\text{D.19})$$

The spherical harmonics satisfy a very important theorem, known as the Addition Theorem, which states that

$$P_l(\cos\gamma) = \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_{lm}^*(\theta', \phi') Y_{lm}(\theta, \phi). \quad (\text{D.20})$$

Using the expressions for  $Y_{lm}$  and  $Y_{l,-m}$  given by Eqs. (D.14) and (D.15), this theorem can be reduced to the useful form

$$\begin{aligned} P_l(\cos\gamma) &= P_l(\cos\theta) P_l(\cos\theta') \\ &+ 2 \sum_{m=1}^l \frac{(l-m)!}{(l+m)!} P_l^m(\cos\theta) P_l^m(\cos\theta') \cos[m(\phi - \phi')]. \end{aligned} \quad (\text{D.21})$$

The significance of the Addition Theorem, as given by Eq. (D.21), should not be missed. This theorem relates the directional change of a neutron in a scattering collision to the associated Legendre functions and Legendre polynomials of the before and after states. The differential angular scattering cross sections, which are only a function of the change in direction, are thereby connected to the actual angular neutron flux distribution. Moreover, the relationship is obtained in terms of functions whose orthogonality properties can be used to greatly simplify the ensuing equations. The result, of course, is the well-known  $P_n$  method of solving the Boltzmann transport equation.



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## Differentiation of an Integral

One of the standard methods that is used to solve an integral equation is to differentiate the equation, manipulate the result and then reintegrate to obtain the final solution. In order to facilitate this operation, we make use of Leibniz's theorem, which states that the derivative of an integral is composed of three parts, namely:

1. the integrand, evaluated at the upper limit of the integral times the derivative of the upper limit;
2. minus the integrand, evaluated at the lower limit of the integral, times the derivative of the lower limit, and
3. the integral of the derivative of the integrand.

In equation form, Leibniz's theorem is written as

$$\frac{d}{dy} \int_{a(y)}^{b(y)} f(x,y) dx = f(b,y) \frac{db}{dy} - f(a,y) \frac{da}{dy} + \int_{a(y)}^{b(y)} \frac{\partial f(x,y)}{\partial y} dx. \quad (\text{E.1})$$

One should note that if either limit is a constant, the corresponding term does not contribute to the result. Likewise, if the variable of differentiation does not appear explicitly in the integrand, then this term contributes nothing.

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