Part II

ELEMENTS OF NEUTRON PHYSICS CALCULATIONS

14 Boltzmann equation

Introduction

The Boltzmann equation was briefly introduced in Chapter 4, with an outline of the principles for solving it (§ 3.2). This topic will now be discussed in greater detail. Firstly we review the operators involved in this equation: the collision operator and the transport operator, and then we present the principles of numerical processing for each of them. For the transport operator there are two variants: the integral approach and the differential approach, which lead to completely different numerical methods. We then examine the behaviour of the solution to this equation in fundamental mode, which is simpler than the general situation, and is often taken as a reference case. Finally, we present the probabilistic "Monte Carlo" method.

This book is intended for engineers who are likely to use these calculation codes or to work with results thus obtained, not for specialists in the development of these codes. The discussion is therefore often limited to presenting the principles of the numerical methods, without providing too many details or mathematical proofs[1].

Because numerical neutron kinetics calculations[2] are not very original compared to what is done in other fields[3] and because, except for the study of accident scenarios, all reactor design and monitoring calculations are performed in a steady-state situation, the variable *time* (t) is not used in this chapter[4].

According to convention, we use the lethargy u to describe the neutron spectrum. The other two categories of variable to be discussed are the usual space variables $\vec{r}$ (three coordinates) and phase variables $\vec{\Omega}$ (two coordinates).

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[1] Moreover, a separate book would be required to provide a reasonably complete description of the methods for solving the Boltzmann equation.

[2] Kinetics as defined in Chapter 4, i.e. fast kinetics with not change in the atomic concentrations by irradiation.

[3] It is, however, appropriate to point out the special nature in neutron physics of two very different timescales: the one related to prompt neutrons, and the one related to delayed neutrons. Certain kinetics codes attempt to deal with phenomena separately according to each of these scales.

[4] The problems related to allowing for evolution and counter-reactions, where time is not really an argument of the flux governed by the Boltzmann equation, but simply a parameter handled by other evolution equations, will be discussed in Chapter 17.

14.1. The two forms of the Boltzmann equation

14.1.1. Incoming density, outgoing density, and neutron flux

The neutron population can be represented equally well by three density functions:

– the *density n* and the *neutron flux* $\Phi = nv$ characterise neutrons that "travel", i.e. that are followed from their starting point to their next collision;

– the *emission density*, also called *outgoing density*, here denoted by Q —often written as χ — (these letters suggest the neutrons that *quit* a point), represents the neutrons emitted by fission sources or other sources and the neutrons re-emitted by scattering;

– the *collision rate*, also called *incoming density* (coming into collision) is the product $\Psi = \Sigma \times \Phi$ of the total cross-section of the material by the neutron flux.

These three functions are connected by the two operators in the Boltzmann equation:

– The *collision operator C* is used to express the outgoing density as a function of the incoming density (if there are any independent sources S_a, they should be added to the outgoing density):

$$Q = C\Psi + S_a;$$

– The *transport operator T* is used to express the flux and therefore, after multiplication by Σ, the incoming density based on the outgoing density:

$$\Psi = TQ.$$

The Boltzmann equation is obtained by eliminating one of the densities, generally Q:

$$\Psi = T(C\Psi + S_a),$$

or, if it is preferable to work with the flux:

$$\Sigma\Phi = T[C(\Sigma\Phi) + S_a].$$

For most practical applications, the independent source can be neglected. Under these conditions, the Boltzmann equation is homogeneous, which has two consequences:

– the (non-trivial) solution cannot be obtained unless a critical condition is fulfilled (physically, this condition expresses the exact equality between the number of neutrons disappearing per unit time and the number of neutrons produced during the same unit time: a necessary equality for the steady-state regime to exist);

– if this condition is satisfied, the solution is obtained only *to within a factor* (physically, the equilibrium corresponding to steady-state can be created at any level).

14.1.2. Collision operator

The collision operator expresses the number of neutrons leaving collisions as a function of the number of neutrons entering collisions. In practice, a distinction is made between the physical processes of scattering and fission:

$$Q = D + S_f + S_a.$$

For the case of fission, if emission is assumed to be isotropic (always an allowable assumption) and that the fission spectrum[5] χ_f is independent of the energy of the neutron that caused the fission and the nucleus that underwent fission (non-mandatory assumptions), this gives:

$$S_f(\vec{r}, u, \vec{\Omega}) = \frac{1}{4\pi}\chi_f(u) \int_0^\infty du' \int_{(4\pi)} d^2\Omega' \nu\Sigma_f(\vec{r}, u')\Phi(\vec{r}, u', \vec{\Omega}'), \tag{14.1}$$

where the integral expresses the total number of neutrons produced by fission at a point $\vec{r}$. (All neutrons are assumed to have positive lethargy.)

The second part of the collision operator [including, where applicable, (n,2n) reactions], is written as:

$$D(\vec{r}, u, \vec{\Omega}) = \int_0^\infty du' \int_{(4\pi)} d^2\Omega' \Sigma_s[\vec{r}, (u', \vec{\Omega}') \rightarrow (u, \vec{\Omega})]\Phi(\vec{r}, u', \vec{\Omega}'), \tag{14.2}$$

where the integral expresses all of the transfers from any lethargy u' and direction $\vec{\Omega}'$ liable to take the neutron to the lethargy u and direction $\vec{\Omega}'$ considered on the left-hand side.

14.1.3. Transport operator (integral form)

Neutrons of lethargy u travelling in direction $\vec{\Omega}$ seen by an imaginary observer at a point O are neutrons that have left (after emission or scattering) one of the points M located a distance s upstream of the observer on the line of direction $\vec{\Omega}$ passing through O (see Figure 14.1), provided that such neutrons have not undergone any collision on the path MO.

The probability of no collisions occurring on the path MO is $\exp(-\tau)$, where τ is the integral along the line segment MO of the total cross-section of the material for neutrons of lethargy u:

$$\tau = \int_0^s \Sigma(\vec{r} - s'\vec{\Omega}, u)\, ds', \tag{14.3}$$

an expression where $\vec{r}$ denotes the position of the observer O. (This parameter τ is called the "optical path".)

By summing over all points M, the flux counted by the observer is found to be:

$$\Phi(\vec{r}, u, \vec{\Omega}) = \int_0^\infty ds \exp(-\tau) Q(\vec{r} - s\vec{\Omega}, u, \vec{\Omega}). \tag{14.4}$$

[5] The notation χ for the fission spectrum is standard: do not confuse χ_f with the outgoing density χ.

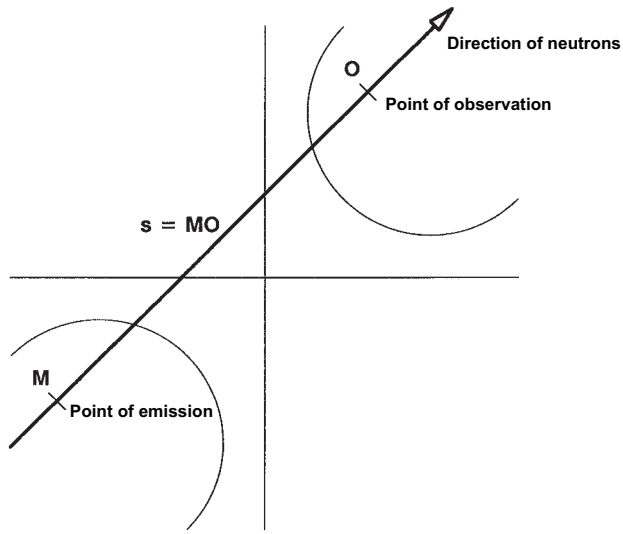


Figure 14.1. Path of neutrons of direction $\vec{\Omega}$ in a structure that can be heterogeneous.

14.1.4. Transport operator (differential form)

The differential form of the transport operator can be obtained *via* physical arguments based on an analysis of the neutron balance, like the reasoning used to obtain the diffusion equation (§ 5.1.1). Let us apply this reasoning again here in the context of a steady-state regime.

Let us consider any domain in space, D, and look at the number X of neutrons of lethargy u and direction $\vec{\Omega}$ it contains (for the sake of simplicity, this will always be understood to mean "per unit lethargy and per unit solid angle"). If a steady-state regime is established, this number does not change with time; its variation over a unit time interval is zero:

$$dX = 0.$$

This means that the algebraic sum of all the variations that can modify X is zero. Three mechanisms can affect this number X:

1/ ***Emission and re-emission*** of neutrons at lethargy u and in the direction $\vec{\Omega}$, which contribute to *increasing* X by the following amount during the unit time interval:

$$d_{(1)}X = \int_D Q(\vec{r}, u, \vec{\Omega})\, d^3r; \tag{14.5}$$

2/ ***Collisions*** between neutrons of lethargy u and direction $\vec{\Omega}$, which contribute to *decreasing* X by the following amount during the unit time interval:

$$d_{(2)}X = \int_D \Sigma(\vec{r}, u)\Phi(\vec{r}, u, \vec{\Omega})\, d^3r, \tag{14.6}$$

(absorptions eliminate neutrons, and scattering events make them go to a different lethargy and send them in a different direction);

3/ ***Inputs and outputs:*** Inputs contribute to *increasing* X and outputs contribute to *decreasing* it. We have seen (§ 3.1.4) that the vector $\vec{J}(\vec{r}, u, \vec{\Omega})$ is used to express this *current*: $\vec{J}(\vec{r}, u, \vec{\Omega}).\vec{N}dS$ is the *algebraic* number of crossings of a surface element dS oriented by its normal vector $\vec{N}$ (it is positive if the vectors $\vec{\Omega}$ and $\vec{N}$ form an acute angle, and therefore if crossings occur in the direction of the normal, and negative if the vectors $\vec{\Omega}$ and $\vec{N}$ form an obtuse angle, therefore if crossings occur in the opposite direction). If the normal is directed towards the outside of the domain D and if we integrate over its entire surface S, we can express the third variation of X (decreasing if positive, increasing if negative):

$$d_{(3)}X = \int_S \vec{J}(\vec{r}, u, \vec{\Omega}).\vec{N}\, dS. \tag{14.7}$$

To write this integral in an analogous form to the previous ones, i.e. in the form of a volume integral, we use the *divergence theorem:*

$$d_{(3)}X = \int_D \mathrm{div}[\vec{J}(\vec{r}, u, \vec{\Omega})]\, d^3r. \tag{14.8}$$

Finally:

$$dX = d_{(1)}X - d_{(2)}X - d_{(3)}X = 0,$$

expresses the balance in D during the unit time.

Because D can be any domain, it can be reduced to the volume element d^3r by removing the summation signs and then simplifying by d^3r :

$$Q(\vec{r}, u, \vec{\Omega}) - \Sigma(\vec{r}, u)\Phi(\vec{r}, u, \vec{\Omega}) - \mathrm{div}[\vec{J}(\vec{r}, u, \vec{\Omega})] = 0. \tag{14.9}$$

Finally, note (§ 3.1.4), that the phase current is simply the product of the phase flux by $\vec{\Omega}$; the transport operator relating Φ to Q is therefore written as follows, with the terms rearranged:

$$\mathrm{div}[\vec{\Omega}\Phi(\vec{r}, u, \vec{\Omega})] + \Sigma(\vec{r}, u)\Phi(\vec{r}, u, \vec{\Omega}) = Q(\vec{r}, u, \vec{\Omega}). \tag{14.10}$$

Note that, unlike the transport operator in integral form, the differential form of the transport operator is not written in the form: $\Psi = TQ$ (where $\Psi = \Sigma\Phi$ and where T is the transport operator), but in the following form:

$$T^{-1}\Psi = Q.$$

Note: The operator $\mathrm{div}(\vec{\Omega}\cdot)$ is called the "*streaming operator*".

14.1.5. Equivalence between the two forms of the transport operator

It can be shown, either by differentiating the integral form or by integrating the differential form, that these two expressions for the transport operator are strictly equivalent from a mathematical point of view[6]. (Compare this to the lethargy reasoning in § 7.1.10.)

[6] If working on a finite geometry, there are a few precautions to be taken (we shall not insist on them here) when defining the boundary conditions.

Physically, this equivalence expresses the comparison of the counts performed by the observer O of Figure 14.1 and an observer O′ shifted from O by an infinitesimal distance *ds* in direction $\vec{\Omega}$: the difference in the counts, i.e. the derivative of the flux, div($\vec{\Omega}\Phi$), along direction $\vec{\Omega}$, comes from:

a/ Neutrons emitted between O and O′, i.e. Q, seen by O′ and not by O;

b/ Neutrons undergoing a collision between O and O′, i.e. $\Sigma\Phi$, seen by O and not by O′;

which gives:

$$\text{div}(\vec{\Omega}\Phi) = Q - \Sigma\Phi.$$

14.1.6. The two deterministic approaches to the Boltzmann equation

Even if the two forms of the transport operator are equivalent from a mathematical point of view, they are not equivalent from a practical point of view, i.e. in terms of the solutions, whether analytical or, more often, numerical, of the Boltzmann equation.

Each form of the equation has been the subject of many studies by mathematicians, computational scientists, and physicists. As we have mentioned, it is not appropriate to attempt an exhaustive review here[7]. We shall limit ourselves to presenting the methods that have turned out to be the most effective cost/accuracy tradeoffs[8]:

– Concerning the integral form of the transport operator, the first collision probabilities method;

– Concerning the differential form of the transport operator, the method of spherical harmonics and the method of discrete ordinates.

In both cases, the collision operator must be processed in parallel. The technique used is the multigroup approximation that was presented in Chapter 10 and which is briefly reviewed below.

14.1.7. Probabilistic approach to the Boltzmann equation

In addition to these deterministic treatments of the Boltzmann equation, probabilistic calculations can be performed, and are often valued by neutron physicists: this is the Monte Carlo approach.

One of the immediate advantages of this approach is that it eliminates the need to write out the Boltzmann equation explicitly[9].

It can also produce results that provide a reference to validate the deterministic methods, which are generally less costly to run.

[7] For more information, please use the bibliography as a guide to further reading.

[8] It has been common to refer to the "cost" of a calculation ever since the days when computer-based calculations were subcontracted out to a service provider. Today, most calculations are performed by the engineers concerned at their own workstations, and so it is more appropriate to think of the "cost" as "machine time".

[9] This remains necessary, however, if "biasing" is to be performed.

Note that this method consists in simulating the neutron paths as closely as possible and, after many simulations, in performing a statistical analysis of the results. For certain problems, it can be useful, or even essential, to "bias" the phenomena to favour the events of interest, thus improving the statistical accuracy. This probabilistic approach will be presented at the end of this chapter.

14.2. Processing the collision operator

Collisions can change both the energy and the direction of neutrons. The directional aspect is closely related to the spatial aspect, i.e. the transport, since the direction of a neutron affects the points it will be able to reach, and will be examined when transport is calculated.

In deterministic solutions of the Boltzmann equation, the energetic aspect is taken into account by a multigroup process (see Chapter 10): the flux $\Phi(u)$ and the cross-sections $\sigma(u)$, as lethargy functions, are replaced by "vectors" Φ_g and σ_g, where the group number is a whole number from 1 to N. Note that Φ_g must be interpreted as the *integral* of flux on the group g, i.e. over the interval $[u_{g-1}, u_g]$, and σ_g as the *flux-weighted average* of the cross-section in this interval. (The multigroup theory approximation relies on the fact that this average is not calculated, in practice, with strictly the exact flux.)

In this formalism, the collision operators take the following form:

– concerning the *fission operator*:

$$S_{f,g}(\vec{r},\vec{\Omega}) = \frac{1}{4\pi}\chi_{f,g}\sum_{h=1}^{N}\nu\Sigma_{f,h}(\vec{r})\int_{(4\pi)}\Phi_h(\vec{r},\vec{\Omega}')d^2\Omega'; \tag{14.11}$$

– concerning the *diffusion operator*:

$$D_g(\vec{r},\vec{\Omega}) = \sum_{h=1}^{N}\int_{(4\pi)}\Sigma_{s,h\to g}(\vec{r'},\vec{\Omega}'\to\vec{\Omega})\Phi_h(\vec{r},\vec{\Omega}')d^2\Omega'. \tag{14.12}$$

(Note that these relationships would be absolutely rigorous if the multigroup cross-sections had been obtained by weighting by the exact flux.)

With regard to Monte Carlo solutions of the Boltzmann equation, the general recommendation in the simulation of collisions is a continuous, and therefore exact, treatment of the lethargy variable. A multigroup treatment can also be introduced, however, either to simplify the simulation calculations[10], or to validate a deterministic calculation that is itself multigroup.

[10] For example, a deterministic calculation by the APOLLO code can give more or less homogeneous structure multigroup cross-sections, which are then input into a Monte Carlo code.

14.3. Treatment of the integral form of the transport operator

14.3.1. Isotropic collision assumption

The transport operator T, in the integral form just written, is more difficult to handle than the inverse operator T^{-1}, which is differential. That is why the integral problem is never considered in this form in calculation codes.

The advantage of the integral approach is that, applying an assumption that is not too drastic, *the integral form lets us eliminate the directional variable* $\vec{\Omega}$ *from the equations*, which is not possible with the differential form. The required assumption is that of *isotropic scattering and sources*, or "isotropic collision".

This is a reasonable assumption because neutrons are emitted by fission in an effectively isotropic manner, and the anisotropy of scattering is not very pronounced, particularly for nuclei that are not too light (§ 7.1.3). Moreover, as we shall see below, most of the error caused by this approximation is easy to correct using transport cross-sections[11].

The isotropic collision assumption means that $\Sigma_{s,h\to g}(\vec{r'}, \vec{\Omega'} \to \vec{\Omega})$, and therefore the density $D_g(\vec{r}, \vec{\Omega})$, is independent of $\vec{\Omega}$ (note that, as written here, $S_{f,g}(\vec{r}, \vec{\Omega})$ is also independent of $\vec{\Omega}$). The sum Q of these densities is therefore also independent of $\vec{\Omega}$.

Returning to the integral form of the transport operator under these conditions, we have:

$$\Phi(\vec{r}, u, \vec{\Omega}) = \int_0^\infty ds \exp(-\tau) Q(\vec{r} - s\vec{\Omega}, u, \vec{\Omega}). \tag{14.13}$$

We can:

- Not write $\vec{\Omega}$ as the last variable of Q.
- Set $\vec{r'} = \vec{r} - s\vec{\Omega}$.
- Integrate both sides of the equation over $\vec{\Omega}$.
- Note that, except for a factor, $ds\, d^2\Omega$ is the volume element about the point $\vec{r'}$:

$$d^3r' = 4\pi s^2\, ds\, d^2\Omega = 4\pi R^2\, ds\, d^2\Omega.$$

In this context, the distance from $\vec{r}$ to $\vec{r'}$ is written as R rather than s:

$$R = |\vec{r'} - \vec{r}|.$$

After performing the calculations, and allowing that the functions that do not contain $\vec{\Omega}$ among their arguments are the *integrals* over $\vec{\Omega}$ of the corresponding phase functions, we obtain the following sets of equations:

[11] Note that it is also possible to construct a nearly exact integral transport theory with an assumption of "linearly anisotropic collision", i.e. with a scattering law that is linearly dependent on the cosine of the scattering angle ψ in the laboratory system.

a/ Continuous form:

$$\begin{aligned} Q &= D + S_f + S_a, \\ S_f(\vec{r}, u) &= \chi_f(u) \int_0^\infty \nu\Sigma_f(\vec{r}, u')\Phi(\vec{r}, u')du', \\ D(\vec{r}, u) &= \int_0^\infty \Sigma_s(\vec{r}, u' \to u)\Phi(\vec{r}, u')du', \\ \Phi(\vec{r}, u) &= \int_{(\infty)} \frac{e^{-\tau}}{4\pi R^2} Q(\vec{r'}, u)d^3r', \end{aligned} \tag{14.14}$$

(τ: optical path from $\vec{r}$ to $\vec{r'}$).

b/ Multigroup form:

$$\begin{aligned} Q_g &= D_g + S_{f,g} + S_{a,g}, \\ S_{f,g}(\vec{r}) &= \chi_{f,g} \sum_{h=1}^{N} \nu\Sigma_{f,h}(\vec{r})\Phi_h(\vec{r}), \\ D_g(\vec{r}) &= \sum_{h=1}^{N} \Sigma_{s,h\to g}(\vec{r})\Phi_h(\vec{r}), \\ \Phi_g(\vec{r}) &= \int_{(\infty)} \frac{e^{-\tau_g}}{4\pi R^2} Q_g(\vec{r'})d^3r', \end{aligned} \tag{14.15}$$

Again we find the simple form of the transport operator that was obtained using the same assumptions in § 3.1.6. This is known as the *Peierls operator*.

Note that these relationships make *no approximation* concerning the phase distribution of travelling neutrons (flux).

14.3.2. Transport correction

The parameters that affect the multiplication factor of a reactor and the power distribution within it are, on the one hand, the number of neutrons regenerated when a neutron is absorbed and, on the other hand, the distance separating one fission from the next. The first aspect is characterised by the ratio $\nu\bar{\Sigma}_f/\bar{\Sigma}_a$ of the average production and absorption cross-sections. The second aspect is described by the Green's function of the migration and, more specifically, as is easily seen by analysing the critical condition of the bare homogeneous pile using one-group theory (Chapter 6), its second-order moment, i.e. the mean square of the crow-fly distance travelled by the neutron from emission to absorption. Allowing for a factor of 1/6, this is called the *migration area* M^2. It is therefore important when carrying out modelling to respect the three synthetic parameters $\nu\bar{\Sigma}_f$, $\bar{\Sigma}_a$, and M^2 as much as possible.

The migration area involves three aspects:

1/ The elementary path of the neutrons between the point of emission or re-emission and the point of the first subsequent collision, governed by the total cross-section Σ.

2/ The number of elementary paths travelled by the neutron during its migration, governed by the ratio Σ_s/Σ.

3/ The scattering deflection angle ψ and particularly the mean value μ of its cosine. For example, if μ is positive, which is the most frequent case, i.e. if scattering tends to occur in a forward direction, then the neutrons tend to travel farther on average than if scattering were isotropic.

Even if it is obvious that the isotropic collision assumption we have introduced does not affect the average cross-sections, it does lead us to replace μ by 0. This assumption therefore does not respect the migration area.

The transport correction is applied to restore the correct migration area value.

In practice, to apply this correction, we use the equation that gives the migration area in monokinetic theory for an infinite homogeneous medium[12]:

$$M^2 = \frac{1}{3\Sigma_a\Sigma_{tr}}, \tag{14.16}$$

where the so-called *"transport" cross-section* is defined by:

$$\Sigma_{tr} = \Sigma - \mu\Sigma_s. \tag{14.17}$$

To avoid modifying Σ_a, the total cross-section Σ is replaced by the transport cross-section Σ_{tr}. In order to respect M^2, we also abandon the constraint of respecting the elementary mean free paths, which is less of a problem than not respecting the migration area.

In a spectrum theory, this correction is applied to each lethargy or in each group. It is not strictly equivalent to respecting M^2, but it can be shown, for the overall migration area, that it is a good approximation.

14.3.3. First collision probabilities

To present the formalism for first collision probabilities, we return to the expression for the isotropic collision transport operator, where the lethargy variable u or the group index g is understood, as well as the transport correction:

$$\Phi(\vec{r}) = \int_{(\infty)} \frac{e^{-\tau}}{4\pi R^2} Q(\vec{r'}) d^3r'. \tag{14.18}$$

To comply with the usual practice, although this is not essential[13], we go from the flux Φ to the *collision density* (or incoming density) $\Sigma\Phi$ by multiplying both sides of the equation by the cross-section at point $\vec{r}$:

$$\Sigma(\vec{r})\Phi(\vec{r}) = \int_{(\infty)} \Sigma(\vec{r}) \frac{e^{-\tau}}{4\pi R^2} Q(\vec{r'}) d^3r'. \tag{14.19}$$

The kernel of the operator is now no longer interpreted as the flux at the point $\vec{r}$, but as the collision density at this point for a neutron emitted isotropically at the point $\vec{r}'$.

The "first collision probabilities" method consists of the following steps:

1/ Cutting up the object to be processed into small volumes V_i, with i from 1 to M;

2/ Approximating the emission density $Q(\vec{r'})$ in each of the little volumes V_j by its average value Q_j, i.e.:

$$Q_j = \frac{1}{V_j} \int_{(j)} Q(\vec{r'}) d^3r'. \tag{14.20}$$

[12] The proof of this formula involves calculating the mean of the square of the vector sum of the elementary paths.

[13] In the APOLLO code, for example, flux is used rather than collision density, so that calculations can be performed even for a vacuum.

In practice, the volumes are homogeneous for practical reasons (for example, one or several volumes for the fuel, one or several volumes for the moderator, etc.), and this is what we assume here. Obviously the choice of smaller volumes will improve the accuracy of the approximation, but at the cost of longer calculation times.

Let Φ_i be the average value of flux in the volume V_i, i.e.:

$$\Phi_i = \frac{1}{V_i} \int_{(i)} \Phi(\vec{r}) d^3 r. \tag{14.21}$$

This average is calculated by integrating the equation over the volume V_i. Moreover, if the integral on the right-hand side is broken down into M integrals on the volumes V_j, we immediately see that:

$$V_i \Sigma_i \Phi_i = \sum_{j=1}^{M} V_j Q_j \tilde{P}_{ji}, \tag{14.22}$$

with:

$$\tilde{P}_{ji} = \frac{1}{V_j Q_j} \int_{(i)} d^3 r \int_{(j)} \Sigma(\vec{r}) \frac{e^{-\tau}}{4\pi R^2} Q(\vec{r'}) d^3 r'. \tag{14.23}$$

This quantity is interpreted as the probability for a neutron emitted isotropically in V_j and according to density $Q(\vec{r'})$ to undergo its first collision in V_i.

This expression is rigorous but impossible to use, because the distribution $Q(\vec{r'})$ of emissions in each volume is unknown. That is why $Q(\vec{r'})$ is replaced by the constant Q_j (which is eliminated between the numerator and the denominator), i.e. the exact probabilities $\tilde{P}_{ji}$ by the probabilities P_{ji} corresponding to uniform emission:

$$P_{ji} = \frac{1}{V_j} \int_{(i)} d^3 r \int_{(j)} \Sigma(\vec{r}) \frac{e^{-\tau}}{4\pi R^2} d^3 r'. \tag{14.24}$$

This quantity is interpreted as the *probability for a neutron emitted* ***uniformly*** *and* ***isotropically*** *in V_j to undergo its first collision in V_i.*

This "flat emission" approximation in terms of space and angle is the only approximation applied by this method. In particular, no space or angle approximation is made concerning the flux. The first collision probabilities method therefore consists of the following steps:

1/ Calculating the double integrals numerically:

$$P_{ji} = \frac{\Sigma_i}{V_j} \int_{(i)} d^3 r \int_{(j)} d^3 r' \frac{e^{-\tau}}{4\pi R^2}, \tag{14.25}$$

by suitable quadrature formulae (the volume elements are assumed to be homogeneous, and the function $\Sigma(\vec{r})$ to be taken in V_i can be replaced by the constant Σ_i that comes out of the double integral);

2/ And then calculating the flux Φ as a function of the emission density Q by simply multiplying a vector by a matrix:

$$V_i \Sigma_i \Phi_i = \sum_{j=1}^{M} V_j Q_j P_{ji}. \tag{14.26}$$

In practice, this must be done for each of the energy groups with which the cross-sections and the spectrum are processed:

1/ Calculating the first collision probabilities $P_{ji,g}$ for each of the groups with the corresponding total cross-sections (or transport cross-sections if appropriate);

2/ And then calculating the flux values of this group according to the emission density in the group:

$$V_i \Sigma_{i,g} \Phi_{i,g} = \sum_{j=1}^{M} V_j Q_{j,g} P_{ji,g}. \tag{14.27}$$

Naturally, Q must also be expressed as a function of the flux values Φ by writing out the collision operators, which can be done in each of the volumes using the multigroup formalism, which can be reduced to multiplications of a flux vector by fission and scattering matrices:

$$\begin{aligned} Q_{j,g} &= D_{j,g} + S_{f,j,g} + S_{a,j,g}, \\ S_{f,j,g} &= \chi_{f,j,g} \sum_{h=1}^{N} \nu \Sigma_{f,j,h} \Phi_{j,h}, \\ D_{j,g} &= \sum_{h=1}^{N} \Sigma_{s,j,h \to g} \Phi_{j,h}. \end{aligned} \tag{14.28}$$

The looping between these two types of formula is usually performed by iteration. To accelerate convergence, scattering is generally isolated in the group:

$$Q_{j,g} = \Sigma_{s,j,g \to g} \Phi_{j,g} + Q'_{j,g},$$

and we work with the vectors Φ and Q'.

14.3.4. Reciprocity and complementarity relationships between the first collision probabilities

Note that the double integral in the formula defining P_{ji} is symmetric; this implies an obvious reciprocity relationship[14]:

$$V_i \Sigma_i P_{ij} = V_j \Sigma_j P_{ji}. \tag{14.29}$$

(This relationship reflects the fact that the probability of a neutron travelling from one point to another without collision does not change if the direction of travel is inverted.)

Moreover, if there is no leakage, every neutron undergoes a collision in the system; the sum of the probabilities on the target volumes for any emission volume is therefore equal to 1:

$$\sum_{i=1}^{M} P_{ji} = 1. \tag{14.30}$$

(These are "complementarity" or "neutron conservation" relationships.)

The number of double integrals to be calculated can be almost halved by applying the reciprocity and complementarity relationships.

[14] In the following equations, the group subscript is understood.

14.3.5. Probabilities involving a surface

In practice, it is often necessary to deal with a *finite* "object" bounded by a surface S, for example an elementary cell or a reactor assembly. This leads to considering the neutrons leaving the "object" on the one hand, and the future of the neutrons entering the neighbouring "object" on the other hand. That is why we must consider not only volume probabilities P_{ji}, but also probabilities P_{jS} for a neutron emitted in V_j to exit *via* the surface S, and first collision probabilities P_{Si} and re-exit probabilities P_{SS} for a neutron entering *via* the surface S.

If the neutrons can exit, the above complementarity relationships no longer apply, because the probability of the "exit" event would need to be added:

$$\sum_{i=1}^{M} P_{ji} + P_{jS} = 1. \tag{14.31}$$

In practice, this formula makes it possible to obtain the probabilities P_{jS} once the probabilities P_{ji} have been calculated.

Just as it was necessary when defining P_{ji} to specify how neutrons were emitted in V_j, likewise it is necessary to specify how the neutrons enter *via* the surface S in order to define P_{Si} and P_{SS} unambiguously. Here again, ***uniformity*** *and* ***isotropy***[15] will be assumed. In this case:

– *Uniformity* means that the same number of neutrons enters *via* any unit surface element; in other words, the probability of the neutron entering *via* an element dS is dS/S;

– *Isotropy* concerns the *incoming* phase *flux* of neutrons; in other words, the number of neutrons entering *via* a solid angle element $\sin\theta\, d\varphi\, d\theta$ defined by $d\varphi$ and $d\theta$ (counting θ from the incoming normal) is $\cos\theta \sin\theta\, d\varphi\, d\theta/\pi$ so that a total of one neutron is concerned for the 2π steradians of input directions.

14.3.6. Reciprocity and complementarity relationships between probabilities involving a surface

Under these conditions, if we write out the integrals we can show that there is a reciprocity relationship between the mixed surface/volume probabilities:

$$P_{Si} = \frac{4V_i\Sigma_i}{S} P_{iS}. \tag{14.32}$$

This means that the P_{Si} probabilities can be deduced from the P_{iS} probabilities.

By listing all the possibilities, we can write the complementarity relationship:

$$\sum_{i=1}^{M} P_{Si} + P_{SS} = 1, \tag{14.33}$$

which then allows us to obtain the probability P_{SS}.

[15] Note that an assumption must be made about the *incoming* neutrons, but no assumption is made concerning the distribution of the *outgoing* neutrons.

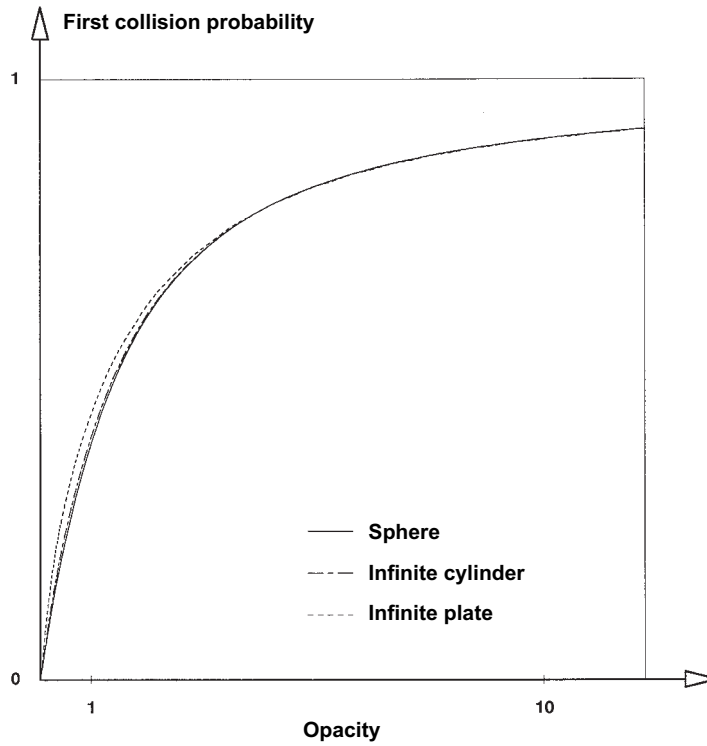


Figure 14.2. Probability P_{VV} for three simple geometries (in schematic form, these are the geometries generally used for reactor fuel elements).

Note that, with the assumptions made, only the $M(M + 1)/2$ P_{ji} probabilities with (for example) $j \leqslant i$ need to be calculated explicitly by quadrature; all others can be deduced using reciprocity and complementarity.

14.3.7. First collision probabilities for a homogeneous convex body

The simplest case is that of a single volume V bounded by its surface S, i.e. the case $M = 1$. There are then four probabilities to consider: P_{VV}, P_{VS}, P_{SV}, and P_{SS}, but only one to be calculated, thanks to the reciprocity and conservation relationships. (Note in the examples below that P_{SS} is the easiest probability to express and calculate.)

The first collision probability P_{VV} in this body for a neutron emitted uniformly and isotropically in the volume V is plotted in Figure 14.2 for three simple geometries: a sphere, a cylinder of infinite height, and a plate of infinite length and width. The variable plotted along the abscissa is not the radius or thickness, but the *opacity* ω: the

dimensionless product $\omega = \Sigma\bar{X}$ of the total cross-section Σ by the average chord[16] $\bar{X} = 4V/S$ (Cauchy's theorem)[17].

A series expansion of the probability P_{SS} allows the expansion of P_{VV} to be deduced:

– for *low values of opacity*:

$$P_{VV} = \frac{Q\omega}{2} + \ldots, \quad Q = \frac{\langle X^2 \rangle}{(\langle X \rangle)^2}. \tag{14.34}$$

The coefficient Q characterises the slope of the curves at the origin. Its value is 9/8 for the sphere, 4/3 for the cylinder, and infinity for the plate;

– for *high values of opacity*:

$$P_{VV} = 1 - \frac{1}{\omega} + \ldots, \quad P_{VV} \simeq \frac{\omega}{1+\omega}. \tag{14.35}$$

(This equation is the Wigner approximation.)

The asymptotic behaviour of the curves is therefore the same for all geometries.

(Note that this observation is the basis for the possible equivalence between the heterogeneous case and a homogeneous case in resonant absorption theory: see § 8.3.2.)

14.3.8. Calculation of collision probabilities in x Geometry and $x - y$ Geometry

In these three examples, probability calculations are possible thanks to geometric symmetries. In general, after a few legitimate simplifications, we often find problems that are independent of the variable z, or independent of y or the azimuth φ. The following equations are useful in these cases because they simplify the general form of the Peierls operator:

$$\Phi(\vec{r}) = \Phi(x, y, z) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{e^{-\tau}}{4\pi R^2} Q(x', y', z') dx'\, dy'\, dz'; \tag{14.36}$$

– for a *planar geometry* problem, meaning one involving the variable x only, it is possible to integrate over y and z to obtain:

$$\Phi(x) = \int_{-\infty}^{+\infty} \frac{1}{2} E_1(\tau_x) Q(x') dx', \tag{14.37}$$

and the resulting formulae for the first collision probabilities. The argument τ_x is the projection of the optical path $\vec{\tau}$ on the $\vec{x}$ axis, and the functions E_n are the *integral exponentials*[18]:

$$E_n(u) = \int_0^1 \exp\left(-\frac{u}{\mu}\right) \mu^{n-2} d\mu; \tag{14.38}$$

[16] To define the average chord, it is necessary to specify the probability distribution with which the chord was chosen. Cauchy selected the chord's point of origin according to a probability that is uniform on the surface, and an incoming direction according to an isotropic distribution. These are the assumptions we have adopted for the distribution of incoming neutrons.

[17] Note that this opacity is also the coefficient that relates the two surface/volume probabilities in this case.

[18] See appendices.

– for a problem involving only the variables x and y, it is possible to integrate over z to obtain:

$$\Phi(\vec{\rho}) = \Phi(x, y) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{Ki_1(\tau_{xy})}{2\pi R_{xy}} Q(x', y') dx'\, dy', \tag{14.39}$$

and the resulting formulae for the first collision probabilities. The argument τ_{xy} is the projection of the optical path $\vec{\tau}$ on the $x - y$ plane, and R_{xy} is the projection of the real path $\vec{R}$ of the neutron on the $x - y$ plane; Ki_n are the *Bickley functions*[19]:

$$Ki_n(u) = \int_0^{\pi/2} \exp\left(-\frac{u}{\sin\theta}\right) \sin^{n-1}\theta\, d\theta. \tag{14.40}$$

For problems in the cylindrical geometry (infinite height), this formula is used, with the revolution symmetry taken into account[20].

For general two-dimensional $x - y$ problems, the first collision probabilities are calculated using the variables R, Φ, t and t' as defined in the diagram below.

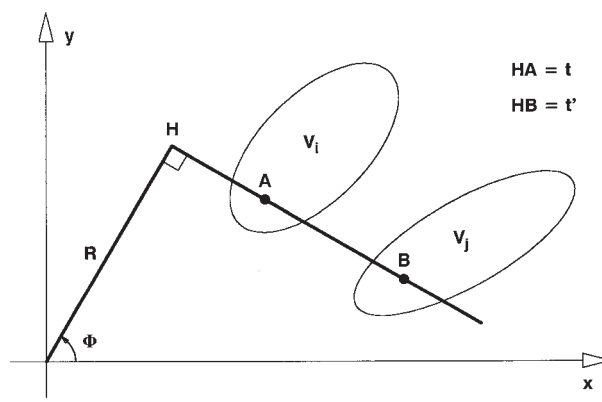


Figure 14.3. Variables used to calculate first collision probabilities.

Under these conditions, the first collision probability is written as follows:

$$P_{ji} = \frac{\Sigma_i}{V_j} \iiint \frac{Ki_1(\tau_{xy})}{2\pi} dR\, d\Phi\, dt\, dt', \tag{14.41}$$

where the variables describe the volumes V_i and V_j.

[19] See appendices.
[20] The formulae can also be simplified in problems with spherical symmetry.

14.3.9. Calculation of probabilities on an infinite lattice of identical cells

The structure used in nuclear reactor cores is often relatively regular, so that each fuel element and its cladding can be associated with a part of the volume of the coolant and the moderator (in the case of a thermal neutron reactor) to form the mesh element of this structure, which neutron physicists call a "cell". By juxtaposing these cells, we obtain what neutron physicists call a *"lattice"*.

These lattices are not always very regular. Four types of cell can be identified in the example presented in Figure 13.3, concerning a pressurised water reactor assembly[21] with consumable poison rods:

- 248 standard fuel cells[22];
- 16 cells with a gadolinium-poisoned fuel;
- 24 cells able to accommodate the control bundle consisting of 24 absorbent rods;
- The central cell, reserved for instrumentation[23].

To simplify the calculations, the lattice is extended to infinity by assuming that the geometry and therefore the neutron flux are periodic; this creates the *regular infinite lattice*, which has become a paradigm in neutron physics, as it is used as a reference between the two steps of the calculation[24]: the fine calculation (on the scale of a cell), and the macroscopic calculation (calculation of the whole core).

Lattices can be:

- One-dimensional, i.e. consisting of flat cells made up of infinite plates,
- Two-dimensional, i.e. consisting of prismatic cells of infinite height,
- Three-dimensional, i.e. consisting of box-shaped cells.

All three cases are found in practice; the two-dimensional case is the most common, and this is the case we shall consider here.

The simplest lattice consists of cells that are all identical; for example, the one represented in Figure 14.4 (imagine that it continues *ad infinitum*), a fictitious lattice made up of fuel cells in a pressurised water reactor. We begin by considering this case, and then we shall look at "multi-cell" lattices.

Whether the lattice is rectangular, hexagonal, or triangular, the planes containing the interfaces between cells are all symmetry planes. When a neutron travelling in a given cell passes through one of these interfaces, the part of the path located beyond it can be replaced by its symmetric counterpart[25]; in other words, without changing the physics, we can reason on this one cell, assuming that the neutrons reaching the surface are sent back to the inside as if by a perfect mirror. This boundary condition is introduced in the processing of the Boltzmann equation, and is called a *specular reflection condition*.

[21] Note that, in water reactors, this fluid acts as both a coolant and a moderator.

[22] In practice, the peripheral cells must also be distinguished; they include the half-water gap between assemblies and the corner cells with two half-water gaps.

[23] On the simplified diagram (Figure 13.3), it is represented like the previous 24 cells.

[24] The link between these two steps (equivalence) will be specified in Chapter 17.

[25] In fact, this symmetry means that the neutron under consideration is replaced by an equivalent symmetric neutron.

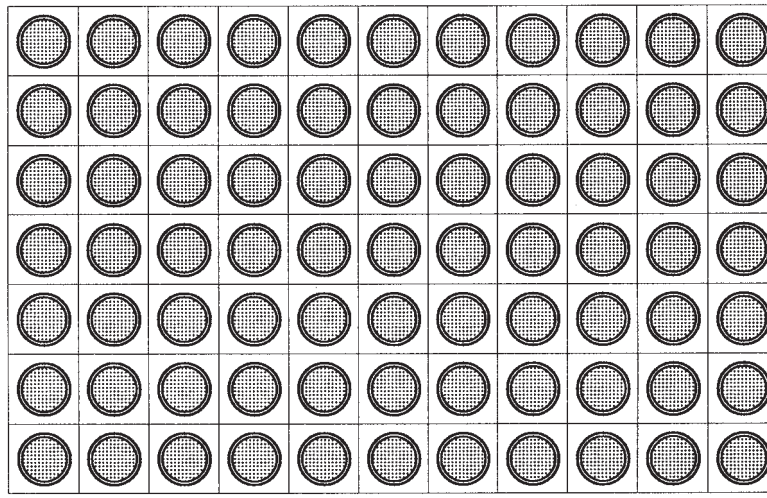


Figure 14.4. The lattice: paradigmatic neutron situation of reactors (here: pressurised water reactor lattice). Note that the contours of the squares correspond to purely fictitious limits.

It is obvious that the use of the first collision probabilities method in this type of problem will involve a two-dimensional $x-y$ calculation, either in the lattice itself by identifying the similar volumes of all the cells[26], or in the isolated cell with the specular reflection conditions[27]. In codes such as APOLLO, this type of calculation is possible, but is still costly. That is why an interface current uniformity and isotropy approximation is often made. This consists of replacing the correct boundary condition (specular reflection) by an approximate condition called *white reflection*, where every neutron reaching the surface of the cell is assumed to "forget" its state (position and direction), and is sent according to a distribution that is uniform along the surface and isotropic towards the inside. Note that this makes it possible to use the surface probabilities introduced above, which do not need to be calculated if the volume-volume probabilities have already been obtained.

The following equations are to be used in the context of this simplifying assumption. Let:

- P_{ji}^{+} be the probability for a neutron emitted in the volume V_j in one of the cells of undergoing its first collision in the volume V_i of the *same* cell;

- P_{jS}^{+} be the probability for a neutron emitted in the volume V_j of one of the cells of leaving this cell;

- P_{Si}^{+} be the probability for a neutron entering one of the cells of undergoing its first collision in the volume V_i of *that* cell.

[26] For P_{ji} to be calculated, the neutrons must be emitted in one of the volumes V_j and the impacts in *all* volumes V_i must be counted.

[27] The path of neutrons reaching the surface must be continued by reflection until the neutrons have had their first collision.

The probability P_{ji} for a neutron emitted in the volume V_j of one of the cells undergoing its first collision in the volume V_i of the same cell or any other cell[28] is calculated by adding the probabilities of events with 0, 1, 2, 3 ... exits:

$$P_{ji} = P_{ji}^{+} + P_{jS}^{+}P_{Si}^{+} + P_{jS}^{+}P_{SS}^{+}P_{Si}^{+} + P_{jS}^{+}P_{SS}^{+}P_{SS}^{+}P_{Si}^{+} + \cdots$$

A geometric series is obtained:

$$P_{ji} = P_{ji}^{+} + \frac{P_{jS}^{+}P_{Si}^{+}}{1 - P_{SS}^{+}}. \tag{14.42}$$

The "no exit" probabilities P^{+} are those that were introduced above (§ 14.3.3 and 14.3.5); we noted that all probabilities involving the surface are deduced from the volume-volume probabilities. This means that only the latter need to be calculated (taking the reciprocity relations into account): there are far fewer of them[29] and they are far more simple to calculate than the true probabilities, because they relate to a single cell which we imagine to be isolated. The true probabilities, on the other hand, involve calculating and summing, for a fixed V_j, the probabilities for the volumes V_i of all the cells[30] and require the handling of complicated optical paths for the outside cells.

When it is acceptable, which it is for most calculations, this simplifying assumption considerably reduces the volume of calculations to be performed.

14.3.10. Cylindrisation of cells

To further simplify the calculations, another (non-mandatory) approximation is often introduced: cell cylindrisation[31].

This idea arises from the observation that, in many reactor concepts, (UNGG, PWR and BWR, FNR, etc.), the unit cell consists of a fuel and a cladding, i.e. a channel with rotational symmetry, where only the outside contour of the cell breaks the symmetry. The cylindrisation approximation (see Figure 14.5) consists of replacing the prismatic contour of the cell with a cylindrical contour[32] in order to obtain complete rotational symmetry, and therefore simplify the calculation of the probabilities P_{ji}^{+}[33].

Conservation of matter is obviously essential in this operation, but this leaves an open choice of radius R. It might be difficult to choose between "Askew cylindrisation", which conserves the exchange surface with the neighbouring cells and therefore the *external perimeter* (with reduction of the moderator density to conserve its mass), and "Wigner cylindrisation", which conserves the *cross-section* (and the density of the moderator). For cells whose cross-section is shaped like a regular polygon (hexagon, square, or triangle), Wigner cylindrisation is usually chosen. For cells with a rectangular cross-section[34] with

[28] Or, in the context of the problem of the unique cell which we imagine to be isolated, in the volume V_i of this cell after any number of reflections on the surface.

[29] For example, six probabilities if three volumes are placed in the cell: the fuel, the cladding, and the moderator.

[30] In practice, for this type of calculation, the infinite series is truncated, neglecting the cells beyond a certain "optical" distance.

[31] Cylindrisation of the cells whilst conserving specular reflection would not make sense, because the probability calculations would not be simplified much; moreover, it has been shown that the errors due to both approximations (white reflection and cylindrisation) partially cancel each other out.

[32] Cylindrisation can only be envisaged in the image of the cell that we imagine to be isolated, because space can obviously not be paved with cylinders.

[33] Rotational symmetry simplifies the integrals expressing these probabilities.

[34] For example, the cells at the edge of a PWR assembly, including the water gap on one of their faces.

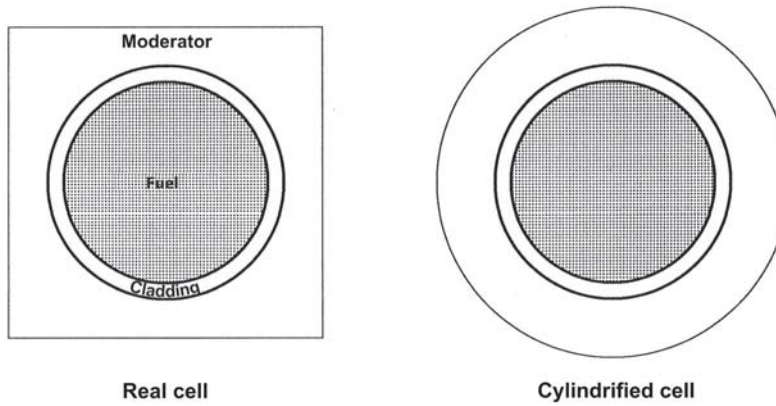


Figure 14.5. Cylindrisation of a cell (here, a pressurised water; real size of the square cell: 12.6 mm).

sides *a* and *b*, it is recommended to use "Lefebvre cylindrisation" (with a density reduction), which is better suited to "multicell" calculations[35] (see next section), and is reduced to Wigner cylindrisation if the rectangle is a square:

$$R = \frac{a+b}{2\sqrt{\pi}}. \tag{14.43}$$

14.3.11. Principle of "multicell" geometry calculations

We have seen that, in practice, the objects dealt with by a neutron physicist are often assemblies of unit cells that are not always identical.

The method presented above can be generalised (with exactly the same assumptions) to the regular infinite lattice whose elementary pattern comprises a set of cells of different types. This is the "multicell" formalism.

The pattern can contain several cells that are identical in geometry and composition. Theoretically, they cannot be considered as being of the same type (from a neutron physics point of view) unless they also have an identical environment (for example, being symmetrical with respect to a general plane of symmetry for the pattern), but in practice, they can be declared to be of the same type even if this condition is not fulfilled. This reduces the number of types, and therefore the calculation cost, but is obviously an additional approximation whose validity needs to be verified.

Let *I*, *J* or *K* be the index used to identify the type, and α_I, α_J or α_K be the proportion in the lattice (or pattern) of cells of type *I*, *J* or *K*, and let S_{JI} be the probability that a neutron leaving a type *J* enters a type *I* cell. To remain consistent with the assumption of uniformity of the currents leaving the cells, S_{JI} must be the proportion of the side surface of all cells *J* of the pattern in contact with a type *I* cell. It is therefore a strictly geometric parameter that characterises the connections between the various types of cell. Because

[35] Because it satisfies the reciprocity relationships on the "contact probabilities" S_{JI}.

S_{JI} are probabilities (for fixed J), the following complementarity relationships exist:

$$\sum_I S_{JI} = 1. \tag{14.44}$$

In addition, because the surfaces of the type J cells in contact with type I cells are obviously the same as the surfaces of the type I cells in contact with type J cells, the S_{JI} values must satisfy the following reciprocity conditions:

$$\alpha_I p_I S_{IJ} = \alpha_J p_J S_{JI}, \tag{14.45}$$

where p_I is the surface of a type I cell, i.e. its perimeter. (These relationships are useful on the one hand to check that no errors were made in calculating the S_{JI} of a pattern, and on the other hand, as we have just seen, to obtain a cylindrisation rule if we also wish to introduce this approximation.)

Using the same type of argument as the one used to express the probabilities P of a lattice as a function of the probabilities P^+ of a cell, the "multicell"[36] formalism provides all the first collision probabilities P_{ji} in a zone i of a type I cell for a neutron emitted in a zone j of a type J cell based on the cell-specific probability sets P^+ — the only ones, finally, that need to be calculated:

1/ Using δ_{JI} to denote the Kronecker symbol and Q_{JI} to denote the number of neutrons entering a type I cell, without an intermediate collision, for a neutron leaving a type J cell, we have:

$$P_{ji} = P^+_{ji}\delta_{JI} + P^+_{jS}Q_{JI}P^+_{Si}; \tag{14.46}$$

2/ By writing out the definition of these probabilities, we obtain the equation used to calculate Q_{JI} :

$$Q_{JI} = S_{JI} + \sum_K S_{JK}P^+_{SS,K}Q_{KI}. \tag{14.47}$$

In a lattice consisting of only one type of cell, there is obviously no need to distinguish between the faces because they are equivalent. In a multicell lattice, however, this assumption of complete uniformity, named after Roth (the author who suggested it), is very much debatable.

For example, in the pattern in Figure 14.6, it is obvious that a neutron leaving a fuel cell adjacent to the absorbent cell is not likely to have the same outcome as if it emerged facing the absorbent or *via* the opposite face. That is why it is helpful to *distinguish the faces* of cells, i.e. to have uniformity of interface currents not over the entire surface of cells, but face by face.

The simplest improvement of the Roth assumption, known as ROTH-4 for square cells and ROTH-6 for hexagonal cells, consists of preventing a neutron that enters a cell and passes through it without collision from exiting *via* the face of entry. It can, however, leave with equal probability *via* the three (or five) other faces. This approximation does not lead to new P^+ probability calculations, but makes it necessary to generalise the matrix Q (distinction of faces).

[36] It can be verified that it gives the formulae for the lattice when there is only one type of cell.

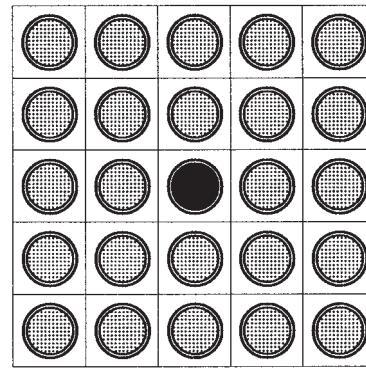


Figure 14.6. Example of heterogeneity in a PWR lattice: an absorbent rod in the centre of a 5 × 5 pattern, where the other twenty-four cells contain fuel (imagine that the edges of the pattern are planes of symmetry).

A more accurate method can also be envisaged: calculating the exact probabilities of crossing a cell from one face to the other. In this case, in addition to the generalisation of the matrix Q, some surface probabilities P^+ must be calculated, because the complementarity and reciprocity relationships do not distinguish between the faces in the surface probabilities that are deduced from the P_{ji}^+.

Note also that the treatment of interface currents can be improved not only with respect to uniformity, but also with respect to isotropy. The assumption of isotropy (over 2π) of the flux of neutrons passing through the interfaces can be abandoned in favour of a *linear anisotropy* assumption, i.e. a flux that is linearly dependent on $\cos\theta$. Here again, on the one hand, certain components must be added to the interface currents and the matrix Q must be generalised. On the other hand, a few additional probabilities P^+ must be calculated.

The multicell method can be generalised to handle any structure that has been imaginarily cut into sub-structures that exchange neutrons *via* their interfaces. The uniformity and isotropy (or linear anisotropy) approximation at each interface can reduce the number of probabilities and considerably simplify the calculation, because only P^+ type probabilities are involved.

14.4. Handling the differential form of the transport operator

14.4.1. Handling the diffusion operator

We have seen that the isotropic collision approximation (possibly with a transport correction) considerably simplifies the integral form of the Boltzmann equation, because the variable $\vec{\Omega}$ can be made to disappear simply by integrating over the phases. The transport operator, on the other hand, can hardly be simplified if written in differential form,

because in that case it is impossible[37] to return to a problem without $\vec{\Omega}$ even if the collisions are isotropic. In contrast, taking the exact angular scattering distribution into account does not make it more difficult to handle the integral/differential equation[38].

In its continuous form, the scattering operator is written as follows:

$$D(\vec{r}, u, \vec{\Omega}) = \int_0^\infty du' \int_{(4\pi)} d^2\Omega' \Sigma_s \left[\vec{r}, (u', \vec{\Omega}') \rightarrow (u, \vec{\Omega})\right] \Phi(\vec{r}, u', \vec{\Omega}'). \tag{14.48}$$

After multigroup discretisation, this takes the following form:

$$D_g(\vec{r}, \vec{\Omega}) = \sum_{h=1}^{N} \int_{(4\pi)} \Sigma_{s,h\rightarrow g}(\vec{r'}, \vec{\Omega}' \rightarrow \vec{\Omega}) \Phi_h(\vec{r'}, \vec{\Omega}') d^2\Omega'. \tag{14.49}$$

In practice, materials placed in reactors can *always* be considered to be *isotropic*; as we have seen, this leads us to separate v (scalar speed, which can be replaced by u) and $\vec{\Omega}$ (direction of speed) since the isotropy of matter means that the cross-sections do not depend on $\vec{\Omega}$. This applies to all reactions, and scattering in particular. This illustrates the fact that writing the differential scattering cross-section in these integrals is not a good idea, because it does not reveal it. With regard to the angular aspect, the differential scattering cross-section is not dependent on four variables (θ', φ', θ and φ), but only one: the scattering angle or, which amounts to the same thing, its cosine, written as μ or $\vec{\Omega}' \cdot \vec{\Omega}$, i.e. the scalar product of two vectors. (Moreover, there can be a partial or total correlation between this angle and the group or lethargy change; this aspect is mentioned here as a reminder only.) These operators are then rewritten as:

$$D(\vec{r}, u, \vec{\Omega}) = \int_0^\infty du' \int_{(4\pi)} d^2\Omega' \Sigma_s \left(\vec{r}, \vec{\Omega}' \cdot \vec{\Omega}, u' \rightarrow u\right) \Phi(\vec{r}, u', \vec{\Omega}'), \tag{14.50}$$

and:

$$D_g(\vec{r}, \vec{\Omega}) = \sum_{h=1}^{N} \int_{(4\pi)} \Sigma_{s,h\rightarrow g}(\vec{r'}, \vec{\Omega}' \cdot \vec{\Omega}) \Phi_h(\vec{r'}, \vec{\Omega}') d^2\Omega'. \tag{14.51}$$

We allow $\vec{r}$, u' and u (or h and g) to be understood, and concentrate on the integral operator:

$$D(\vec{\Omega}) = \int_{(4\pi)} \Sigma_s(\vec{\Omega}' \cdot \vec{\Omega}) \Phi(\vec{\Omega}') d^2\Omega', \tag{14.52}$$

with kernel $\Sigma_s(\vec{\Omega}' \cdot \vec{\Omega})$.

As a function of $\mu = \vec{\Omega}' \cdot \vec{\Omega}$, this kernel can be broken down into Legendre polynomials[39]:

$$\Sigma_s(\mu) = \sum_{n=0}^{\infty} \frac{2n+1}{2} \Sigma_{s,n} P_n(\mu), \tag{14.53}$$

with:

$$\Sigma_{s,n} = \int_{-1}^{+1} \Sigma_s(\mu) P_n(\mu) d\mu. \tag{14.54}$$

[37] Unless an approximation such as the diffusion approximation is applied.
[38] Note again that emission by fission is isotropic.
[39] The definitions and main properties of Legendre polynomials are reviewed in an Appendix.

In particular, $\Sigma_{s,0}$ is the usual scattering cross-section Σ_s (including all angles), and $\Sigma_{s,1}$ is the product $\bar{\mu}\Sigma_s$ of this cross-section by the average cosine of the deflection angle of the neutron when scattered.

The following theorem describes the advantage of this breakdown: *the scattering operator, whose kernel depends only on* $\vec{\Omega}' \cdot \vec{\Omega}$, *is rotationally invariant*; *its eigenfunctions are the spherical harmonics*[40] $Y_n^m(\vec{\Omega})$; the associated eigenvalues are the coefficients $\Sigma_{s,n}$:

$$\int_{(4\pi)} \Sigma_s(\vec{\Omega}' \cdot \vec{\Omega}) Y_n^m(\vec{\Omega}') d^2\Omega' = \Sigma_{s,n} Y_n^m(\vec{\Omega}). \tag{14.55}$$

14.4.2. Spherical harmonic method

The spherical harmonics $Y_n^m(\vec{\Omega})$ are the equivalent for three-dimensional space of the trigonometric functions used to perform a Fourier expansion of a periodic function; they are functions of $\vec{\Omega}$ (or of the angles θ and φ), i.e. of a point on the unit sphere. Just as trigonometric functions return to the same value after one full revolution, i.e. when the argument changes by 2π, spherical harmonics are invariant after one full rotation around the unit sphere along, for example, a large circle or a parallel circle. These functions can be numbered with two subscripts: a main subscript n with values from zero to infinity, and a secondary subscript m with values (for fixed n) from $-n$ to $+n$.

The functions of $\vec{\Omega}$ that can be encountered in physics, for example a neutron phase flux, can be expanded using spherical harmonics[41]:

$$\Phi(\vec{r}, u, \vec{\Omega}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \Phi_n^m(\vec{r}, u) Y_n^m(\vec{\Omega}). \tag{14.56}$$

Because spherical harmonics are normed, by definition the coefficients of the expansion are as follows[42]:

$$\Phi_n^m(\vec{r}, u) = \int_{(4\pi)} \Phi(\vec{r}, u, \vec{\Omega}) Y_n^{*m}(\vec{\Omega}) d^2\Omega, \tag{14.57}$$

where the asterisk denotes the complex conjugate function.

The formulae are analogous in the multigroup approximation.

By writing this expansion into the integral/differential Boltzmann equation and then:

a/ using the property that spherical harmonics are eigenfunctions of the diffusion operator, and

b/ expressing the products $\Omega_k Y_n^m(\vec{\Omega})$ (with $k = x$, y or z) as a function of the neighbouring spherical harmonics using the recurrence relationships between these functions,

we reach an infinite system of equations numbered with the subscripts n and m *where the variable* $\vec{\Omega}$ *no longer appears*.

[40] The definitions and main properties of spherical harmonics are reviewed in an Appendix. Legendre polynomials are the spherical harmonics that dependent on the angle θ (or its cosine μ) only.

[41] This is the same idea as expanding the cross-section, except that for the cross-section the invariance along φ leads to an expansion along n only, i.e. in Legendre polynomials.

[42] A formula comparable to the one defining $\Sigma_{s,n}$.

In practice, we truncate this system by eliminating all terms of rank n greater than a given value N, and then process it according to $\vec{r}$ and u using the usual numerical methods. This approach is traditionally called the $\mathbf{P_N}$ *approximation*.

The number of coefficients $\Phi_n^m(\vec{r}, u)$ to be calculated is:

$$1 + 3 + 5 + 7 + \cdots + (2N + 1) = (N + 1)^2.$$

To illustrate this general principle on a simple example, let us examine a monokinetic problem in planar geometry. In monokinetic theory, the equation to be solved has the following form[43]:

$$\operatorname{div}\left[\vec{\Omega}\Phi(\vec{r}, \vec{\Omega})\right] + \Sigma(\vec{r})\Phi(\vec{r}, \vec{\Omega}) = Q(\vec{r}, \vec{\Omega}) + \int_{(4\pi)} d^2\Omega' \Sigma_s(\vec{r}, \vec{\Omega}' \to \vec{\Omega})\Phi(\vec{r}, \vec{\Omega}'), \tag{14.58}$$

where $Q(\vec{r}, \vec{\Omega})$ is assumed to be known, at least provisionally.

"In planar geometry" means that, in terms of space, the problem involves the variable x only (the system is assumed to consist of a series of infinite plates along y and z). In this case, concerning $\vec{\Omega}$, it is advisable to identify the colatitude from the direction of the $\vec{x}$ axis, since the longitude will not be involved for reasons of symmetry. If we set $\mu = \cos\theta$, the equation is reduced to:

$$\mu\frac{\partial\Phi(x, \mu)}{\partial x} + \Sigma(x)\Phi(x, \mu) = Q(x, \mu) + \int_{-1}^{+1} \Sigma_s(x, \mu' \to \mu)\Phi(x, \mu')d\mu'. \tag{14.59}$$

Under these conditions, the Legendre polynomials (except for a factor, the φ-independent spherical harmonics) are sufficient to expand the phase flux. We therefore set:

$$\Phi(x, \mu) = \sum_{n=0}^{\infty} \Phi_n(x)P_n(\mu), \tag{14.60}$$

where the coefficients are interpreted like the integrals[44]:

$$\Phi_n(x) = \frac{2n + 1}{2} \int_{-1}^{+1} \Phi(x, \mu)P_n(\mu)d\mu. \tag{14.61}$$

In the first instance, we replace the flux appearing under the "summation" sign by its expansion, bearing in mind that Legendre polynomials are eigenfunctions of the diffusion operator. The equation then takes on the following form:

$$\mu\frac{\partial\Phi(x, \mu)}{\partial x} + \Sigma(x)\Phi(x, \mu) = Q(x, \mu) + \sum_{k=0}^{\infty} \frac{2k + 1}{2}\Sigma_{s,k}P_k(\mu) \int_{-1}^{+1} \Phi(x, \mu')P_k(\mu')d\mu', \tag{14.62}$$

[43] In multigroup theory, the equations would have the same form in each group, because, in order to improve the convergence of the iteration between Q and Φ, it is advisable to place the scattering within the group itself on the right-hand side. In this case, in addition to the absorptions, the term $\Sigma\Phi$ on the left-hand side includes transfers to other groups, and the term Q on the right-hand side represents the transfers from other groups (as well as fissions).

[44] Unlike spherical harmonics, Legendre polynomials are not normed. The coefficient $2/(2n+1)$ representing the square of the norm of polynomial P_n is therefore placed in an arbitrary position, which different authors choose differently. Here, a different convention was used for the diffusion cross-section and the flux, in order to simplify the formulae.

where the integrals that appear implicitly represent the coefficients of the Legendre expansion of the flux[45].

This form suggests handling the equation by "internal" iteration (as opposed to the "external" iteration between Q and Φ): based on an initial estimate of the last term, Φ is calculated by inverting the transport operator on the left-hand side[46]; after obtaining Φ, we re-evaluate the integrals on the right-hand side; we then re-calculate Φ; and so on until convergence.

Strictly speaking, the method of spherical harmonics consists of introducing on the left-hand side also the expansion according to these base functions to invert the advection operator.

In the current example, where only Legendre polynomials appear, the recurrence formula for these polynomials can be used:

$$nP_{n-1}(\mu) - (2n+1)\mu P_n(\mu) + (n+1)P_{n+1}(\mu) = 0, \tag{14.63}$$

to transform the terms of the μP_n form. We now expand the "source" Q like the flux:

$$Q(x,\mu) = \sum_{n=0}^{\infty} Q_n(x)P_n(\mu), \tag{14.64}$$

with:

$$Q_n(x) = \frac{2n+1}{2}\int_{-1}^{+1} \Phi(x,\mu)P_n(\mu)d\mu. \tag{14.65}$$

By stating that the algebraic sum of the coefficients in front of each of the polynomials is identical to zero, we finally obtain an infinite system of differential equations governing the functions Φ_n of the space variable x. In practice, this system will be truncated at the *Nth* order:

$$\begin{aligned}
&-\tfrac{1}{3}\Phi_1' - \Sigma\Phi_0 + \Sigma_{s,0}\Phi_0 + Q_0 = 0,\\
&-\Phi_0' - \tfrac{2}{5}\Phi_2' - \Sigma\Phi_1 + \Sigma_{s,1}\Phi_1 + Q_1 = 0,\\
&-\tfrac{n}{2n-1}\Phi_{n-1}' - \tfrac{n+1}{2n+3}\Phi_{n+1}' - \Sigma\Phi_n + \Sigma_{s,n}\Phi_n + Q_n = 0,\\
&-\tfrac{N}{2N-1}\Phi_{N-1}' - \Sigma\Phi_N + \Sigma_{s,N}\Phi_N + Q_N = 0.
\end{aligned} \tag{14.66}$$

This system of $N+1$ equations governs $N+1$ functions. Note that the equations of this system are relatively uncoupled because each equation only involves three successive unknown functions. Even by combinations, however, it is not possible in the general case to obtain a system of decoupled equations.

For reasons that will be explained below, related to an equivalence between the $\mathbf{P_N}$ and $\mathbf{S_{N+1}}$ approximations, an odd value of N is usually chosen.

14.4.3. Diffusion approximation and transport correction

The $\mathbf{P_0}$ approximation would lead us to assume the flux to be everywhere isotropic, which would eliminate any migration. The "minimum" approximation is therefore $\mathbf{P_1}$:

$$\begin{aligned}
&-\tfrac{1}{3}\Phi_1' - \Sigma\Phi_0 + \Sigma_{s,0}\Phi_0 + Q_0 = 0,\\
&-\Phi_0' - \Sigma\Phi_1 + \Sigma_{s,1}\Phi_1 + Q_1 = 0.
\end{aligned} \tag{14.67}$$

[45] In the general case, these would be the coefficients of the spherical harmonic expansion.
[46] The tricky part is the "advection operator".

If we also assume that the "sources" are isotropic, i.e. taking Q_1 to be zero and noting that:

- Φ_0 is $\Phi/2$ where Φ is the usual flux integrated over the phases, because $P_0 = 1$;
- similarly, Q_0 is $Q/2$;
- Φ_1 is $3J/2$ where J is the usual current integrated over the phases, because $P_1 = \mu$;
- $\Sigma - \Sigma_{s,0} = \Sigma - \Sigma_s$ is the absorption section Σ_a;
- $\Sigma - \Sigma_{s,1} = \Sigma - \bar{\mu}\Sigma_s$ is the transport section Σ_{tr},

we see that this system can be rewritten in the following form:

$$\begin{aligned} -J' - \Sigma_a \Phi + Q &= 0, \\ -\Phi' - 3\Sigma_{tr} J &= 0. \end{aligned}$$

The first equation sets out the neutron balance per unit volume (including all neutron directions); the second is the approximate expression for the current, known as *"Fick's Law"*:

$$\vec{J} = -D\overrightarrow{\text{grad}}\,\Phi \tag{14.68}$$

(§ 5.1.2), with the *transport correction* (§ 5.1.8) for the expression of the diffusion coefficient $D = 1/3\Sigma_{tr}$.

More generally, the approximation $\mathbf{P_1}$ that consists of representing the phase flux by the zeroth-order spherical harmonic (a constant) and the three first-order spherical harmonics (linear combinations of the three components of the vector $\vec{\Omega}$) amounts to approximating the phase flux at each point by an expression of the following type:

$$\Phi(\vec{r}, \vec{\Omega}) \simeq A + \vec{B} \cdot \vec{\Omega}.$$

By identification, we can see that, except for a factor, the scalar constant A is the integrated flux and the vector constant $\vec{B}$ is the integrated current:

$$\Phi(\vec{r}, \vec{\Omega}) \simeq \frac{1}{4\pi}\Phi(\vec{r}) + \frac{3}{4\pi}\vec{\Omega} \cdot \vec{J}(\vec{r}). \tag{14.69}$$

This approach to the diffusion approximation as a $\mathbf{P_1}$ approximation is the mathematical justification for the physical and intuitive approach suggested in Chapter 5.

Note: In monokinetic theory, the transport correction is equivalent to approximating linearly anisotropic diffusion (probability distribution for the deflection of the neutron during a linear collision at $\cos\theta$); in multigroup theory, the transport correction is "concentrated" on the initial group, when it should be "broken down" in the arrival groups. The practical effects of this second approximation turn out not to be very major.

14.4.4. Method of simplified spherical harmonics

The spherical harmonics method quickly produces a large number of unknown functions to be calculated if a somewhat high order N is used. On the other hand, limiting the calculation to $N = 1$, i.e. the diffusion approximation, can sometimes turn out to be insufficient[47]. The method of "simplified" spherical harmonics can be a good compromise between the cost and the precision of the calculation.

The idea is to identify the direction of the *current* $\vec{J}$ at each point of the reactor, described in two- or three-dimensional geometry; this means describing the axis along which migration mainly occurs and assuming that, according to this axis, the *local* phase flux has *rotational symmetry*. This assumption allows it to be represented by a Legendre expansion only (taking a local reference with its axis along $\vec{J}$ to measure θ) and therefore without the φ-dependent harmonics. Under these conditions, at the Nth order, this "$\mathbf{SP_N}$" approximation involves $N+3$ unknown functions instead of $(N+1)^2$ for the standard $\mathbf{P_N}$ approximation; for example, 12 instead of 100 for $N = 9$.

The advantage of the $\mathbf{SP_N}$ approximation is its ability to improve the diffusion approximation at little additional cost, by taking, for example, $N = 3$ or 5. The disadvantage is that the solution does not converge towards the exact solution when N tends to infinity: adopting very high values of N brings only an illusory improvement, and does not allow the error to be evaluated (to do this, it is necessary to perform an "exact" calculation, for example a complete $\mathbf{P_N}$ approximation).

14.4.5. Method of discrete ordinates

As we saw in § 6.2.1, there are two main types of method used to represent functions by a finite number of numerical values: discretisation, and series representation. Where functions of the variable $\vec{\Omega}$ are concerned, the method of spherical harmonics illustrates the series representation; the method of "discrete ordinates" illustrates the concept of discretisation (here, "ordinates" refers to the variable $\vec{\Omega}$).

The difficulty in discretising the variable $\vec{\Omega}$, i.e. the point on a unit sphere, is obviously caused by the curvature: a finite number of points and associated area elements on the sphere must be distributed as uniformly as possible. The most frequently used technique is illustrated on the diagrams in Figure 14.7. This technique can be improved, as is discussed below. To construct these "$\mathbf{S_N}$" diagrams, we start by cutting up the sphere into N bands delineated by circles that are parallel to the equator at regularly spaced colatitudes, i.e. multiples of π/N. Then, from the north pole down to the equator, these bands are cut up, from the meridian of origin, by meridian segments into 4, 8, 12, etc. identical trapezoidal elements; the southern hemisphere is cut up symmetrically from the south pole. The "discrete ordinates" are the directions $\vec{\Omega}_n$ associated with the points placed at the centres of the mesh elements; the corresponding weights are the mesh element areas normalised to 4π.

Discrete ordinates $\vec{\Omega}_n$ on the equator should be avoided, because the value $\mu = \cos\theta = 0$ could cause some difficulties for the numerical processing; that is why an even value of N is always used.

[47] Example: processing of core-reflector or standard assembly-plutonium assembly interface transients.

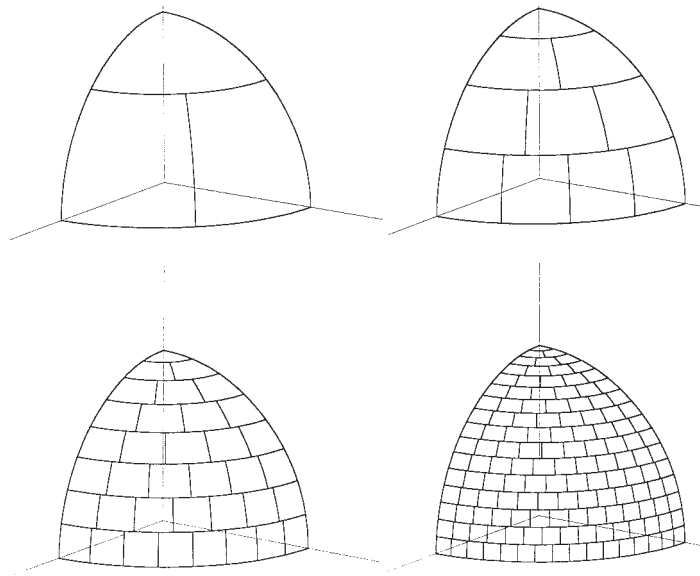


Figure 14.7. Representation on an octant of meshes S_4, S_8, S_{16} and S_{32} (24, 80, 288 and 1088 mesh elements respectively, therefore discrete ordinates).

A first possible way to improve this meshing consists of replacing the regular latitude divisions by a discretisation of the variable μ along the Gauss points: for a given *N* and with the associated Gauss weights, these values lead to the best possible quadrature formula in μ. The longitudinal discretisation is performed in the same way. It can be shown that, for a problem that is dependent on μ only, the $\mathbf{S_N}$-Gauss and $\mathbf{P_{N-1}}$ approximations are rigorously equivalent.

Another possible improvement, but one which is incompatible with the previous one, consists of seeking a partitioning that is symmetric with respect to the three Cartesian axes[48], which is not the case for the previous partitionings because they give a special role to the $\vec{z}$ axis. A symmetric meshing can be of interest if there is no direction that plays a special part in the problem, but this is not usually the case in neutron physics, where the $\vec{z}$ axis along which the coolant flows[49] is different from the perpendicular axes.

14.4.6. Ray effects

An artefact related to the method of discrete ordinates, known as the "ray effect", is illustrated below (Figure 14.8) for an extreme example.

For a two-dimensional case, which is easier to represent, we have considered the problem of a point source in a purely absorbent medium. The arrows represent the directions of the discrete ordinates, and the squares represent the meshing of the spatial discretisation. Because neutrons are obliged to travel along the discrete directions, we note that only the

[48] This is shown to be possible; there is even a degree of freedom.
[49] Generally vertical, but sometimes horizontal as in *CANDU* reactors.

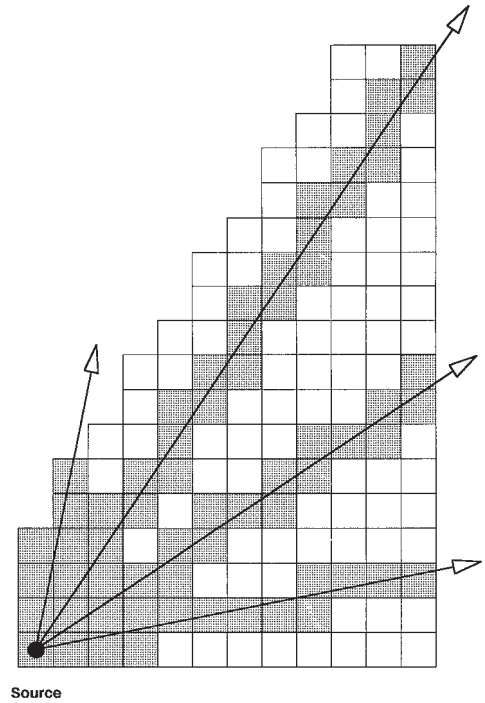


Figure 14.8. Example of the ray effect.

shaded mesh elements will "see" a certain neutron flux, since the others cannot receive any neutrons. The resulting lines are clearly visible on the diagram.

In practical cases, the artefact is never so clear, since the sources are spread out and there is scattering, but it can still be identified. The only way to improve this situation is to refine the angular meshing.

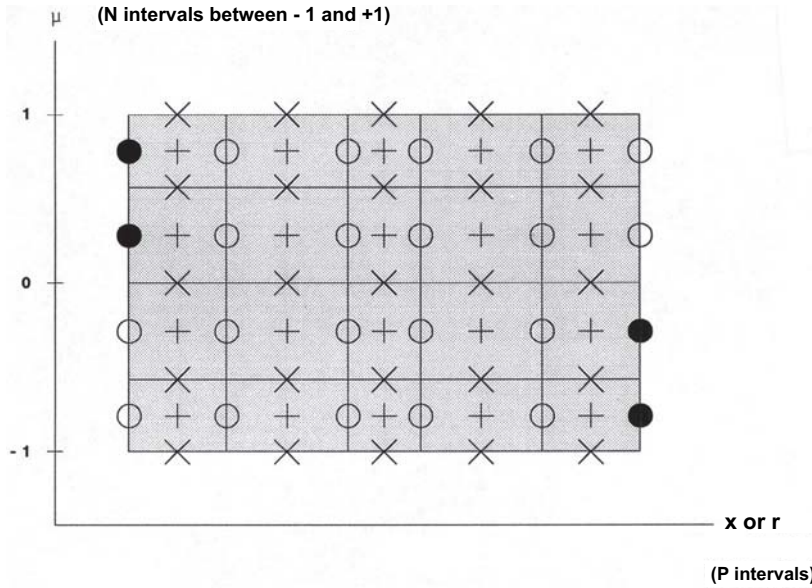
14.4.7. Handling the space variable

In any phase flux calculation, the handling of the space variable $\vec{r}$ is always associated with the handling of the angular variable $\vec{\Omega}$. If it was decided to handle the angular variable with discrete ordinates, there are many possible variants for processing the space variable. The most classic method is known as the "diamond scheme". More recently, several other methods have been suggested.

The diamond scheme[50] is illustrated in Figure 14.9 for a two-variable case only: a space variable x or r, and an angular variable μ[51].

[50] The term "$\mathbf{S_N}$ method" is often associated with "discrete ordinates + diamond scheme"; here we shall use the term "$\mathbf{S_N}$ method" to refer solely to the processing of angular variables by "discrete ordinates".

[51] Note that problems with a cylindrical symmetry, and of course problems with two or three space variables, must involve **both** angular variables.



$$2\Phi(M) = \Phi(A) + \Phi(B) = \Phi(C) + \Phi(D)$$

Figure 14.9. Identification of the unknowns in the S_N + finite difference method.

During the iterative process, the equation to be processed at each step of the "internal" iteration is, for example for a problem that depends on x and μ:

$$\mu \frac{\partial \Phi(x, \mu)}{\partial x} + \Sigma(x)\Phi(x, \mu) = E(x, \mu), \tag{14.70}$$

where E is known (emissions calculated using the flux estimated at the previous iteration).

The angular variable μ was discretised according to N values μ_n (4 on the diagram, shown by horizontal lines of "circles"). In an analogous way, the space variable is discretised in P intervals (5 on the diagram).

The above neutron physics equation is written for each "box" centre identified by the + sign and the letter M; the derivative with respect to x or r is replaced by the finite difference

quotient:

$$\frac{\Phi(D) - \Phi(C)}{x_D - x_C}, \quad \text{or:} \quad \frac{\Phi(D) - \Phi(C)}{r_D - r_C}, \tag{14.71}$$

and, similarly, the derivative with respect to μ (which does not appear in the above equation, but would enter into the similar equation with r because of the curvature) is approximated by: $[\Phi(B) - \Phi(A)]/(\mu_B - \mu_A)$.

Because there are more unknowns — all the circles, + signs and × symbols — than equations — one per + sign — the "diamond" equations are used in addition (refer to the bottom of Figure 14.9), which is equivalent to stating that the flux variation in a "box" is *assumed to be linear with respect to each of the variables*.

Under these conditions, the equation can be solved very quickly (inversion of the advection operator giving Φ if E is known) because the unknowns can be calculated from one term to the next, working line by line, i.e. with fixed μ, from the point of entry of the neutrons where the phase flux is known. That is the boundary condition of the problem (this input flux is often assumed to be zero)[52]. Note that these known values (black circles on Figure 14.9) are located to the left if μ is positive, and to the right if μ is negative. The line by line process is therefore carried out from left to right if μ is positive, and from right to left if μ is negative[53].

The method can be extended to problems with a greater number of variables, where the rectangular "boxes" become 3, 4, or 5-dimensional parallelepiped boxes, and the parallelograms *ABCD* become true "diamonds", hence the name of the method.

The disadvantage of the diamond scheme is that it can lead to negative flux values. This problem is solved by replacing an equation of the following type:

$$\Phi(M) = \frac{1}{2}\Phi(C) + \frac{1}{2}\Phi(D),$$

with:

$$\Phi(M) = \alpha\Phi(C) + (1 - \alpha)\Phi(D), \tag{14.72}$$

and by choosing α suitably to eliminate the problem. This inevitably leads to the iterations converging more slowly.

It is worth mentioning some of the other methods that use discrete ordinates:

– *Finite element*-type methods (the principle is explained in Chapter 6);

– "*Nodal*" methods. Their principle is as follows for the example of the planar geometry problem and a linear approximation in x:

$$\mu\frac{\partial\Phi(x, \mu)}{\partial x} + \Sigma(x)\Phi(x, \mu) = E(x, \mu). \tag{14.73}$$

- The equation is written for a direction μ_n and a homogeneous spatial mesh element, assuming that $E(x, \mu_n)$ was previously approximated by an expression that is linear in x:

$$\mu\frac{\partial\Phi(x, \mu_n)}{\partial x} + \Sigma\Phi(x, \mu_n) = E_0 + E_1 x. \tag{14.74}$$

[52] The boundary condition is often also a reflection condition, in which case an iteration is necessary.

[53] To be precise, it should be noted that there are only $3PN$ equations for $3PN + P$ unknowns; an additional assumption must therefore be made to obtain the P missing equations.

- This equation is integrated analytically by x.
- The integration constant is calculated from the incoming flux, which is known because it is the flux leaving the previous mesh element (or the boundary condition).
- The outgoing flux is deduced from this.
- By projection on the polynomials 1 and x, we approximate the flux that was calculated in the mesh element with a linear expression $\Phi_0 + \Phi_1 x$.
- This linear approximation is used to calculate the linear approximation $E_0 + E_1 x$ of $E(x, \mu)$, which will be used for the next iteration;

– The so-called *"characteristics"* methods. These are similar in principle to nodal methods, but instead of integrating the neutron physics equation along the directions of the coordinate axes, we integrate along the direction $\vec{\Omega}_n$ of neutrons travelling parallel to the discrete ordinate under consideration. These methods are of particular interest in dealing with complicated geometries.

The calculation is performed by iteration, as with all numerical methods for solving the Boltzmann equation:

- In a given spatial mesh element, where the right-hand side E is assumed to be known, the flux Φ is calculated analytically along $\vec{\Omega}_n$ according to the abscissa s on the characteristic using:

$$\text{div}\left[\vec{\Omega}_n \Phi(\vec{r}, \vec{\Omega}_n)\right] + \Sigma\Phi(\vec{r}, \vec{\Omega}_n) = E(\vec{r}, \vec{\Omega}_n). \tag{14.75}$$

The integration constant is determined from the current entering the mesh element along direction Ω_n.

- All other spatial mesh elements are handled in a similar way; the calculation is explicit if the mesh elements are processed according to the path of the neutrons for the direction concerned.
- Using the flux thus obtained, E is re-evaluated. The integrals on the direction are evaluated using the quadrature formula:

$$I = \int_{(4\pi)} F(\vec{\Omega}) d^2\Omega \simeq \sum_n w_n F(\vec{\Omega}_n). \tag{14.76}$$

With respect to space, the function E is approximated by a constant in each mesh element, obtained by taking the average over space of the mesh elements of the functions considered (where appropriate, for Cartesian geometries, a polynomial approximation, first-order at the most, can be performed). The currents leaving the faces of the mesh element are also evaluated in this way (currents entering the next mesh element).

- We recalculate Φ, and then E, and then Φ, and then E, and so on until convergence. In practice, the iterations are separated into internal iterations (handling of scattering in the group) and external iterations (handling of inter-group transfers and fissions).

Finally, note that it is possible to construct a simplified $\mathbf{S_N}$ method, called $\mathbf{SS_N}$, which is similar to the simplified spherical harmonic method; by assuming rotational symmetry of the local phase flux around the direction of the overall current, we can greatly reduce the number of discrete directions to be handled because the azimuth is no longer involved.

14.5. Concept of fundamental mode

14.5.1. Why is the fundamental mode of interest?

The "fundamental mode" is the name given to the neutron physics situation observed in an infinite homogeneous medium or an infinite regular lattice. The symmetry of the system leads to a solution of the Boltzmann equation that is simpler than the solution of a general case. This alone makes it of interest to study the problem, in order to reveal physical or mathematical aspects that can be more or less generalised. More specifically, the fundamental mode will be introduced very naturally when seeking to simplify the problem of a two-stage reactor calculation: the "mesh", handled as finely as possible, and the whole core, handled with a simpler model that is adjusted according to the fine mesh calculation.

For the elementary mesh calculation, the boundary conditions must be specified: the simplest way, even if it is not exactly realistic, is to use a *zero flux derivative*; in other words, as we have seen (§ 14.3.9), we imagine inserting this mesh element in an infinite, regular lattice of identical mesh elements, i.e. we place it in fundamental mode.

In this section, we begin by examining a few simple solutions of the Boltzmann equation in an infinite, homogeneous medium and in monokinetic theory: these will reveal the mathematical nature of the solutions in fundamental mode. We shall then generalise to spectrum theory, and then to the case of the infinite regular lattice.

14.5.2. A few analytical solutions of the Boltzmann equation in monokinetic theory

a) No-absorption case

In monokinetic theory, we consider an infinite, homogeneous medium that is purely scattering, with a given angular scattering distribution. In the absence of a source, we shall look for a solution that depends on space by x only, and therefore depends on the phase by μ only. If we seek this solution in the form of a Legendre expansion (see the equations in § 14.4.2), we note that only the coefficients Φ_0 and Φ_1 are nonzero; the phase flux has the following form:

$$\Phi(x, \mu) = A \left(x - \alpha - \frac{\mu}{\Sigma_{tr}} \right), \tag{14.77}$$

where A and α are constants. This solution is obviously physically acceptable only in the area of space where the flux is positive. It assumes sources at infinity, either to the right or to the left according to the sign of A.

It is remarkable that the Legendre expansion of the flux involves only two terms, even if the scattering cross-section involves all of the terms.

We also note that the integrated flux is:

$$\Phi(x) = 2A(x - \alpha), \tag{14.78}$$

and the integrated current is (directed along the $\vec{x}$ axis):

$$J(x) = -\frac{2A}{3\Sigma_{tr}}, \tag{14.79}$$

and therefore that these parameters are related by Fick's law with the following scattering coefficient:

$$D = \frac{1}{3\Sigma_{tr}}\cdot \tag{14.80}$$

b) Linearly anisotropic scattering distribution; absorbent medium

Still in monokinetic theory, we now assume the homogeneous material to be scattering and absorbent and, as before, we look for a solution without a source at finite distance that is dependent only on x and μ.

By direct examination of either the Boltzmann equation for this case or the system of equations $\mathbf{P_N}$, we see that the flux can only depend on x by an exponential distribution, either increasing or decreasing, according to whether the sources are at infinity to the right or to the left. Let us take the latter case as an example:

$$\Phi(x, \mu) = \varphi(\mu)e^{-\kappa x}.$$

The constant κ and the phase distribution $\varphi(\mu)$ must be determined by the Boltzmann equation.

The equations $\mathbf{P_N}$ could be used, but this would require manipulating an algebraic system of infinite dimension (whatever the scattering distribution). If the scattering distribution is represented by a finite number of terms (expansion to order K), it is simpler to work directly on the integral/differential Boltzmann equation in the form shown in § 14.4.2, eq. (14.62), which is written out with a finite sum. After substituting in the factorised form of the phase flux, and then simplifying by $e^{-\kappa x}$, it gives:

$$-\kappa\mu\varphi(\mu) + \Sigma\varphi(\mu) = \sum_{k=0}^{k} \frac{2k+1}{2}\Sigma_{s,k}P_k(\mu)\int_{-1}^{+1}\varphi(\mu')P_k(\mu')d\mu'. \tag{14.81}$$

If we divide this equation by $\Sigma - \kappa\mu$, multiply it by $P_l(\mu)$ (for values of l from 0 to K) and integrate from -1 to $+1$, we obtain a linear system of $K + 1$ equations giving the $K + 1$ unknown integrals:

$$\varphi_k = \frac{2k+1}{2}\int_{-1}^{+1}\varphi(\mu')P_k(\mu')d\mu', \tag{14.82}$$

appearing on the right-hand side. This system involves the following coefficients:

$$G_{kl} = \int_{-1}^{+1}\frac{P_k(\mu)P_l(\mu)}{\Sigma - \kappa\mu}d\mu, \tag{14.83}$$

which are calculated analytically:

$$G_{00} = \frac{1}{\kappa} \ln \frac{\Sigma + \kappa}{\Sigma - \kappa}, \quad G_{01} = G_{10} = \frac{1}{\kappa} G_{00} - \frac{2}{\kappa}, \quad G_{11} = \frac{\Sigma^2}{\kappa^2} G_{00} - \frac{2\Sigma}{\kappa^2}, \tag{14.84}$$

and so on. For example, for $K = 1$, i.e. the so-called $\mathbf{B_1}$ approximation, the system is written as:

$$\begin{aligned} 2\varphi_0 &= \Sigma_{s,0} G_{00} \varphi_0 + \Sigma_{s,1} G_{01} \varphi_1, \\ \tfrac{2}{3}\varphi_1 &= \Sigma_{s,0} G_{10} \varphi_0 + \Sigma_{s,1} G_{11} \varphi_1. \end{aligned} \tag{14.85}$$

This system is homogeneous; the compatibility condition (zero determinant) gives the value of the constant κ; this is the solution of the following equation:

$$\frac{\kappa[\kappa^2 + 3\bar{\mu} c(1-c)\Sigma^2]}{c\Sigma[\kappa^2 + 3\bar{\mu}(1-c)\Sigma^2]} = \frac{1}{2} \ln \frac{\Sigma + \kappa}{\Sigma - \kappa} = \operatorname{argth} \frac{\kappa}{\Sigma}, \tag{14.86}$$

with $c = \Sigma_s/\Sigma$, called the *"number of secondaries per collision"*. The constant κ is called the "*relaxation constant"* and its inverse $1/\kappa$ is the *relaxation length*.

c) Linearly anisotropic scattering distribution; multiplying medium

If the medium is multiplying, but remaining in monokinetic theory (assuming therefore that neutrons emitted by fission are at the same energy as that where neutrons are scattered and absorbed), a similar approach can be used by adding the cross-section of production by fission, $\nu\Sigma_f$, to the scattering cross-section Σ_s. We now set:

$$c = \frac{\nu\Sigma_f + \Sigma_s}{\Sigma}. \tag{14.87}$$

– If c is less than 1, all the above formulae apply exactly as they are[54].

– If c is greater than 1, i.e. if production wins out over absorption (k_∞ greater than 1), the constant κ becomes purely imaginary. We therefore set $\kappa = i\chi$ and look for a flux of the following form:

$$\Phi(x, \mu) = \varphi(\mu) e^{-i\chi x}.$$

The calculations are similar if we set:

$$G_{kl} = \int_{-1}^{+1} \frac{P_k(\mu) P_l(\mu)}{\Sigma - i\chi\mu} d\mu, \tag{14.88}$$

i.e.:

$$\begin{aligned} &G_{00} = \tfrac{2\xi}{\chi}, \quad G_{01} = G_{10} = \tfrac{2i(1-\xi)}{\chi}, \quad G_{11} = \tfrac{2\Sigma(1-\xi)}{\chi^2}, \\ &\text{with} \quad \xi = \tfrac{\Sigma}{\chi} \operatorname{Arctg} \tfrac{\chi}{\Sigma}. \end{aligned} \tag{14.89}$$

For example, for $K = 1$ (linearly anisotropic scattering), the relaxation constant is given by the following equation:

$$\frac{\chi[\chi^2 + 3\bar{\mu} c(c-1)\Sigma^2]}{c\Sigma[\chi^2 + 3\bar{\mu}(c-1)\Sigma^2]} = \operatorname{Arctg} \frac{\chi}{\Sigma}. \tag{14.90}$$

[54] In the formulae, $\bar{\mu}$ is now the average cosine of the deflection angle of **all** re-emitted neutrons, whether re-emitted by scattering or by fission.

d) Linear combinations of the above solutions

If the medium in which the neutrons scatter is isotropic, which it is in most media, the $\vec{x}$ axis that we chose plays no special role.

In the above formulae, we can therefore replace:

$$\Phi(x, \mu) = \varphi(\mu)e^{-\kappa x} \quad \text{or} \quad \Phi(x, \mu) = \varphi(\mu)e^{-i\chi x},$$

by:

$$\Phi(\vec{r}, \vec{\Omega}) = \varphi(\mu)e^{-\kappa \vec{u}\cdot\vec{r}} \quad \text{or} \quad \Phi(\vec{r}, \vec{\Omega}) = \varphi(\mu)e^{-i\chi \vec{\mu}\cdot\vec{r}}, \tag{14.91}$$

where $\vec{u}$ is any unit vector in space, and μ is the scalar product $\vec{u} \cdot \vec{\Omega}$.

Moreover, because neutron physics is linear, any linear combination of the above functions with a weight $\Delta(\vec{u})$:

$$\Phi(\vec{r}, \vec{\Omega}) = \int_{(4\pi)} \Delta(\vec{u})\varphi(\mu)e^{-\kappa \vec{u}\cdot\vec{r}} d^2u, \tag{14.92}$$

or:

$$\Phi(\vec{r}, \vec{\Omega}) = \int_{(4\pi)} \Delta(\vec{u})\varphi(\mu)e^{-i\chi \vec{u}\cdot\vec{r}} d^2u, \tag{14.93}$$

is also a solution of the Boltzmann equation.

14.5.3. Concept of fundamental mode in a homogeneous medium in monokinetic theory

This solution, which appears in the infinite homogeneous and, strictly speaking, multiplying (k_∞ greater than 1) medium, is called the "fundamental mode". The equations we have just seen show that it can also be considered in a submultiplying medium or non-multiplying medium provided that sources are placed at infinity to "feed" the exponential.

This fundamental mode can be generalised:

- to exponential functions $e^{-i\vec{b}\cdot\vec{r}}$ that are space-dependent *via* any vector $\vec{b}$; in practice, the real values of this vector are the most interesting ones to consider, but the extension to complex vectors is possible[55];
- to the general Boltzmann equation, i.e. to a spectrum theory;
- to the case of the infinite regular lattice.

We shall examine each of these three points in turn.

In monokinetic theory and in an infinite and homogeneous medium, let the source be isotropic and of the following form:

$$S(\vec{r}) = se^{-i\vec{b}\cdot\vec{r}}. \tag{14.94}$$

[55] The notation b is generally chosen for the argument of Fourier transforms. It is used in discussions of the fundamental mode because there is a close connection between this mode and the Fourier transform of the kernel of the Boltzmann equation, i.e. its solution for a point source in an infinite homogeneous medium.

By substituting it into the Boltzmann equation:

$$\text{div}\left[\vec{\Omega}\Phi(\vec{r},\vec{\Omega})\right] + \Sigma\Phi(\vec{r},\vec{\Omega}) = \int_{(4\pi)} \Sigma_s(\vec{\Omega}' \to \vec{\Omega})\Phi(\vec{r},\vec{\Omega}')d^2\Omega' + S(\vec{r}), \tag{14.95}$$

we note that the flux must be of the form

$$\Phi(\vec{r},\mu) = \varphi(\mu)e^{-i\vec{b}\cdot\vec{r}}, \tag{14.96}$$

with $\mu = (\vec{b}/b)\cdot\vec{\Omega}$ and:

$$-ib\mu\varphi(\mu) + \Sigma\varphi(\mu) = \int_{-1}^{+1} \Sigma_s(\mu' \to \mu)\varphi(\mu')d\mu' + s, \tag{14.97}$$

If the source comes from fission, it is expressed as a function of the flux:

$$S(\vec{r}) = \nu\Sigma_f\Phi(\vec{r}) \quad \text{with:} \quad \Phi(\vec{r}) = \int_{(4\pi)} \Phi(\vec{r},\vec{\Omega})d^2\Omega. \tag{14.98}$$

Therefore:

$$s = \nu\Sigma_f\varphi \quad \text{with:} \quad \varphi = \int_{-1}^{+1} \varphi(\mu)d\mu. \tag{14.99}$$

It is convenient to study this mode in the context of the so-called $\mathbf{B_K}$ approximation, which involves expanding the scattering angular cross-section to the order K in Legendre polynomials (bearing in mind that no additional approximation concerning the phase flux is applied). For example, approximation $\mathbf{B_1}$, the flux and the source are related by the following equations:

$$\begin{aligned} -2\varphi_0 + \Sigma_{s,0}G_{00}\varphi_0 + \Sigma_{s,1}G_{01}\varphi_1 + G_{00}\tfrac{s}{2} = 0, \\ -\tfrac{2}{3}\varphi_1 + \Sigma_{s,0}G_{10}\varphi_0 + \Sigma_{s,1}G_{11}\varphi_1 + G_{10}\tfrac{s}{2} = 0, \end{aligned} \tag{14.100}$$

with:

$$s = 2\nu\Sigma_f\varphi_0 \quad \text{since:} \quad \varphi = 2\varphi_0.$$

The coefficients G_{kl} are those written above in Paragraph **c**, replacing χ with b.

We have mentioned that, *a priori*, $\vec{b}$ is any vector; however, if we substitute the expression for the source s into the flux equations, we see that the system becomes homogeneous and that, therefore, there is no non-trivial solution unless its determinant is zero, i.e. unless *the modulus b of the vector* $\vec{b}$ *is equal to the relaxation constant* χ which is a solution of the equation written in Paragraph **c** above. Physically, this expresses the concept of a *critical condition*.

Linear combinations of solutions of this type with vectors $\vec{b}$ having the same modulus b are still solutions of the Boltzmann equation, and can therefore still be considered as "fundamental mode":

$$\begin{aligned} S(\vec{r}) &= \int_{(4\pi)} \Delta(\vec{u})se^{-ib\vec{u}\cdot\vec{r}}d^2u, \\ \Phi(\vec{r},\vec{\Omega}) &= \int_{(4\pi)} \Delta(\vec{u})\varphi(\mu)e^{-ib\vec{u}\cdot\vec{r}}d^2u \quad \text{with:} \quad \mu = \vec{u}\cdot\vec{\Omega}. \end{aligned} \tag{14.101}$$

They correspond to a critical situation if and only if b is equal to χ.

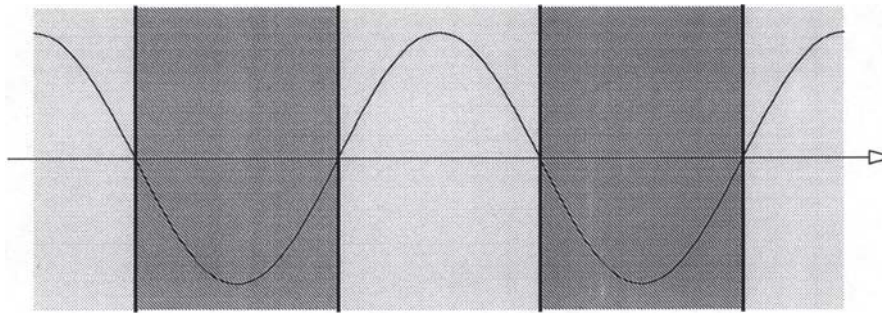


Figure 14.10. Image piles of a bare homogeneous pile, here in the form of an infinite plate. The curve represents the flux as a function of the abscissa *x*.

14.5.4. Physical interpretation of the fundamental mode

These equations might satisfy mathematicians because they satisfy the Boltzmann equation, but they can cause puzzlement to the poor physicist who is looking for a flux, which is by its nature both real and positive. They can represent a physical situation:

a/ If we select linear combinations that lead to real functions,

b/ If we restrict them to a region where they remain positive or zero.

For example, by combining the exponential functions e^{-ibx} and e^{+ibx} with the same weight, 1/2, we obtain $\cos(bx)$. If considered in the interval $-\pi/2b < x < +\pi/2b$, $\cos(bx)$ represents the flux that would be obtained in a homogeneous reactor in the shape of a plate bounded by these two planes, and therefore of thickness π/b, including the extrapolation distance. By other linear combinations it would be possible to find the flux for other pile shapes; for example: parallelepiped, cylinder, sphere, etc.

The fundamental mode therefore generalises, by analytical extension of the functions over all space, neutron physics situations encountered in bare homogeneous piles (including the extrapolation distance in the dimensions).

If the medium is multiplying, the curvature induced by a nonzero value of b simulates the leaks in an actual pile. For example, with the function $\cos(bx)$, fictitious (negative) piles can be seen to appear on either side of the actual pile, in plates where the cosine is negative. These negative piles are adjacent to positive piles, etc. (Figure 14.10). "Negative" neutrons emitted by the "negative" image piles can migrate to the "positive" piles and annihilate the "positive" neutrons emitted by the positive piles, and vice-versa. This mechanism provides a strictly equivalent replacement for leaks *via* the surface of a real pile of finite dimensions.

14.5.5. Existence and calculation of the leakage coefficient

The fundamental mode is characterised by a very interesting property: proportionality at every point between the current (integrated over the phases) and the flux gradient (integrated over the phases). In other words, Fick's law, which we proposed and attempted to

justify in Chapter 5, to simplify the Boltzmann equation:

$$\vec{J}(\vec{r}) = -D\overrightarrow{grad}\,\Phi(\vec{r}), \tag{14.102}$$

becomes rigorously satisfied for this fundamental mode. In the first instance, we shall demonstrate the existence of this law. In the second instance, we shall examine the calculation of the coefficient of proportionality, D.

Assume the phase flux has the following form:

$$\Phi(\vec{r}, \vec{\Omega}) = \varphi(\mu)e^{-ib\vec{u}\cdot\vec{r}}, \tag{14.103}$$

with $\mu = \vec{u}\cdot\vec{\Omega}$. On the one hand, we conclude that:

$$\Phi(\vec{r}) = e^{-ib\vec{u}\cdot\vec{r}}\int_{-1}^{+1}\varphi(\mu)d\mu, \tag{14.104}$$

$$\overrightarrow{grad}\Phi(\vec{r}) = -ib\vec{u}e^{-ib\vec{u}\cdot\vec{r}}\int_{-1}^{+1}\varphi(\mu)d\mu, \tag{14.105}$$

and, on the other hand, since the phase current is the product of phase flux by $\vec{\Omega}$, that:

$$\vec{J}(\vec{r}) = \int_{(4\pi)}\vec{\Omega}\Phi(\vec{r}, \vec{\Omega})d^2\Omega = \vec{u}e^{-ib\vec{u}\cdot\vec{r}}\int_{-1}^{+1}\mu\varphi(\mu)d\mu, \tag{14.106}$$

(Only the integral along the $\vec{u}$ axis is nonzero, for symmetry reasons.) Note that these two vectors are in fact proportional at every point.

This remains true for the general fundamental mode, i.e. if we take any combination of functions of this type with various vectors $\vec{u}$ and weights $\Delta(\vec{u})$, but the same modulus b. Indeed, $\varphi(\mu)$ depends on the modulus of $\vec{b}$ *via* the coefficient $ib\mu$ appearing in the equation that governs this function and the coefficients G_{kl} that are introduced in the handling of $\mathbf{B_K}$, but not its direction[56].

These formulae also show that the diffusion coefficient is given by the following formula:

$$D = \frac{\int_{-1}^{+1}\mu\varphi(\mu)d\mu}{ib\int_{-1}^{+1}\varphi(\mu)d\mu}. \tag{14.107}$$

If we break down $\varphi(\mu)$ into Legendre polynomials:

$$\varphi(\mu) = \sum_{k=0}^{\infty}\varphi_k P_k(\mu) \quad \text{with:} \quad \varphi_k = \frac{2k+1}{2}\int_{-1}^{+1}\varphi(\mu')P_k(\mu')d\mu', \tag{14.108}$$

and if we note that $P_0(\mu) = 1$ and that $P_1(\mu) = \mu$, we can also write:

$$D = \frac{\varphi_1}{3ib\varphi_0}. \tag{14.109}$$

[56] If the medium were anisotropic, $\varphi(\mu)$ would also depend on $\vec{u}$ and Fick's law would no longer be exactly satisfied for linear combinations of exponential modes.

Note that the diffusion coefficient defined in this way in fundamental mode is *dependent*[57] on the value of the parameter b. That is why this coefficient $D(b)$ appearing in the fundamental mode is sometimes called the *leakage coefficient*[58] to distinguish it from the usual diffusion coefficient of Fick's phenomenological law.

For example, in the $\mathbf{B_1}$ approximation, the system of two equations (14.100) gives the two coefficients φ_0 and φ_1 (both proportional to s), giving D. After performing all necessary calculations, we obtain:

$$D = \frac{1}{3(\gamma\Sigma - \Sigma_{s,1})}, \tag{14.110}$$

with:

$$\gamma = \frac{1}{3}\frac{\frac{b}{\Sigma}\text{Arctg}\frac{b}{\Sigma}}{1 - \frac{\Sigma}{b}\text{Arctg}\frac{b}{\Sigma}} = 1 + \frac{4}{15}\left(\frac{b}{\Sigma}\right)^2 + \cdots \tag{14.111}$$

Note that, at the limit $b \to 0$, i.e. a pile whose dimensions tend to infinity, the coefficient γ tends to 1 and the diffusion coefficient tends to the usual value of $1/3\Sigma_{tr}$.

14.5.6. Balance in fundamental mode

Returning to the first of the $\mathbf{B_K}$ equations, the one expressing the neutron balance for all phases[59]:

$$-2\varphi_0 + \Sigma_{s,0}G_{00}\varphi_0 + \Sigma_{s,1}G_{01}\varphi_1 + G_{00}\frac{s}{2} = 0. \tag{14.112}$$

If we substitute in $\varphi_1 = 3ib\varphi_0 D$ and then perform certain algebraic manipulations, we obtain:

$$-Db^2\varphi - \Sigma_a\varphi + s = 0.$$

Here we have the equation expressing the neutron balance of a bare homogeneous pile dealt with using one-group theory (see Chapter 6). This observation again shows the complete equivalence between the bare homogeneous pile problem (with the neglected extrapolation distance) and the fundamental mode problem. The only detail that this latter approach changes, is to replace the constant D with a function $D(b)$ that depends on the modulus of the vector $\vec{b}$.

Even if $\vec{b}$ can be any vector *a priori*, in practice we generally take the value that lets us "loop" the neutron balance in a chain, i.e. such as:

$$s = \nu\Sigma_f\varphi.$$

This value is therefore given by the following equation:

$$Db^2\varphi + \Sigma_a\varphi = \nu\Sigma_f\varphi,$$

i.e.:

$$Db^2 + \Sigma_a = \nu\Sigma_f,$$

[57] This is a weak dependence in practice.
[58] It refers to leaks in the sense of "image piles".
[59] This equation is the projection on P_0 of the equation giving the phase flux, and thus the integral of this equation over all neutron directions.

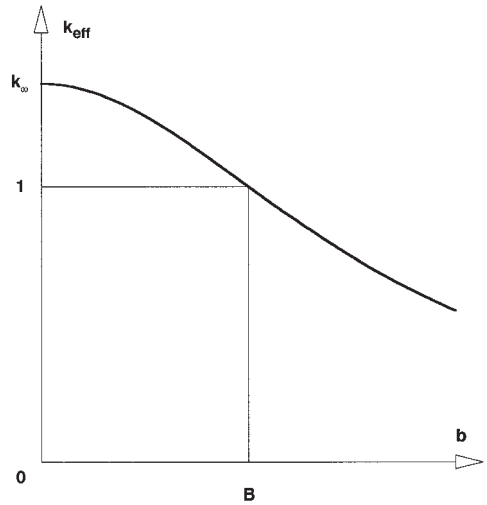


Figure 14.11. Critical value *B* of the parameter *b*, square root of the material buckling.

(where the diffusion coefficient depends on *b*). This *critical condition* expresses the equality between production and elimination (leakage and absorption) that ensures the existence of a *steady-state mode*. This is usually written in the following form:

$$k_{\text{eff}} = \frac{\nu\Sigma_f}{\Sigma_a + Db^2} = 1, \tag{14.113}$$

or

$$k_{\text{eff}} = \frac{k^*}{1 + M^{*2}b^2} = 1, \tag{14.114}$$

by setting:

$$k^* = \frac{\nu\Sigma_f}{\Sigma_a}, \quad \text{and:} \quad M^{*2} = \frac{D}{\Sigma_a}\cdot \tag{14.115}$$

These expressions are reminiscent of those we write in "one group-diffusion theory". The factor k^* is here identified with the usual factor k_∞ (production by absorption in the absence of leakage), but this will no longer hold true, as we shall see, in spectrum theory, where k^* becomes a function of b; the area M^{*2} — which depends on b even in monokinetic theory — is similar to the migration area.

The value of b that achieves criticality (see Figure 14.11) is generally written as B (in monokinetic theory it is the relaxation constant χ for the multiplying medium that we introduced and calculated below, § 14.5.2, in theory $\mathbf{B_1}$).

The square B^2 of this parameter generalises the concept of "material buckling" (§ 6.1.2). Note that b^2 is a "geometric buckling", since:

$$\Delta e^{-i\vec{b}\cdot\vec{r}} = -b^2 e^{-i\vec{b}\cdot\vec{r}}.$$

The critical condition in fundamental mode can therefore be written, as for a bare homogeneous pile, in the following form:

$$\textit{material buckling} = \textit{geometric buckling}$$

14.5.7. Generalisation to the spectrum case

All of the results seen above and the proofs used to establish them remain practically unchanged when going from a monokinetic theory to a spectrum theory. The essential points can be summarised using, for example, the variable v to describe the spectrum:

– if the neutron source is an exponential:

$$S(\vec{r}) = s\mathrm{e}^{-i\vec{b}\cdot\vec{r}}, \tag{14.116}$$

the same applies to the flux, which thus appears in *factorised* form:

$$\Phi(\vec{r}, v, \mu) = \varphi(v, \mu)\mathrm{e}^{-i\vec{b}\cdot\vec{r}}, \tag{14.117}$$

with $\mu = \vec{b} \cdot \vec{\Omega}$;

– the spectral and angular part of the flux is obtained by substituting these expressions into the Boltzmann equation; the exponentials representing the behaviour in space are simplified:

$$-ib\mu\varphi(v, \mu) + \Sigma(v)\varphi(v, \mu) = \int_0^{\infty} \int_{-1}^{+1} \Sigma_s[(v', \mu') \rightarrow (v, \mu)]\varphi(v', \mu')dv'\, d\mu' + s\chi(v); \tag{14.118}$$

– if the source is from fissions, it can be expressed as a function of the flux:

$$S(\vec{r}) = \int_0^{\infty} \nu\Sigma_f(v)\Phi(\vec{r}, v)dv, \tag{14.119}$$

with:

$$\Phi(\vec{r}, v) = \int_{(4\pi)} \Phi(\vec{r}, v, \vec{\Omega})d^2\Omega. \tag{14.120}$$

And therefore:

$$s = \int_0^{\infty} \nu\Sigma_f(v)\varphi(v)dv \quad \text{with:} \quad \varphi(v) = \int_{-1}^{+1} \varphi(v, \mu)d\mu; \tag{14.121}$$

– *Fick's law* is strictly satisfied with a diffusion coefficient that depends not only on v, but also on b. If the medium is isotropic, this result remains valid for combinations of modes with $\vec{b}$ vectors with the same modulus;

– the *flux* integrated over the phases is a solution of the following equation:

$$-D(v)b^2\varphi(v) - \Sigma(v)\varphi(v) + \int_0^{\infty} \Sigma_s(v' \rightarrow v)\varphi(v')dv' + s\chi(v) = 0; \tag{14.122}$$

– it can be established that in the $\mathbf{B_1}$ approximation, the *diffusion coefficient* is itself given by an integral equation:

$$D(v) = \frac{1}{3\gamma(v)\Sigma(v)}\left[1 + 3\int_0^{\infty} \Sigma_{s,1}(v' \rightarrow v)\frac{\varphi(v')}{\varphi(v)}D(v')dv'\right]. \tag{14.123}$$

This integral equation can be treated as a multigroup approximation, like the one giving the flux. Iterations between the two equations (flux and diffusion coefficient) must be performed;

– by integrating the flux equation over all speeds, scattering is simplified between the second and third terms; there remains an equation expressing the overall evaluation in any finite or infinitesimal volume:

$$\int_0^\infty D(v)b^2\varphi(v)dv + \int_0^\infty \Sigma_a(v)\varphi(v)dv = \int_0^\infty \nu\Sigma_f(v)\varphi(v)dv, \tag{14.124}$$

(total production equal to the total number of eliminations by absorption and leakage);

– by setting:

$$k^* = \frac{\int_0^\infty \nu\Sigma_f(v)\varphi(v)dv}{\int_0^\infty \Sigma_a(v)\varphi(v)dv} \quad \text{and:} \quad M^{*2} = \frac{\int_0^\infty D(v)\varphi(v)dv}{\int_0^\infty \Sigma_a(v)\varphi(v)dv}, \tag{14.125}$$

it is possible to write this balance equation in an identical form to the one obtained in monokinetic theory:

$$k_{\text{eff}} = \frac{k^*}{1 + M^{*2}b^2} = 1. \tag{14.126}$$

Note that, now, not only M^{*2} but also k^* are dependent on b, since φ and D are dependent on it:

– we can show that, *when b tends to zero:* **a/** k^* *tends to the multiplication factor in the absence of leakage* k_∞; **b/** M^{*2} *tends to the migration area* M^2, i.e. a sixth of the mean square of the crow-fly distance of neutrons from birth to absorption in the infinite homogeneous medium;

– the concept of material buckling B^2 as a value of b^2 reaching criticality ($k_{\text{eff}} = 1$) remains unchanged.

14.5.8. Concept of fundamental mode in a regular lattice

A fundamental mode does not appear only in infinite homogeneous media, but also in infinite regular lattices. The theory is similar, but more difficult. The essential aspects are as follows:

– for a source of the form $S(\vec{r}) = s(\vec{r})e^{-i\vec{b}\cdot\vec{r}}$ the flux is *factorised* and has the form $\Phi(\vec{r}, v, \vec{\Omega}) = \varphi(\vec{r}, v, \mu)e^{-i\vec{b}\cdot\vec{r}}$; in these expressions, s and φ are *functions with lattice periodicity* with respect to space, meaning that they return to the same value at analogous points of the various mesh elements;

– the functions s and φ have complex values; the real parts of $s(\vec{r})e^{-i\vec{b}\cdot\vec{r}}$ and $\varphi(\vec{r}, v, \mu)e^{-i\vec{b}\cdot\vec{r}}$, when positive, simulate the situation in a pile made up of this lattice. If we set $\varphi = f - ig$, where f and g are real and periodic, the flux appears as the sum of two terms: in each mesh element (assumed to be symmetric), it is the sum of a *symmetric* part $f\cos\vec{b}\cdot\vec{r}$ and an *antisymmetric* part $g\sin\vec{b}\cdot\vec{r}$;

– to calculate the functions f and g, which are also space-dependent, a transport calculation on the mesh scale must be performed. In the APOLLO code, for example, this is done using the method of collision probabilities (only the symmetric term is calculated in this code);

– on a macroscopic scale, a lattice is more or less anisotropic. The same applies to the diffusion coefficient, which is now a *tensor*, not a scalar. A theory $\mathbf{B_K}$ of this tensor is possible, but it would become complicated because transport problems would arise in addition to the aspects already discussed. (In the APOLLO code, only reasonably simplified calculation options are offered.) The material buckling concept also becomes anisotropic.

14.6. Use of Monte Carlo techniques in neutron physics

14.6.1. Outline of the Monte Carlo method

The Monte Carlo method is often used in physics; increasingly so as computing power grows. Methods like Monte Carlo are found to be useful because they can handle problems with few approximations. Their disadvantage is that they require many simulations and therefore use a great deal of machine time: especially when great accuracy is required, because the statistical uncertainty of a result obtained by the Monte Carlo method decreases with the number N of simulations only as an inverse square root (for example, a ten-times increase in accuracy requires 100 times more simulations, and therefore that much more computer time).

The Monte Carlo method takes its name from the fact that it is based on the random selection of random events — an activity for which this city in Monaco is renowned.

The following definition of the Monte Carlo method was stated by Iván Lux and László Koblinger (refer to bibliography):

In all applications of the Monte Carlo Method a stochastic model is constructed in which the expected value of a certain random variable is equivalent to the value of a physical quantity to be determined. This expected value is then estimated by the average of several independent samples representing the random variable introduced above. For the construction of the series of independent samples, random numbers following the distributions of the variable to be estimated are used.

14.6.2. Analogous simulation and non-analogous simulation

We generally draw a distinction between:

– *analogous* simulations, when the stochastic model *copies* the physical phenomenon concerned as closely as possible (e.g. path of a neutron), and

– *non-analogous* simulations otherwise (e.g. calculation of an integral);

– and *intermediate* cases (e.g., calculation of a biological protection with a particle path biasing technique).

The stochastic model is called a *game*. This game is a random process which, when carried out, attributes a value X to a random variable. The value obtained is called the *score*.

If we are examining a physical problem whose solution is characterised by a numerical value Y and we wish to use the Monte Carlo method to solve the problem, we must choose a game and a score such that:

$$E(X) = Y, \tag{14.127}$$

where $E(X)$ denotes the mathematical expectation of the random variable. The value of Y will be estimated by playing many times and taking the arithmetic mean of the scores X obtained. In accordance with the law of large numbers, its value will tend towards the mathematical expectation of this variable.

Buffon's needle is a simple, classic example of a non-analogous simulation. The purpose of this game is to estimate π. It consists of throwing a needle of length b on a parquet floor with slats of width a, and scoring as follows:

– $X = 1$ if the needle cuts across two slats;

– $X = 0$ if the needle rests on only one slat,

and then evaluating the mean value of X after a large number of throws.

It can easily be shown that this stochastic model satisfies the objective; for example, if $a = b$:

$$E(X) = 2/\pi.$$

Although Buffon's game might be very entertaining, it is clearly not very effective[60] at evaluating π.

Another application of the Monte Carlo method is to evaluate an integral:

$$S = \int_{(D)} f(p)dp, \tag{14.128}$$

where D is a multi-dimensional domain, and p is the "point" running in this domain[61]. If we choose a point P at random in D with a normed probability distribution $g(p)\,dp$ (for example, a uniform distribution: $g(p)dp = dp/V$, where V is the volume of D) and if we calculate the random variable $X = f(P)/g(P)$, we immediately see that the mathematical expectation of X is the sought-after integral S:

$$E(X) = \int_{(D)} Xg(p)dp = \int_{(D)} \frac{f(p)}{g(p)} g(p)dp = \int_{(D)} f(p)dp = S. \tag{14.129}$$

Note: Calculation of the variance under the same conditions shows that the *ideal game* is obtained by choosing $g(p)$ equal to $f(p)/S$, because the score is then equal to S irrespective

[60] A well-chosen series expansion, for example, performs far better.

[61] For example, the Monte Carlo method can be used to evaluate the no-collision flux and the associated dose in a given location for a source of ionising radiation; p is then the set of variables "emission point + emission direction + emission energy". Note that, in this context, the simulation is analogous, but this is not necessarily true in general for problems in which the Monte Carlo method is used to calculate integrals.

of the P that is drawn and the variance is zero; but this ideal case is theoretical because it assumes that S is known, i.e. the problem has been solved. This does however illustrate the fact that it is preferable to choose an (integrable) function g that is "similar" to f to reduce the statistical error of the Monte Carlo calculation.

14.6.3. Overview of sampling problems

Whatever the problem being examined, the use of Monte Carlo involves the drawing of one or more random variables according to probability distributions that are given. We use a capital letter, e.g. X, to denote the random variable concerned or the value obtained by drawing. The probability distribution governing this variable will be characterised by the *probability density f (x)* or the *distribution function F(x)*:

$$\begin{aligned} &Pr\{x < X \leqslant x + dx\} = f(x)dx, \\ &Pr\{X \leqslant x\} = F(x), \end{aligned} \tag{14.130}$$

where $Pr\{\ldots\}$ is the probability of the event shown between curly brackets. We can see that the distribution function is the integral of the probability density:

$$\begin{aligned} &F(x) = 0 && (x < a), \\ &F(x) = \int_a^x f(x')dx' && (a \leqslant x \leqslant b), \\ &F(x) = \int_a^b f(x')dx' = 1 && (x > b), \end{aligned} \tag{14.131}$$

where a and b denote the limits between which X can be selected.

In practice, whether a table, a calculator, or a computer is used, it is possible to generate a random variable[62] Ξ that is uniformly distributed[63] between 0 and 1:

$$\begin{aligned} &f(\xi) = 0,\ F(\xi) = 0,\ (\xi < 0), \\ &f(\xi) = 1,\ F(\xi) = \xi,\ (0 \leqslant \xi < 1), \\ &f(\xi) = 0,\ F(\xi) = 1,\ (\xi \geqslant 1). \end{aligned} \tag{14.132}$$

To go from the selection of Ξ to that of a random variable X of density $g(x)$, *we identify the probabilities of events* $\Xi \leqslant \xi$ and $X \leqslant x$, i.e. *the values of the distribution functions*:

$$F(\xi) = \xi = G(x). \tag{14.133}$$

In other words, if the value Ξ was chosen for the variable equidistributed between 0 and 1, we deduce X from this by writing:

$$X = G^{-1}(\Xi), \tag{14.134}$$

where G^{-1} is the inverse function of G.

If this inverse function is simple, this calculation can be performed directly.

[62] This is actually a pseudo-random variable, i.e. one obtained by a perfectly deterministic process but generating numbers with all the properties of a random variable. For example: the decimals of the number π. In practice, we use the remainder of a whole-number division by a carefully-chosen large prime divisor.

[63] We shall assume that 0 can be obtained but that 1 cannot. If necessary, replace ξ by $1 - \xi$ if taking the logarithm, for example; this avoids possibly having to perform computer troubleshooting later on.

– *Example 1:* selection of a longitude Φ distributed isotropically between $-\pi$ and $+\pi$: $\Phi = \pi(2\Xi - 1)$.

– *Example 2 :* selection of an optical path Ω of probability density $e^{-\omega}$ between zero and infinity: $\Omega = -\ln(1 - \Xi)$.

– *Example 3:* selection of a discrete variable k, e.g. of the *k type* of a nuclear reaction, knowing that it took place:

$$\sum_{i=1}^{k-1} \frac{\sigma_i}{\sigma_t} < \Xi \leqslant \sum_{i=1}^{k} \frac{\sigma_i}{\sigma_t}. \tag{14.135}$$

The probability of reaction i is the quotient of the cross-section σ_i of this reaction divided by the total cross-section σ_t; the distribution function of the discrete variable k rises in steps as a function of k. Another, similar, example: determining the element struck by a neutron if the collision took place in a mixture.

If the function G is not a simple analytical function, but has been tabulated, we can return to the previous case in each interval if we assume that the variation is linear between the tabulated points. *Example:* selecting the deflection angle Θ of a scattered neutron from a table of $G(\theta)$ (we generally tabulate the $n + 1$ $\cos\theta_i$ values leading to intervals of equal probability $1/n$).

For certain probability distributions, methods that are more economical in terms of calculation time than the direct determination of G^{-1} have been developed. *Example:* for the variable X governed by the power law:

$$g(x) = (n + 1)x^n, \quad G(x) = x^{n+1},$$

generating Ξ from $n + 1$ draws, and then finding the maximum:

$$X = \max(\Xi_1, \Xi_2, \ldots, \Xi_{n+1}), \tag{14.136}$$

turns out to be more economical than calculating an $(n + 1)^{th}$ root:

$$X = \Xi^{1/(n+1)}.$$

(*Proof:* the probability that X is less than x is the probability that Ξ_1 is less than x, multiplied by the probability that Ξ_2 is less than x,..., multiplied by the probability that Ξ_{n+1} is less than x, i.e., since each of these independent probabilities is equal to x: $x \times x \times \cdots \times x = x^{n+1}$.)

Another example: to select a point in a circle uniformly, it can be more economical to uniformly choose the Cartesian coordinates in the circumscribed square and to reject any points that are outside the circle, rather than selecting the azimuth and the distance to the centre, r, according to a distribution function in r^2.

An analogous principle is seen in the *rejection method,* which can usually be used when g is calculable: Ξ_1 is drawn uniformly between a and b, and then Ξ_2 uniformly between 0 and the value g_{max} that g can reach in the interval $[a, b]$. The selection is accepted if $\Xi_2 < g(\Xi_1)$, and we take $X = \Xi_1$; otherwise, this dual draw is repeated.

(*Proof:* a/ The probability of obtaining Ξ_1 in the interval $]x, x + dx]$ is $dx/(b - a)$; b/ The probability of obtaining X_2 less than $g(x)$ is $g(x)/g_{max}$; c/ By taking the product of these two probabilities and renormalising the distribution thus obtained to 1 to take the success rate into account, we do indeed find the desired distribution $g(x)\,dx$ for the probability of obtaining X between x and $x + dx$.)

14.6.4. Analogous simulation of a neutron path

The path of a neutron from emission to disappearance by absorption in the system or outside (leakage) is a series of *independent random events,* which are either *transport*-type events (travelling through space in a straight line) or *collisions* with an atomic nucleus. The process is *Markovian*[64], which means, in this case, that the event about to occur is dependent only on the current state of the neutron (its position and velocity), and is independent of the details of what occurred before[65].

Figure 14.12, shows how the simulated "life story" of a neutron might look if plotted on a flowchart. In practice, the selection of random variables and the calculations are programmed in a computer code so that many stories — typically, anywhere from a few thousand to a few million — can be simulated before the statistical processing of the results.

In this diagram, the story starts at the "emission" box and continues until the "end of story" box, taking various paths through the chart. A shaded rectangle represents the selection of a random variable. A circle represents a direction imposed according to the result of the selection. A white rectangle represents a calculation.

The source is assumed to be distributed in space, energy, and angle according to given distributions: the flowchart begins with the corresponding selections. The diagram is centred on the selection of the optical path. We examine whether the neutron remains in or leaves the homogeneous medium. If it remains, we deal with the interaction; if it leaves, we see whether the interface it crossed is at the surface of the domain under consideration, or whether it is an internal interface. If the neutron has reached the limit, we evaluate the leak or handle the reflection, according to the chosen distribution, if applicable. If the neutron crosses an internal interface in the domain concerned, we must calculate the trajectory beyond and repeat the test; rather than working with the remainder of the optical path beyond the interface reached, it is simpler (and strictly equivalent given the Markovian nature of the process) to reposition the neutron at the interface with its velocity, and repeat the selection of an optical path as if the point were an emission point. For a collision, the element concerned, and then the reaction concerned, must be defined by random selection. In the case of absorption, the story is brought to an end. In the event of scattering, we must define whether it is elastic or inelastic (and, in this case, choose the excitation energy), randomly select both scattering angles and, finally, calculation the post-collision energy using the laws of conservation of momentum and energy.

14.6.5. Estimating the multiplication factor

In problems where neutrons are emitted by fission, the source is unknown but results from the flux. Moreover, if the calculation is performed at steady state, a critical parameter must be introduced. In general, the effective multiplication factor k_{eff} is used. This is defined as the number by which the fission products must be divided to achieve system criticality.

These two aspects require an iterative calculation:

$$S^{(0)} \rightarrow \Phi^{(0)} \rightarrow S^{(1)} \rightarrow \Phi^{(1)} \rightarrow S^{(2)} \rightarrow \Phi^{(2)} \rightarrow \cdots$$

[64] Andrei Andreyevich Markov, Russian mathematician (1856–1922).

[65] In more descriptive terms: as the neutron goes about living its life, it forgets its past and is only aware of its present state.

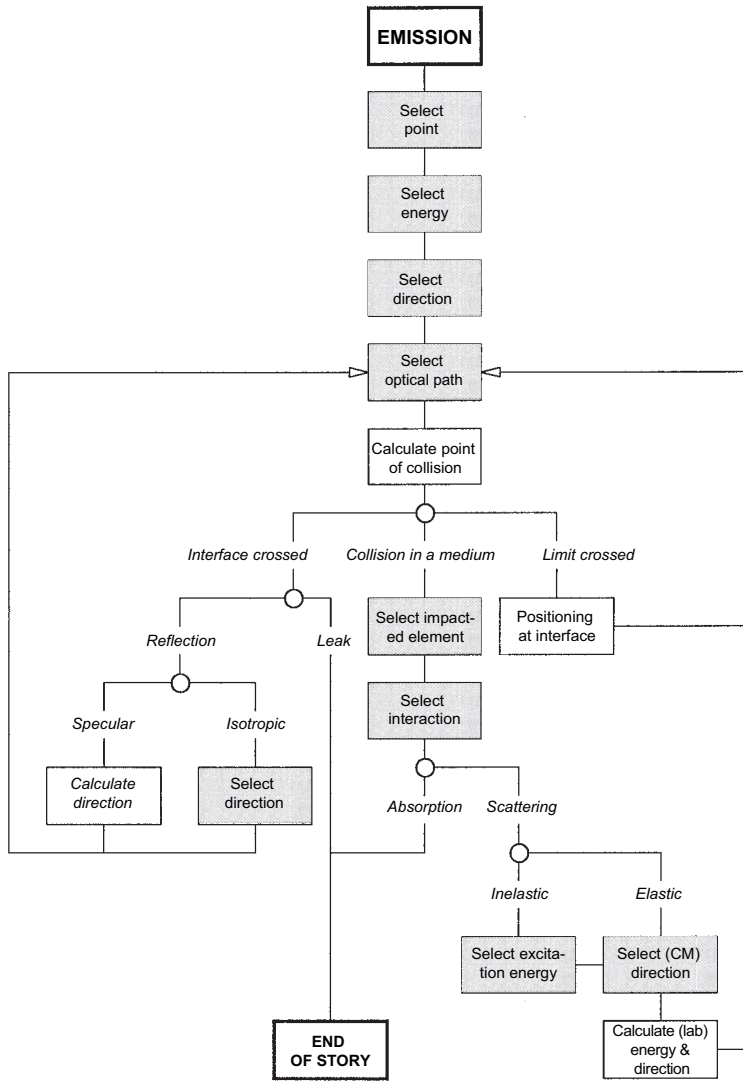


Figure 14.12. Simulation of the life story of a neutron using the Monte Carlo method.

It is standard practice to simulate successive batches of neutrons. The first batch is emitted according to $S^{(0)}$, giving $\Phi^{(0)}$ and $S^{(1)}$; the second is emitted according to $S^{(1)}$, giving $\Phi^{(1)}$ and $S^{(2)}$; and so on. The multiplication factor $k^{(n)}$ is calculated at each stage as the ratio of the number of neutrons obtained by fission to the number of neutrons emitted in the batch (the same number of neutrons is generally emitted in each batch).

The multiplication factor k_{eff} is finally obtained by taking the arithmetic mean of all[66] $k^{(n)}$. Note: To calculate this mean, and to avoid any bias, it is necessary to eliminate the *first*

[66] Weighted by the number of neutrons in each batch if the batches are not equal.

generations[67], for which the sources do not have their energy and space equilibrium distribution, and for which the number of descendants has not reached its asymptotic value.

Note: Working on successive batches also has the advantage of providing statistical distributions for the parameters of interest (reaction rate, multiplication factor, etc.) and therefore, in addition to an estimate of the parameter, an estimate of the standard deviation with which it is obtained. After dividing by the square root of the number N of batches used, we then have the estimate of the standard deviation on the average of the N batches.

14.6.6. Semi-analogous simulation of neutron paths

In reactor core neutron physics problems, flux levels are relatively uniform and analogous simulations are sufficient. In protection calculations, however, we often have to deal with problems where the flux varies by several decades between the level observed in the neighbourhood of sources (e.g. in the core) and the level of the room in which the dose of ionising radiation must be evaluated. In this type of problem[68], an analogous simulation would perform very badly. For example, if the protection attenuates the flux by a factor of 10^6, then 1,000,000 particles must be simulated, of which 999,999 unnecessarily, to obtain the one particle that provides the pertinent information (or: a thousand million to obtain a thousand useful ones with the desired information). Clearly, under these conditions, the Monte Carlo approach would be useless. That is why *biased simulation* (or semi-analogous) methods were developed.

References to many biasing techniques are given in the bibliography, and so we shall not discuss them in detail. Two ideas should however be mentioned:

– the idea of giving a weight to the particles, in proportion to their likely contribution to the result being sought. This should be associated with the Russian roulette consisting of "killing" particles whose weight is too low, with a probability that is proportional to the weight, and the *"duplication"* or *"splitting"* of particles that are too heavy. It can also sometimes be of interest to replace absorptions (capture and fission) by weight changes, without stopping the particles;

– the idea being to change the cross-sections to favour trajectories in the desired direction, by replacing the section Σ with:

$$\Sigma^* = \Sigma(1 - a\cos\theta),$$

where a is a biasing coefficient between 0 and 1, and θ is the angle between the direction of the neutron and the direction of interest. This obviously leads to the true flux Φ being replaced by a biased flux Φ^*, but when we substitute into the Boltzmann equation, we can see that the biasing factor Φ^*/Φ is fairly simple to evaluate.

[67] To give a rough idea, let us say that this means about ten generations.
[68] The problem arises in a similar way (the same Boltzmann equation) for the transport of neutrons and gamma photons.

We should also mention *correlated* Monte Carlo simulations, where a simulation is repeated with the same selection of pseudo-random numbers in two very slightly different situations. This provides an evaluation of the sensitivity coefficients (reactivity effects, sensitivity to cross-sections or composition, etc.) without having the effect of the great statistical error on the difference between two neighbouring results that would exist if they had been obtained by independent simulations.

Along the same lines, a Monte Carlo calculation can also be used to evaluate not only a given physical parameter, but also its derivatives with respect to a given parameter, so that the variations can then be evaluated using a Taylor series expansion.

Exercises

A. Study of the Boltzmann equation

Exercise 14.1: equivalence of the two forms of the transport operator

Let $Q(\vec{r}, v, \vec{\Omega}, t)$ and $\Phi(\vec{r}, v, \vec{\Omega}, t)$ be the emission density and the resulting flux, respectively. Recall that the transport operator links Φ to Q.

a) Show this operator in its integral form.

b) Apply a small shift of magnitude ds, to the location of a notional detector, along $\vec{\Omega}$, with the operator.

c) Derive the differential form of the transport operator from the effect on it of the shift $\vec{\Omega}ds$.

d) Give a physical interpretation of the difference between observations made by two notional detectors separated by $\vec{\Omega}ds$.

Exercise 14.2: exact solution without absorption

In a homogeneous, non-absorbent material, without neutron sources at finite distances, show the general solution of the monokinetic, stationary, one-dimensional Boltzmann equation.

Exercise 14.3: relaxation length

a) In a homogeneous, diffusive, absorbing material, without neutron sources, show that the solution of the monokinetic, stationary, one-dimensional Boltzmann equation, is in the form $\Phi(x, \mu) = \varphi(\mu)e^{-\kappa x}$. Recall that the quantity $L^* = 1/\kappa$ is called the 'relaxation length' (see exercise **5.18**).

b) Using the Boltzmann equation for this case in its differential form, and assuming that the scattering is isotropic in the laboratory system, derive the equation giving κ.

c) Based on the same assumptions as used previously, derive the equation giving κ, from the Boltzmann equation in its integral form.

d) Compare the relaxation length with the diffusion length (see exercise **3.2**) for several example values of the number of secondaries per collision $c = \Sigma_s/\Sigma_t$.

e) Repeat part **b** for the linearly anisotropic collision hypothesis.

Exercise 14.4: diffusion length

The aim of this exercise is to find the general expressions describing the diffusion length L for a homogeneous, infinite medium, as in Exercise **3.2**, except no longer assuming that scattering is isotropic.

a) Begin by considering the neutrons performing exactly n elementary paths $\vec{\rho}_i$ ($i = 1, \cdots, n$), and define

$$\vec{R}_n = \vec{\rho}_1 + \vec{\rho}_2 + \cdots + \vec{\rho}_n;$$

thereby taking the average,

$$\langle \vec{R}_n{}^2 \rangle = \langle \vec{\rho}_1{}^2 \rangle + \langle \vec{\rho}_2{}^2 \rangle + \cdots + \langle \vec{\rho}_n{}^2 \rangle + 2 \langle \rho_1 \cdot \rho_2 \cdot \cos\theta_{12} \rangle + \cdots,$$

where θ_{ij} is the angle between the vectors $\vec{\rho}_i$, and $\vec{\rho}_j$. Write out the sum in full. Then show that the variables ρ and θ are independent, and hence simplify the result.

b) Define $\bar{\mu}$ to be the average cosine of the scattering angle. This angle, $\theta_{i,i+1}$ is a random variable, independent of i. Employ recursion and spherical trigonometry to show that $\langle \cos\theta_{i,i+k} \rangle = \bar{\mu}^k$. A spherical triangle drawn on the surface of a sphere is described by either its three dihedral *face-angles* A, B, C measured at the centre of the sphere, or the three angles a, b, c of its *sides* on the surface of the sphere. They are related by the formula

$$\cos a = (\cos b)(\cos c) + (\sin b)(\sin c)(\cos A).$$

c) Find the expression for $\langle \vec{R}_n{}^2 \rangle$.

d) Weighting the $\langle \vec{R}_n{}^2 \rangle$ by the probability p_n that a neutron carries out exactly n paths (see exercise **3.1**), find $\langle \vec{R}^2 \rangle$.

e) Show that the diffusion area $L^2 = \langle \vec{R}^2 \rangle / 6$ can be written in the form $L^2 = D/\Sigma_a$ with $D = 1/(3\Sigma_{tr})$ and $\Sigma_{tr} = \Sigma_t - \bar{\mu}\Sigma_s$. Notice that this diffusion area — calculated exactly here — is expressed using only the first moment, $\bar{\mu}$, of the collision law.

Exercise 14.5: integral kernel in one- and two-dimension geometries

Recall that the point kernel of the integral transport operator is $e^{-\tau}/(4\pi R^2)$, provided emission occurs isotropically.

a) Show by taking the integral along y and z that for a system with planar geometry, i.e. depending on x only, the kernel becomes $E_1(\tau_x)/2$. Substitution by other variables is necessary. Define τ_x to be the projection of the optical path $\vec{\tau}$ on the $\vec{x}$ axis.
Recall of the definition of the integral exponentials,

$$E_n(u) = \int_0^1 \exp\left(-\frac{u}{\mu}\right) \mu^{n-2}\, d\mu.$$

b) Show by taking the integral along z only that the kernel becomes $Ki_1(\tau_{xy})/(2\pi\rho)$ when the geometry of the system depends on x and y only. Again, it is necessary to make a suitable substitution. Define ρ to be the projection on the x-y plane of the true neutron path $\vec{R}$, and τ_{xy} the projection of the optical path $\vec{\tau}$ on this plane.
Recall of the definition of the Bickley functions,

$$\mathrm{Ki}_n(u) = \int_0^{\pi/2} \exp\left(-\frac{u}{\sin\theta}\right) \sin^{n-1}\theta\, d\theta.$$

B. Treatment of energy and time

Exercise 14.6: multigroup theory and treatment of the time derivative

a) In multigroup theory, any function $f(u)$ of the lethargy u is replaced by a set of discrete group values f_g, which can be interpretated as averaged values, while the lethargy integrals are replaced by corresponding sums over the groups.
For example, in exercise **7.8**, the integral equation

$$\int_{u-\varepsilon}^{u} f(u')\,P(u-u')\,du' = (1+a)\,f(u),$$

is replaced by the algebraic expression

$$\sum_{h} f_h\,P_{g-h} = (1+a)\,f_g,$$

where h is taken for the groups in the interval $[u-\varepsilon, u]$. Also assume that the groups are divided up over intervals with equal lethargy width $\Delta = \varepsilon/n$, where n is integer.
The solutions to these equations take the form

$$f(u) = C^{\mathrm{t}}\,\exp(-mu),$$

and

$$f_g = C^{\mathrm{t}}\,\exp\left(-\tilde{m}\,\Delta\,g\right).$$

To simplify matters, assume that the probability $P = 1/\varepsilon$, and is constant over the interval $[u-\varepsilon, u]$. This approximation is accurate for a heavy nucleus. Compare m and $\tilde{m}$ according to a and n.

b) Consider the differential equation

$$\frac{df(t)}{dt} = f(t),$$

together with the discrete forms divided into equal time intervals Δ, which are either

$$\frac{f_{i+1} - f_i}{\Delta} = f_i,$$

or

$$\frac{f_{i+1} - f_{i-1}}{2\Delta} = f_i.$$

Compare the exact and approximate solutions — notice that they are exponential functions. Apart from its symmetry, what other advantage does the second discrete form have?

C. Collision probabilities

Exercise 14.7: Cauchy's theorem

Consider any convex body of volume V and surface S. The mean chord X, averaged isotropically over all directions is $\langle X \rangle = 4V/S$.

This theorem is due to Augustin Cauchy (1789-1857). It is important in neutron physics because the mean chord multiplied by the macroscopic cross-section represents in effect the 'opacity' of a volume 'seen' by the neutrons.

Previously, in chapter **3**, Exercise **7**, this theorem was demonstrated using a model with a physical basis, i.e. monokinetic particles, such as neutrons, flowing uniformly and isotropically throughout all space, and passing through a body. This exercise takes a more formal mathematical approach to the problem.

a) Define AB to be a chord and X its length. The point A on the surface is chosen at random with equal probability, i.e. proportional to the surface element d^2S. The direction of entry $\vec{\Omega}$ of the chord is made proportional to $d^2\Omega \cos\theta$, where $\theta < \pi/2$ is the angle between $\vec{\Omega}$ and the normal at A, meaning that the angular distribution is isotropic. This determines where B is. Give the expression for the probability density governing chords.

b) Show the double integral giving the mean chord $\langle X \rangle$.

c) Show that the integral with d^2S is equal to the volume. Then deduce the Cauchy theorem.

Exercise 14.8: reciprocity theorem (and absorption probabilities)

In Exercise **8.3** a direct demonstration of the reciprocity relationship between the probabilities P_{VS} and P_{SV} was proposed. This relationship can also be obtained using a notional physical model similar to the one in Exercise **3.7**.

The volume V — which is assumed to contain homogeneous, diffusive, absorbing material — with surface S, is divided and distributed evenly, thereby transfoming it into an infinite, homogeneous medium. A uniform, isotropic neutron source with intensity s is located in this infinite medium; consequently, a flux Φ is generated. Assume also that the neutrons are monokinetic with a velocity v.

a) Express, as functions of s, and the cross-sections of the medium, the flux Φ, the number of neutrons J_- crossing the surface per unit time and area, in the direction opposite to the normal, and the emission density $Q = s + \Sigma_s\Phi$.

b) How many collisions are observed per unit time in volume V?

c) By considering that these collisions represent both, the first ones occuring to neutrons produced or scattered in V before they exit, and the collisions of neutrons entering through S and suffering their first collision in V, show the relationship linking P_{VV} with P_{SV}.

d) Deduce the reciprocal relationship connecting P_{VS} with P_{SV}.

e) By following a similar argument, next establish the relationship between the *absorption* probabilities P^*_{VV} and P^*_{SV} in volume V for a neutron emitted uniformly and isotropically in V, and a neutron entering uniformly and isotropically through S, respectively.

Exercise 14.9: moments of the chord

Show the integrals giving the moments $\langle X^n \rangle$ of the chord X, with isotropic entry. Then find expressions for the first values of n for,

a) an infinite slab of thickness $2a$;

b) an infinite cylinder of radius R;

c) a sphere of radius R.

Exercise 14.10: first collision probability for a sphere

a) Find the probability P_{SS} for a homogeneous sphere of radius R.

b) Deduce the probabilities P_{SV}, P_{VS} and P_{VV}.

Exercise 14.11: first collision probabilities in a checkerboard pattern

Consider an 'infinite checkerboard' consisting of two types of alternating cells A and B. Define i or j to be regions in type A cells, and k or ℓ are regions in type B cells.

Find expressions giving the first collision probabilities P_{ij}, P_{ik}, P_{ki}, and $P_{k\ell}$, assuming that neutrons crossing the interfaces between the two types of cells exhibit isotropic, uniform behaviour. Why is this problem interesting?

Exercise 14.12: calculation of the disavantage factor

Consider a cell containing two regions labelled 1 and 2, representing fuel and moderator, respectively. The objective is to find the thermal utilisation factor f, which is the probability that a neutron emitted uniformly and isotropically in the moderator is eventually absorbed in the fuel.

a) Assuming that the neutrons are monokinetic, and considering the total reaction rates in each zone, show the equations giving the fluxes Φ_1 and Φ_2 as functions of the cross-sections, of the volumes, and of the first collision probabilities P_{ij} (i, j = 1 or 2).

b) From these equations, find the disavantage factor Φ_2/Φ_1, and the thermal utilisation factor f. *Hint:* use the reciprocity and conservation relationships in order to keep only the probability P_{11}.

c) Let P_{11}^+ be the probability for a neutron generated uniformly and isotropically in a fuel element to suffer its first collision in this fuel element, without exit; and the Dancoff factor C, which is the probability that a neutron leaving uniformly and isotropically a fuel element enters another fuel element without an intermediate collision in the moderator. Find the probability P_{11} as a function of both these probabilities, and the physical and geometrical characteristics on the cell. Define S to be the area of the fuel-moderator interface, and assume that the neutrons cross the moderator-fuel interface uniformly and isotropically.

d) According to tabulated values in the literature, the Dancoff factor for square cells is $C_{\text{exact}} = 0.179$, while the corresponding figure for cylindrical cells is $C_{\text{cylinder}} = 0.158$. Given that $f \approx 0.94$ and $4V_2\Sigma_{a2}/S \approx 0.015$, estimate the error in f when a cylindrical geometry is adopted. Is this amount significant?

Exercise 14.13: numerical calculation of the collision probabilities

The first collision probability method introduces two approximations which have to be distinguished:

- the so-called 'flat flux' approximation which assumes that the flux, and the related quantities, reaction rates, sources, etc., are constant relative to the space variable $\vec{r}$ in each elementary volume. This constant can be interpretated as the mean value over the volume;
- the use of approximate numerical quadrature formulae for the calculation of the first collision probabilities.

Both approximations are illustrated here for a fictitious, elementary example: one-dimensional neutron migration. Imagine a 'string' made from a homogeneous medium. Scattering in the string is assumed to be isotropic, meaning that when it occurs there is an equal probability for a scattered neutron to go in either direction. It is also assumed that the neutrons are monokinetic. In these circumstance the Boltzmann equation reduces to

$$\Phi(x) = \int \frac{1}{2}\, \mathrm{e}^{-|x-x'|} \left[S(x') + c\, \Phi(x') \right] dx',$$

where $c = \Sigma_s/\Sigma_t$, and where $1/\Sigma_t$ is taken as unit of length. It can be proved that, in this case, the diffusion equation becomes rigourous; however, we wish to examine an integral treament of the first collision probability type.

a) Firstly, consider the relaxation mode $\Phi(x) = A\, \mathrm{e}^{-\kappa x}$ without a source, then find the exact value of the parameter κ.

b) The $\vec{x}$ axis is divided into finite intervals of length h labelled i or j, and the discretised expression of the previous equation is then

$$\Phi_i = \sum_{j=-\infty}^{+\infty} P_{ji} \left[S_j + c\, \Phi_j \right].$$

Calculate the exact values of the first collision probabilities P_{ji}. Verify that their sum over $i = 1$, exactly. Show that the solution of the discretised equation is in the form $\Phi_i = A\, \mathrm{e}^{-\tilde{\kappa} x}$. Show the equation giving $\tilde{\kappa}$, and show that

$$\frac{\tilde{\kappa}}{\kappa} = 1 - \frac{ch^2}{6} + \cdots$$

c) Now, the exact calculation of the probabilities is replaced with

$$P_{ji} \simeq \frac{h}{2} \mathrm{e}^{-h|i-j|} \quad (i \neq j); \qquad P_{jj} = 1 - \sum_{i \neq j} P_{ji}.$$

Repeat the previous problem, and show that, owing to a fortuitous compensation, the error on κ is smaller than in the preceding case.

Exercise 14.14: Wigner, Bell-Wigner, and Carlvik approximations

Apart from in a few cases such as the sphere (Exercise **14.10**), the formulae for the first collision probabilities are complicated, and have no analytical solution. For this reason approximate formulae sometimes are employed. Three examples are given below. These are based on a (infinite) cylinder, the most usual geometry of the fuel elements.

a) Recall that the probability P_{VV} is a function, for a given form, of only one parameter, namely the opacity $\omega = \Sigma\langle X\rangle$, which is the product of the macroscopic total cross-section and the mean chord. How does this function behave for the small and the large opacities? *Hints:* for small opacities, see exercise **8.4**; large opacities, start from $P_{SS} \simeq 0$, then use the complementarity and reciprocity relationships.

b) *Wigner's approximation:*

$$P_{VV} \simeq \frac{\omega}{1+\omega}.$$

Show this is consistent with the asymptotic behaviour.

c) *Bell-Wigner's approximation:* this is a generalization of the previous approximation by virtue of an adjustable coefficient b, defined by

$$P_{VV} \simeq \frac{\omega}{b+\omega}.$$

Which value of b is consistent with the behaviour at the origin?

d) *Carlvik's approximation:* it is a generalization of the previous approximation, with two rational fractions instead of one:

$$P_{VV} \simeq \omega \left[\frac{\alpha}{\beta+\omega} - \frac{\gamma}{\delta+\omega} \right].$$

Show that the set $\alpha = 2$; $\beta = 2$; $\gamma = 1$; $\delta = 3$ is consistent with both the asymptotic behaviour and the behaviour at the origin.

e) Compare numerically these three approximations with the exact values given in the table below.

Table showing the first collision probability for an infinite cylinder

ω	P	ω	P	ω	P
0.04	0.02561	0.6	0.28351	3	0.69843
0.08	0.04967	0.8	0.34838	4	0.76355
0.2	0.11498	1.2	0.45225	5	0.80677
0.4	0.20697	2	0.59285	10	0.90077

D. Treatment of the integral and differential forms

Exercise 14.15: unknowns of the 'diamond scheme' calculation

For geometries depending only on the variable x (planar symmetry) or the variable r (spherical symmetry), the monokinetic transport equation contains only one angular variable, the angle θ, or of the cosine of this angle, $\mu = \cos\theta$, between the direction of the neutron and either the axis $\vec{x}$ or the direction $\vec{r}$. In a planar geometry, the only derivative is the one with respect to x; however, in spherical geometry, there is not only a derivative with respect to r but also with respect to μ, owing to the curvature of the coordinate system.

When the numerical treatment employs an angular 'discrete ordinate' and a spatial 'finite difference' approach, which unknowns are required in each case?

Exercise 14.16: maximum of the space mesh

In a planar geometry and for neutron directions characterized by a given value of μ, the transport equation is

$$\mu \frac{\partial \Phi(x, \mu)}{\partial x} + \Sigma(x)\, \Phi(x, \mu) = \left[\text{Second member}\right],$$

where Σ is the total macroscopic cross-section.

Consider now the general solution of the equation without the second member, in a homogeneous zone, and in a given direction $\Phi(x, \mu) = C^{\mathrm{t}}\, e^{\kappa x}$, with $\kappa = \Sigma/\mu$.

When using a finite difference treatment, this equation without the second member is replaced by

$$\mu \frac{\Phi_i - \Phi_{i-1}}{h} + \Sigma \frac{\Phi_i + \Phi_{i-1}}{2} = 0,$$

where $h = x_i - x_{i-1}$ and $\Phi_i = \Phi(x_i, \mu)$.

Assuming the mesh h is regular, show that the solution remains of the same exponential type, $\tilde{\Phi}_i = C^{\mathrm{t}}\, e^{\tilde{\kappa} i h}$, with $\tilde{\kappa}$ instead of κ. Compare the two constants $\tilde{\kappa}$ and κ. In what way is h constrained?

When applying one-group theory to a homogeneous, spherical system, the value $h = \varepsilon\mu_1/\Sigma$ is chosen such that μ_1 is the smallest absolute value of μ in the 'discrete ordinates', and $\varepsilon = 0.1$. How many spatial meshes are necessary?

Numerical example: Find the number of meshes needed for a 50-litre sphere containing an aqueous solution, where $\Sigma = 300\ \mathrm{m}^{-1}$, when using $\mathbf{S_4}$, $\mathbf{S_8}$, and $\mathbf{S_{16}}$ schemes.

Exercise 14.17: Milne's problem

Consider the Milne problem for the simplest case:

- planar interface between a homogeneous medium and a vacuum;
- monokinetic neutrons;
- no absorption;
- isotropic scattering;
- sources situated deep within the homogeneous medium.

a) Write the system of $\mathbf{P_N}$ equations for this problem.

b) Examine the $\mathbf{P_1}$ approximation, then compare two possibilities for taking into account the boundary condition $\Phi(0, \mu) = 0$ for μ negative, which are either

$$\int_{-1}^{0} \Phi(0, \mu)\, d\mu = 0,$$

or

$$\int_{-1}^{0} \Phi(0, \mu)\, \mu\, d\mu = 0,$$

and calculate the extrapolation distance in each case.

c) Apply the $\mathbf{P_3}$ approximation to the problem.

Exercise 14.18: even-odd formulation of the Boltzmann equation

a) Write the Boltzmann equation in its integral/differential form for the following conditions.

- Stationary situation.
- Monokinetic neutrons.
- Isotropic sources.
- Streaming operator given by $\vec{\Omega} \cdot \overrightarrow{\text{grad}}$.
- Linearly anisotropic scattering, i.e.

$$\Sigma_s(\vec{r}, \vec{\Omega}) = \frac{1}{4\pi}\Sigma_{s0}(\vec{r}) + \frac{3}{4\pi}\Sigma_{s1}(\vec{r})\, \vec{\Omega}' \cdot \vec{\Omega},$$

  where Σ_{s0} is the scattering cross-section integrated over all directions, and Σ_{s1} is the mean cosine of the deflecting angle multiplied by Σ_{s0}.

b) The phase flux $\Phi(\vec{r}, \vec{\Omega})$ is split into the sum of its even part ψ and its odd part χ with respect to $\vec{\Omega}$:

$$\Phi(\vec{r}, \vec{\Omega}) = \psi(\vec{r}, \vec{\Omega}) + \chi(\vec{r}, \vec{\Omega}),$$

where

$$\psi(\vec{r}, \vec{\Omega}) = \frac{\Phi(\vec{r}, \vec{\Omega}) + \Phi(\vec{r}, -\vec{\Omega})}{2},$$

$$\chi(\vec{r}, \vec{\Omega}) = \frac{\Phi(\vec{r}, \vec{\Omega}) - \Phi(\vec{r}, -\vec{\Omega})}{2}.$$

The Greek letters ψ and χ are used to indicate the symmetry or antisymmetry of the state; the notations Φ^+ and Φ^- are also used.

By substitution into the Boltzmann equation, find the system of two equations (even and odd parts) coupling the even and odd parts with respect to $\vec{\Omega}$.

c) Assume temporarily that the scattering is isotropic, i.e. that Σ_{s1} is equal to zero, then express χ from the second equation and, by substituting the result into the first equation, find the equation governing only ψ.

d) For a given fixed direction $\vec{\Omega}$ (for instance, during a treatment by discrete ordinates), compare the previous equation with the diffusion equation.

e) To treat the second equation when $\Sigma_{s1} \neq 0$, a '$\mathbf{P_1}$' hypothesis is introduced, meaning it is assumed that $\chi(\vec{r}, \vec{\Omega})$ is given approximately by

$$\chi(\vec{r}, \vec{\Omega}) \simeq \vec{u}(\vec{r}) \cdot \vec{\Omega}.$$

Calculate the vector $\vec{u}(\vec{r})$ using the second equation, then write the equation governing ψ by substituting χ into the first equation.

f) Show that the '$\mathbf{P_1}$' hypothesis made in the previous question for Σ_s, and for χ can, in fact, be made only for Σ_s, and avoided for χ. In other words, a '$\mathbf{B_1}$' instead of a '$\mathbf{P_1}$' treatment can be made for the second equation. Find the equation for ψ with this '$\mathbf{B_1}$' treatment.

E. Fundamental mode

Exercise 14.19: elementary eigenfunctions of the Laplace operator

Consider a linear combination with the same weight of $e^{-i\vec{b}.\vec{r}}$ functions with vectors $\vec{b}$ whose extremity is situated on,

a) a point of the sphere of radius b and its seven symmetrical points with respect of the coordinate planes,

b) two parallel circles symmetrical with respect to the equator,

c) the whole sphere.

Show this yields the eigenfunctions of the Laplace operator which, respectively, go to zero on,

a) the faces of a rectangle parallelepiped,

b) the surface of a cylinder,

c) the surface of a sphere.

Recall:

$$\frac{1}{2\pi} \int_{(2\pi)} \exp(-i\, u\, \cos\varphi)\, d\varphi = J_0(u).$$

Exercise 14.20: diffusion coefficient in fundamental mode

For the fundamental mode in a homogeneous medium — meaning the situation where the flux and the reaction rates varies in space as $e^{-i\vec{b}.\vec{r}}$ — it can be observed that Fick's law is rigorous. Thus, there is proportionality between the current $\vec{J}(\vec{r})$ and the gradient of the flux $\Phi(\vec{r})$, with a proportionality coefficient which can depend on the neutron velocity, but not on the position in space. This coefficient (after changing the sign) is called 'diffusion coefficient' or 'leakage coefficient' according to its association with the neutron migration, or with the neutron balance. This exercise examines the calculation of this coefficient, employing monokinetic theory in order to simplify matters. An extension to the polykinetic case is possible.

a) Since the medium can be assumed to be isotropic, the vector $\vec{b}$ can take any direction, e.g. $\vec{x}$. Then, the source and the flux are

$$S(x,\mu) = \frac{1}{2} s\, e^{-ibx}; \qquad \Phi(x,\mu) = \varphi(\mu)\, e^{-ibx},$$

respectively. Find the equation governing φ and the integral giving s from $\varphi(\mu)$.

b) The phase distribution $\varphi(\mu)$ can be expanded in Legendre polynomials:

$$\varphi(\mu) = \sum_{n=0}^{\infty} \varphi_n P_n(\mu).$$

Show that the integrated flux is $\Phi(x) = 2\,\varphi_0\, e^{-ibx}$; therefore, that the component of its gradient along the axis $\vec{x}$ is $-2ib\,\varphi_0\, e^{-ibx}$. Then show that the component along $\vec{x}$ of the integrated current is $J_x(x) = (2/3)\,\varphi_1\, e^{-ibx}$, and consequently that Fick's law is consistent with the diffusion coefficient

$$D = \frac{\varphi_1}{3ib\varphi_0}.$$

c) To find φ_0 and φ_1, express the equation governing $\varphi(\mu)$ in terms of an expansion in Legendre polynomials. Since the Legendre polynomials are eigenfunctions of the scattering operator, notice that

$$\int_{-1}^{+1} \Sigma_s(\mu' \rightarrow \mu)\, P_n(\mu')\, d\mu' = \Sigma_{s,n}\, P_n(\mu),$$

Thus, the eigenvalues $\Sigma_{s,n}$ are the moments of the differential scattering cross-section.

d) Divide the previously obtained equation by $\Sigma - ib\mu$. Next, multiply by one of the Legendre polynomials, $P_k(\mu)$, and integrate over μ in order to obtain its projection on this polynomial. Introduce the coefficients

$$G_{nk} = \int_{-1}^{+1} \frac{P_k(\mu)\, P_n(\mu)}{\Sigma - ib\mu}\, d\mu,$$

and calculate G_{00}, $G_{01} = G_{10}$, and G_{11}.

e) Assuming that only the first moment $\Sigma_{s0} \equiv \Sigma_s$ (scattering cross-section integrated over the angles) is not zero, find φ_0 and φ_1 from the two first equations, and deduce D.

f) Supposing now that only the two first moments Σ_{s0} and $\Sigma_{s1} \equiv \bar{\mu}\,\Sigma_s$ — where $\bar{\mu}$ is the mean cosine of the deflecting angle — are not zero, find D from the two first equations, and compare with the previous result.

g) Finally, express D in a general form. In pratice, such as in the APOLLO code, $\mathbf{B_1}$ theory is employed to estimate the diffusion coefficient in a manner similar to **f** with Σ_{s0} and Σ_{s1}; however, multigroup theory is used instead of the monokinetic assumption.

Exercise 14.21: Behrens's correction

In a heterogeneous medium, such as a reactor lattice, the theory of the fundamental mode and of the diffusion coefficient is much more difficult. It appears that, owing to streaming effects, the use of simple averages of cross-sections or their inverses (mean free paths) is not sufficient to take into account the heterogenity effect on the diffusion coefficient[69].

Behrens studied the regular, infinite lattice constituted by a homogeneous moderator, and empty cavities. This is similar to a natural uranium-gas-graphite UNGG system, when the fuel element is neglected because its volume in the gas duct is relatively small. The (thermal) neutrons — which are assumed to be monokinetic — are emitted by a uniform source in the moderator. This represents neutrons near the end slowing down. Consequently, the flux everywhere — in the moderator as well as in the cavities — is uniform and isotropic.

As the flux is constant, the averaged macroscopic absorption cross-section can be defined by the homogenization formula:

$$\bar{\Sigma}_a = \frac{V_m}{V_m + V_c}\Sigma_{am}.$$

Then, conservation of the diffusion area[70] L^2 implies D. This criterion is correct at the limit $b \longrightarrow 0$, leading to

$$L^2 = \frac{D}{\bar{\Sigma}_a}, \qquad D = L^2\,\bar{\Sigma}_a.$$

Therefore, the diffusion area must be obtained from its definition,

$$L^2 = \frac{1}{6}\langle \vec{R}^2 \rangle.$$

Behrens performed this calculation of $\langle \vec{R}^2 \rangle$ by generalizing the argument made in exercises **3.1** and **3.2**. He also assumed that isotropic scattering occurs; hence,

$$\langle \vec{R}^2 \rangle = \bar{n}\,\langle \vec{\rho}^{\,2} \rangle, \qquad \bar{n} = \frac{\Sigma_m}{\Sigma_{am}}.$$

To calculate $\langle \vec{\rho}^{\,2} \rangle$, he distinguished the neutron paths crossing a cavity or not, and neglected paths crossing more than one cavity. This is a reasonable assumption for a UNGG system of this type. The following exercise demonstrates his reasoning.

a) By counting, the numbers of collisions and neutrons entering a cavity per unit of time, calculate the proportion γ of neutron paths crossing a cavity.

b) Calculate $\langle \rho_m \rangle$ and $\langle \rho_m^2 \rangle$ for a path which does not cross a cavity.

c) The vector representing a neutron path crossing a cavity can be given as the sum $\vec{\rho}_{m1} + \vec{\rho}_c + \vec{\rho}_{m2}$, where the terms are the parts of the path before, within, and after the cavity,

[69] D. J. Behrens Proc. Phys. Soc. A, **62**(10) 607–616 (1949), and P. Benoist, thesis, University of Paris (1964); CEA-R-2278.

[70] The diffusion area is one sixth of the averaged square direct distance between the creation of the neutron and its absorption. In diffusion theory, this area is equal to the diffusion coefficient divided by the macroscopic absorption cross-section. Here, the diffusion area will be calculated, and the diffusion coefficient defined in order to obtain this equality.

respectively. The averages $\langle \rho_{m2} \rangle$ and $\langle \rho_{m2}^2 \rangle$ are equal to the averages $\langle \rho_m \rangle$ and $\langle \rho_m^2 \rangle$ calculated in part **b**. Symmetry in time dictates that the averages $\langle \rho_{m1} \rangle$ and $\langle \rho_{m1}^2 \rangle$ are equal to the averages $\langle \rho_{m2} \rangle$ and $\langle \rho_{m2}^2 \rangle$. Find $\langle \rho_c \rangle$ and $\langle \rho_c^2 \rangle$ as functions of the parameters S (surface), V_c (volume) and Q (form parameter — see exercise **8.4**) of the cavities. Deduce the average of the square of the length of a path crossing a cavity.

d) Using these results, give the formula for the diffusion coefficient. What size is the ratio between this coefficient and that for the moderator? Show that this ratio is not the expression of a simple homogenization.

e) *Numerical example:* apply the previous results to a lattice containing cylindrical cavities 100 mm in diameter, embedded inside square-section 200 × 200 mm graphite blocks, with infinite length in the z-direction. Assume that the neutron mean free path in graphite is 26 mm.

F. Monte Carlo method

N.B: in the following exercises, ξ is the random variable governed by a uniform law in the interval $[0, 1[$. A pseudo-random algorithm is employed to generate ξ, in practice.

Exercise 14.22: power law probability distribution

Assume that n random values of ξ are taken, and that the largest one is selected. Show that this maximum is the random variable X governed by the probability law $P(x)\,dx = n\,x^{n-1}\,dx$ in the interval $[0, 1[$. How can this variable be obtained in a single step? What is the best way to generate it?

Exercise 14.23: random point inside a circle

Consider the following methods for picking a random point inside a circle, where ξ_1 and ξ_2 are two random numbers used to generate the coordinates.

a) Why is $\rho = \xi_1$ and $\varphi = 2\pi\xi_2$ unsatisfactory?

b) How can the previous method be modified to yield a better outcome?

c) An alternative might be to generate Cartesian coordinates using

$$x = 2\xi_1 - 1, \qquad y = 2\xi_2 - 1,$$

and discard points outside the circle when $x^2 + y^2 \geq 1$. Does it produce a satisfactory result? What proportion of the points are discarded?

d) Which of these methods is best?

Exercise 14.24: Buffon's needle

Recall that the Buffon experiment consists of throwing a needle of length b on a plane divided into parallel strips of width a, and observing how often the needle lies across a boundary between two strips. The result is related to the constant π.

a) Taking $a = b$, give the probability that the needle lies across a boundary.

b) How do the variance and standard deviation in the estimate for π depend on the number of trials n?

Exercise 14.25: evaluation of a resonance escape probality

a) Assume that neutron slowing down occurs in a monoatomic material by elastic, isotropic scattering in the centre of mass system. Devise a 'Monte Carlo' algorithm to evaluate the probability that a neutron emitted at high energy escapes a resonance simulated by a unique 'black trap' (infinite absorption cross-section in the trap and no absorption outside the trap).

b) Perform some numerical simulations, and compare the outcome with the result given by the exact analytical expression for the resonance escape probability.

Solutions

A. Study of the Boltzmann equation

Exercise 14.1: equivalence of the two forms of the transport operator

a) The integral form of the transport operator is

$$\Phi\left(\vec{r}, v, \vec{\Omega}, t\right) = \int_0^{\infty} \mathrm{e}^{-\tau}\, Q\left(\vec{r} - s\vec{\Omega}, v, \vec{\Omega}, t - s/v\right)\, ds,$$

where

$$\tau = \int_0^{s} \Sigma\left(\vec{r} - s'\vec{\Omega}, v\right)\, ds'.$$

The integral expressing Φ makes explicit the neutron paths without collision over a distance s, at the velocity v, and in the direction $\vec{\Omega}$ from the emission point, to the point where the flux is evaluated. Q is the emission density; $\mathrm{e}^{-\tau}$ is the probability that the neutron performs the path without collision; the integral sums all the possible contributions.

b) In order to express a shift in the direction $\vec{\Omega}$ of the point where the neutron flux is observed, it is convenient to *fix* a point on the path taken by the neutrons to define the origin of the abscissa s — which can be different from the observation point — and to rewrite the equation giving the flux when the observation point is located at the abscissa s as follows.

$$\Phi\left(\vec{r} - s\vec{\Omega}, v, \vec{\Omega}, t - s/v\right) = \int_s^{\infty} \mathrm{e}^{-\tau}\, Q\left(\vec{r} - s'\vec{\Omega}, v, \vec{\Omega}, t - s'/v\right)\, ds',$$

where

$$\tau = \int_s^{s'} \Sigma\left(\vec{r} - s''\vec{\Omega}, v\right)\, ds''.$$

For the sake of clarity, s in the integral expressing the transport operator is replaced with s', and s' in the expression of the optical path with s''.

c) All that remains is to differentiate with respect to s everywhere it appears, as follows.

$$-ds\,\vec{\Omega}.\overrightarrow{\text{grad}}\,\Phi\left(\vec{r}-s\vec{\Omega},\,v,\,\vec{\Omega},\,t-s/v\right)$$

$$-\frac{ds}{v}\frac{\partial}{\partial t}\left[\,\Phi\left(\vec{r}-s\vec{\Omega},\,v,\,\vec{\Omega},\,t-s/v\right)\,\right]$$

$$=-ds\,Q\left(\vec{r}-s\vec{\Omega},\,v,\,\vec{\Omega},\,t-s/v\right)$$

$$+\int_s^{\infty} ds\,\Sigma\left(\vec{r}-s\vec{\Omega},\,v\right)\,\mathrm{e}^{-\tau}\,Q\left(\vec{r}-s'\vec{\Omega},\,v,\,\vec{\Omega},\,t-s'/v\right)\,ds'.$$

In the third term, the exponential for $\tau = 0$ occurs; hence, it is omitted. For the last term, $ds\,\Sigma$ can be outside the integral. The remaining integral is the flux Φ. Finally, by simplifying ds, changing the sign, and setting $s = 0$ gives

$$\vec{\Omega}.\overrightarrow{\text{grad}}\,\Phi\left(\vec{r},\,v,\,\vec{\Omega},\,t\right)+\frac{1}{v}\frac{\partial}{\partial t}\Phi\left(\vec{r},\,v,\,\vec{\Omega},\,t\right)$$

$$=Q\left(\vec{r},\,v,\,\vec{\Omega},\,t\right)-\Sigma\left(\vec{r},\,v\right)\,\Phi\left(\vec{r},\,v,\,\vec{\Omega},\,t\right).$$

This can be recognized as being the differential form of the transport operator. *Recall,*

$$\vec{\Omega}.\overrightarrow{\text{grad}}\,\Phi\left(\vec{r},\,v,\,\vec{\Omega},\,t\right)\equiv\text{div}\,\left[\,\vec{\Omega}\,\Phi(\vec{r},\,v,\,\vec{\Omega},\,t)\,\right].$$

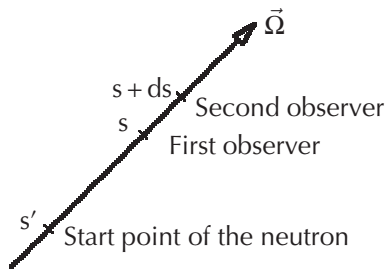


Figure 3

d) The left hand side describes the difference between the observations made in two points separated by $\vec{\Omega}\,ds$ (see figure **3**). These observations — which compare two instants shifted by $dt = ds/v$ — concern almost the same neutrons. The only differences — described by the right hand side — are as follows.

- The neutrons emitted along the line segment joining both the points, seen by the 'observer' located downstream, but not by the 'observer' upstream.
- The neutrons undergoing a collision on this segment, seen by the upstream 'observer' but not by the downstream 'observer'.

Exercise 14.2: exact solution without absorption

The equation to be solved is

$$-\mu\frac{\partial\Phi\left(x,\mu\right)}{\partial x}-\Sigma\,\Phi\left(x,\mu\right)+\int_{-1}^{+1}\Sigma_s\left(\mu'\longrightarrow\mu\right)\,\Phi\left(x,\mu'\right)\,d\mu'=0.$$

This has a solution linear with x and with μ,

$$\Phi\left(x,\mu\right)=A\left(x-a-\frac{\mu}{\Sigma_{tr}}\right),$$

where A and a are any constants, and where $\Sigma_{tr}=\Sigma-\bar{\mu}\Sigma_s$ is the transport cross-section (here $\Sigma_s=\Sigma$). It is noteworthy that only the moments of order 0 and 1 of the scattering law appear.

Exercise 14.3: relaxation length

a) The equation to solve is the same as the previous one, except now with $\Sigma_s\neq\Sigma$. A factorized solution appears, $\Phi(x,\mu)=\varphi(\mu)\,e^{-\kappa x}$, where

$$\kappa\mu\,\varphi\left(\mu\right)-\Sigma\,\varphi\left(\mu\right)+\int_{-1}^{+1}\Sigma_s\left(\mu'\longrightarrow\mu\right)\,\varphi\left(\mu'\right)\,d\mu'=0.$$

b) Provided the scattering is isotropic,

$$\kappa\mu\,\varphi(\mu)-\Sigma\,\varphi\left(\mu\right)+\frac{\Sigma_s}{2}\int_{-1}^{+1}\varphi\left(\mu'\right)\,d\mu'=0.$$

Dividing by $\Sigma-\kappa\mu$, then integrating over μ, yields

$$I=\frac{1}{\kappa}\ln\left(\frac{\Sigma+\kappa}{\Sigma-\kappa}\right)\,\frac{\Sigma_s I}{2},$$

where I is the integral of $\varphi(\mu)$. Following simplification by I, the equation giving κ is obtained:

$$\ln\frac{\Sigma+\kappa}{\Sigma-\kappa}=\frac{2\kappa}{\Sigma_s}.$$

c) The equation for this problem, in the integral form, is

$$\Phi(x)=\int_{-\infty}^{+\infty}\frac{1}{2}E_1\left(\Sigma\mid x-x'\mid\right)\,\Sigma_s\,\Phi(x')\,dx',$$

where

$$E_1(u)=\int_0^1\exp\left(-\frac{\mu}{u}\right)\frac{d\mu}{\mu}.$$

See exercise **14.5** for a demonstration of this problem in one dimension x geometry.

Replacing $\Phi(x)$ with $A\,e^{-\kappa x}$, and simplifying by $A\,e^{-\kappa x}$, the equation giving κ is obtained. The double integral can be calculated by integrating firstly over x' and then over μ. Thus, we obtain again the equation of the paragraph **b**.

d) When the collisions are isotropic, the diffusion length L is given by the formulae

$$L^2 = \frac{D}{\Sigma_a}, \qquad D = \frac{1}{3\Sigma}.$$

Some numerical values for various values of $c = \Sigma_s/\Sigma$ are provided in the following table, where the unit of length is $1/\Sigma$.

c	κ	$1/L$	Difference (%)
0.99	0.17251	0.17321	0.40
0.9	0.52543	0.54772	4.24
0.8	0.71041	0.77460	9.03
0.5	0.95750	1.22474	27.91
0.2	0.99991	1.54919	54.93
0.1	1.00000	1.64317	64.32

e) Expanding $\varphi(\mu)$ into Legendre polynomials, dividing by $\Sigma - \kappa\mu$, and projecting out the two first polynomials, i.e. 1 and μ, yields a homogeneous system governing the two integrals I_0 and I_1, similar to I. The equivalence of the system gives the equation for κ:

$$\ln \frac{\Sigma + \kappa}{\Sigma - \kappa} = \frac{2\kappa}{\Sigma_s} \frac{\kappa^2 + 3\bar{\mu}\Sigma_s\Sigma_a}{\kappa^2 + 3\bar{\mu}\Sigma\Sigma_a}.$$

Exercise 14.4: diffusion length

a) For the neutrons performing exactly n paths, the sum to be calculated is

$$\langle \vec{R}_n^2 \rangle = \langle \vec{\rho}_1^2 \rangle + \langle \vec{\rho}_2^2 \rangle + \cdots + \langle \vec{\rho}_n^2 \rangle + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \langle \rho_i \rho_j \cos\theta_{ij} \rangle.$$

The various random variables are independent, owing to the neutron migration being a Markovian process; hence,

$$\langle \rho \rangle = \frac{1}{\Sigma}, \qquad \langle \rho^2 \rangle = \frac{2}{\Sigma^2}, \qquad \langle \cos\theta_{i,i+1} \rangle = \bar{\mu}.$$

b) Assuming $\vec{\rho}_{i,i+1}$ is located at the vertex A, and defining φ to be the dihedral angle at this vertex, using spherical trigonometry gives

$$\cos\theta_{i,i+2} = \cos\theta_{i,i+1} \cos\theta_{i+1,i+2} + \sin\theta_{i,i+1} \sin\theta_{i+1,i+2} \cos\varphi.$$

The average value of $\cos\varphi$ is zero owing to symmetry; hence,

$$\langle \cos\theta_{i,i+2} \rangle = \bar{\mu}^2.$$

Repeating the reasoning, it can be seen that

$$\langle \cos\theta_{i,j} \rangle = \bar{\mu}^{j-i}.$$

c) This allows the expression

$$\langle \vec{R}_n^2 \rangle = \left[n - \frac{\bar{\mu}\left(1-\bar{\mu}^n\right)}{1-\bar{\mu}} \right] \frac{2}{\left(1-\bar{\mu}\right)\Sigma^2}$$

to be evaluated.

d) Weighting by the probabilities p_n, gives

$$\langle \vec{R}^2 \rangle = \frac{2}{\Sigma_a\left(\Sigma - \bar{\mu}\Sigma_s\right)}.$$

e) Hence, this allows $D = 1/(3\Sigma_{tr})$ to be found.

Exercise 14.5: integral kernel in one- and two-dimension geometries

a) Use $\mu = \cos\theta$, where θ is the angle between the axis $\vec{x}$ and the vector $\vec{R}$ representing the neutron path.

b) Express the integral as a function of the angle θ between the axis $\vec{z}$ and the vector $\vec{R}$ representing the neutron path.

B. Treatment of energy and time

Exercise 14.6: multigroup theory and treatment of the time derivative

a) The exact value of m is given by the equation

$$\frac{e^{m\varepsilon} - 1}{m\varepsilon} = 1 + a,$$

or, with $x = m\varepsilon$,

$$\frac{e^{x} - 1}{x} = 1 + a.$$

When the parameter a characterizing the intensity of the absorption ($a = \Sigma_a/\Sigma_s$) is small, this allows an expansion in powers of a:

$$x = 2a\left(1 - \frac{2a}{3} + \cdots\right).$$

If a regular dicretization is made, with n groups in the interval ε, then $n+1$ probabilities appear in the sum on the left hand side. Integrating $P = 1/\varepsilon$ over the departure and arrival groups, yields

$$P_{gg} = P_{g-n,g} = \frac{1}{2n}; \qquad P_{g-k,g} = \frac{1}{n} \qquad (1 \le k \le n-1).$$

It can be seen by algebraic substitution that it is possible to replace m with $\tilde{m}$ or x with $\tilde{x}$ such that

$$\frac{e^{\tilde{x}} - 1}{2n} \coth \frac{\tilde{x}}{2n} = 1 + a.$$

This formula can be applied even for $n = 1$ and $n = 2$, but then can be simplified:

$$\tilde{x}_{(n=1)} = \ln(1 + 2a); \qquad \tilde{x}_{(n=2)} = 2 \ln \left(2\sqrt{1 + a} - 1 \right).$$

If the parameter a is small, then a series expansion can be employed:

$$x = 2a \left[1 - \frac{2a}{3} \left(1 + \frac{1}{2n^2} \right) + \cdots \right].$$

The term $1/2n^2$ represents, approximately, the error due to the use of the multigroup theory.

When a is not sufficiently small to do this expansion, only numerical solution of the equations giving x and $\tilde{x}$ permits the error to be estimated. For example, for $a = 1/2$ and some values of n, the results are as follows.

n	x	Error (%)
1	0.693147	−9.72
2	0.742423	−2.66
3	0.753381	−1.22
5	0.759279	−0.45
10	0.761830	−0.11
∞	0.762688	0

b) The solutions are exponential functions. Without the normalisation factor, they are $f = e^t$, $\check{f} = e^{i\Delta\alpha}$, and $\hat{f} = e^{i\Delta\beta}$, respectively. The quantities α and β describe the errors due to the numerical calculations of the derivatives by quotients of finite differences. Without the error, these numbers would be equal to one. The equations giving α and β can be found by substitution:

$$e^{\Delta\alpha} = 1 + \Delta; \qquad \sinh \Delta\beta = \Delta.$$

The expansions in powers of Δ,

$$\alpha = 1 - \frac{\Delta}{2} + \frac{\Delta^2}{3} + \cdots, \qquad \beta = 1 - \frac{\Delta^2}{6} + \frac{\Delta^4}{12} + \cdots,$$

show that the error in the first formula is of order Δ, while it is of order Δ^2 in the second. This result also demonstrates that the tangent at a point on a curve is better approximated by a line joining two points at either side of the point than by a line from the point to a point on one side of it.

C. Collision probabilities

Exercise 14.7: Cauchy's theorem

a) After normalisation, the probability law is $d^2S\, d^2\Omega \cos\theta/(\pi S)$.

b) The mean chord is given by the double integral

$$\langle X \rangle = \frac{1}{\pi S} \int_{(S)} d^2S \int_{(4\pi)} d^2\Omega \cos\theta\, X\, \Upsilon(\cos\theta),$$

where $\Upsilon(\cos\theta) = 1$ when the cosine is positive, otherwise is zero.

c) Notice that $d^2S \cos\theta\, X$ is the element of volume and that the integral of this term — when taking the Heaviside function is into account — is the total volume:

$$\int_{(S)} d^2S \cos\theta\, X\, \Upsilon(\cos\theta) = V.$$

Therefore, the double integral is

$$\int_{(4\pi)} d^2\Omega\, V = 4\pi\, V,$$

i.e. the Cauchy theorem.

Exercise 14.8: reciprocity theorem (and absorption probabilities)

a) The neutron densities are described by

$$\Phi = \frac{s}{\Sigma_a}, \qquad J_- = \frac{s}{4\Sigma_a}, \qquad Q = \frac{s\,\Sigma_t}{\Sigma_a}.$$

b) There are $V\,\Sigma_t\,\Phi$ collisions in the volume V per unit of time.

c) Distinguishing both these categories of neutrons, gives

$$V\,\Sigma_t\,\Phi = V\,Q\,P_{VV} + S\,J_-\,P_{SV}.$$

d) Therefore, owing to $1 - P_{VV} = P_{VS}$,

$$P_{SV} = \frac{4\,V\,\Sigma_t}{S} P_{VS}.$$

e) Similarly,

$$P^*_{SV} = \frac{4\,V\,\Sigma_a}{S} P^*_{VS} = \frac{4\,V\,\Sigma_a}{S}\left(1 - P^*_{VV}\right).$$

Exercise 14.9: moments of the chord

a) *Slab:* the $\vec{z}$ axis is normal to the surface at the point of entry; hence,

$$\langle X^n \rangle = 2 \int_0^1 \left(\frac{2a}{\mu} \right)^n \mu \, d\mu.$$

Only the first moment, $\langle X \rangle = 4a$, is finite.

b) *Cylinder:* the $\vec{x}$ axis is normal to the surface at the point of entry, and the axis $\vec{z}$ is along the generatrix; hence,

$$\langle X^n \rangle = \frac{1}{\pi} \int_{-\pi/2}^{+\pi/2} d\varphi \int_0^{\pi} \sin\theta \, d\theta \left(\frac{2R \cos\varphi}{\cos\theta} \right)^n \sin\theta \cos\varphi.$$

In particular,

$$\langle X \rangle = 2R, \qquad \langle X^2 \rangle = \frac{16\,R^2}{3}, \qquad Q = \frac{4}{3}.$$

c) *Sphere:* the $\vec{z}$ axis is normal to the surface at the point of entry; hence

$$\langle X^n \rangle = 2 \int_0^1 \left(2R\mu \right)^n \mu \, d\mu.$$

Particularly:

$$\langle X \rangle = \frac{4}{3} R, \qquad \langle X^2 \rangle = 2\,R^2, \qquad Q = \frac{9}{8}.$$

Exercise 14.10: first collision probabilities for a sphere

When $u = R\Sigma$, the formula is

$$P_{SS} = \frac{1 - (1 + 2u)\,\mathrm{e}^{-2u}}{2u^2}; \qquad P_{VV} = 1 - \frac{3\left[2u^2 - 1 + (1 + 2u)\,\mathrm{e}^{-2u} \right]}{8u^3}.$$

Exercise 14.11: first collision probabilities in a cherckerboard pattern

Owing to the hypothesis the calculation is reduced to the probabilities without exit for each type of cell. For two zones in the same cell,

$$P_{ij} = P_{ij}^{+} + P_{iS}^{+} P_{SS,B}^{+} P_{Sj}^{+} + P_{iS}^{+} P_{SS,B}^{+} P_{SS,A}^{+} P_{SS,B}^{+} P_{Sj}^{+}$$
$$+ P_{iS}^{+} P_{SS,B}^{+} P_{SS,A}^{+} P_{SS,B}^{+} P_{SS,A}^{+} P_{SS,B}^{+} P_{Sj}^{+} + \cdots;$$
$$P_{ij} = P_{ij}^{+} + \frac{P_{iS}^{+} P_{SS,B}^{+} P_{Sj}^{+}}{1 - P_{SS,A}^{+} P_{SS,B}^{+}}.$$

For two zones in different cells,

$$P_{ik} = P_{iS}^{+} P_{Sk}^{+} + P_{iS}^{+} P_{SS,B}^{+} P_{SS,A}^{+} P_{Sk}^{+} + P_{iS}^{+} P_{SS,B}^{+} P_{SS,A}^{+} P_{SS,B}^{+} P_{SS,A}^{+} P_{Sk}^{+} + \cdots;$$
$$P_{ik} = \frac{P_{iS}^{+} P_{Sk}^{+}}{1 - P_{SS,A}^{+} P_{SS,B}^{+}};$$

and similar formulae for P_{ki} and $P_{k\ell}$.

Exercise 14.12: calculation of the disavantage factor

a) The numbers of collisions in each zone are

$$V_1\,\Sigma_{t1}\,\Phi_1 = V_1\,\Sigma_{s1}\,\Phi_1\,P_{11} + (\,V_2\,\Sigma_{s2}\,\Phi_2 + 1\,)\,P_{21},$$
$$V_2\,\Sigma_{t2}\,\Phi_2 = V_1\,\Sigma_{s1}\,\Phi_1\,P_{12} + (\,V_2\,\Sigma_{s2}\,\Phi_2 + 1\,)\,P_{22}.$$

b) Owing to these equations, both fluxes Φ_1 and Φ_2, their ratio Φ_2/Φ_1 (disavantage factor), and the thermal utilisation factor f can be calculated:

$$\frac{1}{f} - 1 = \frac{\Sigma_{a2}}{\Sigma_{t2}}\left[\frac{V_2\,\Sigma_{t2}}{V_1\,\Sigma_{t1}}\left(\frac{P_{11}}{1-P_{11}} + \frac{\Sigma_{t1}}{\Sigma_{a1}}\right) - 1\right].$$

c) Expressing the series of all the possible events as

$$P_{11} = P^+_{11} + P^+_{1S}\,C\,P^+_{S1} + P^+_{1S}\,C\,P^+_{SS}\,C\,P^+_{S1} + P^+_{1S}\,C\,P^+_{SS}\,C\,P^+_{SS}\,C\,P^+_{S1} + \cdots,$$

$$P_{11} = P^+_{11} + \frac{P^+_{1S}\,C\,P^+_{S1}}{1 - C\,P^+_{SS}},$$

with

$$P^+_{1S} = 1 - P^+_{11}, \qquad P^+_{S1} = \frac{4V_1\Sigma_{t1}}{S}P^+_{1S}, \qquad P^+_{SS} = 1 - P^+_{S1},$$

gives

$$\frac{P_{11}}{1-P_{11}} = \frac{P^+_{11}}{1-P^+_{11}} + \frac{C}{1-C}\frac{4V_1\Sigma_{t1}}{S}.$$

The value of f is, therefore, obtained when this expression is substituted into the equation in part **b**.

d) Differentiating the formulae gives

$$\frac{\Delta f}{f} = -f\frac{4V_2\Sigma_{a2}}{S}\frac{\Delta C}{(1-C)^2}.$$

Example: $\Delta f/f = 44$ pcm; the error in f due to the cylindrical approximation is not important. Notice that, for a similar reason, there is also an error of opposite sign in p.

Exercise 14.13: numerical calculation of the collision probabilities

a) The relaxation parameter is obtained by substitution of the exponential solution into the equation without source:

$$\kappa = \sqrt{1-c}.$$

b) The first collision probabilities in the given 'string' can be evaluated exactly using

$$P_{ji} = \frac{(e^h - 1)(1 - e^{-h})}{2h}e^{-|i-j|h} (j \neq i);$$
$$P_{jj} = \frac{h - e^{-h} - 1}{h}.$$

It can be verified that the sum over the second index is one.

The relaxation constant $\tilde{\kappa}$ is solution of the equation

$$\frac{h}{c} = h + \mathrm{e}^{-h} - 1 + \frac{\left(\mathrm{e}^{h} - 1\right)\left(1 - \mathrm{e}^{-h}\right)}{2} E,$$

where

$$E = \frac{\mathrm{e}^{-(1+\tilde{\kappa})h}}{1 - \mathrm{e}^{-(1+\tilde{\kappa})h}} + \frac{\mathrm{e}^{-(1-\tilde{\kappa})h}}{1 - \mathrm{e}^{-(1-\tilde{\kappa})h}}.$$

Limited expansion gives the result

$$\frac{\tilde{\kappa}}{\kappa} = 1 - \frac{ch^2}{6} + \cdots$$

c) Using

$$P_{ji} \simeq \frac{h}{2} \mathrm{e}^{-h|i-j|} \quad (j \neq i),$$

and P_{jj}, owing to complementarity

$$P_{jj} = 1 - \sum_{i \neq j} P_{ji} = 1 - \frac{h\mathrm{e}^{-h}}{1 - \mathrm{e}^{-h}}.$$

Hence, $\tilde{\kappa}$ is given by

$$\frac{1}{c} = 1 - \frac{h\mathrm{e}^{-h}}{1 - \mathrm{e}^{-h}} + \frac{h}{2} E,$$

with the same formula for E. Then, by limited expansions

$$\frac{\tilde{\kappa}}{\kappa} = 1 - \frac{c^2 h^4}{120} + \cdots$$

Owing to a fortuitous cancellation of errors, the terms of order h^2 vanish!

Exercise 14.14: Wigner, Bell-Wigner, and Carlvik appproximations

a) The boundary conditions are

$$\omega \longrightarrow 0 : \; P_{VV} \simeq \frac{Q}{2}\omega; \qquad \omega \longrightarrow \infty : \; P_{VV} \simeq 1 - \frac{1}{\omega};$$

where $Q = \langle X^2 \rangle / \langle X \rangle^2$.

b) The Wigner approximation obeys the asymptotic behaviour

$$\omega \longrightarrow 0 : \; P_{VV,W} \simeq \omega; \qquad \omega \longrightarrow \infty : \; P_{VV,W} \simeq 1 - \frac{1}{\omega}.$$

c) For the Bell-Wigner approximation,

$$\omega \longrightarrow 0 : \; P_{VV,B-W} \simeq \frac{\omega}{b}; \qquad \omega \longrightarrow \infty : \; P_{VV,B-W} \simeq 1 - \frac{b}{\omega},$$

it obeys the behaviour at the origin — but not at infinity — provided that $b = 2/Q$. For example, $b = 3/2$ for a cylinder. For intermediate ω, intermediate values of b can be used.

d) The Carlvick approximation gives

$$\omega \longrightarrow 0 : \; P_{VV,C} \simeq \omega\left(\frac{\alpha}{\beta} - \frac{\gamma}{\delta}\right); \qquad \omega \longrightarrow \infty : \; P_{VV,C} \simeq \alpha - \gamma - \frac{\alpha\beta - \gamma\delta}{\omega}.$$

This suggests that

– *Origin:* $\alpha/\beta - \gamma/\delta = Q/2$;

– *Infinity:* $\alpha - \gamma = 1 \qquad \alpha\beta - \gamma\delta = 1$.

However, there are only three equations with four unknowns; the proposed choice is the simplest one.

e) The following table gives some numerical examples.

ω	Exact	Wigner	(%)	Bell-W.	(%)	Carlvik	(%)
0.04	0.02561	0.03846	50.18	0.02597	1.42	0.02606	1.75
0.08	0.04967	0.07407	49.13	0.05063	1.94	0.05095	2.58
0.2	0.11494	0.16666	44.95	0.11765	2.32	0.11932	3.77
0.4	0.20697	0.28571	38.05	0.21053	1.72	0.21579	4.21
0.6	0.28351	0.37500	32.27	0.28571	0.78	0.29487	4.01
0.8	0.34838	0.44444	27.57	0.34783	−0.16	0.36090	3.59
1.2	0.45225	0.54545	20.61	0.44444	−1.73	0.46429	2.66
2	0.59285	0.66667	12.45	0.57143	−3.61	0.60000	1.21
3	0.69843	0.75000	7.38	0.66667	−4.55	0.70000	0.22
4	0.76355	0.80000	4.77	0.72727	−4.75	0.76190	−0.22
5	0.80677	0.83333	3.29	0.76923	−4.64	0.80357	−0.40
10	0.90077	0.90909	0.92	0.86957	−3.46	0.89744	−0.37

Notice that the Wigner approximation always overestimates the probability P_{VV}, and by a large relative amount for the small values of the opacity ω. The Bell-Wigner approximation improves the situation for the small opacities, but greatly underestimates the exact values of P_{VV} for the large values of ω. The Carlvik approximation satisfies both for the small and large values of ω, with good accuracy for the intermediate opacities. Furthermore, within the Bell-Wigner approximation, the sign of the error changes according to ω, and some compensation may occur; for example, in resonant-absorption calculations.

D. Treatment of the integral and differential forms

Exercise 14.15: unknows of the 'diamond scheme' calculation

The treatment of the Boltzmann equation must be performed in a rectangle limited horizontally by $x_{\min} \le x \le x_{\max}$, or $r_{\min} \le r \le r_{\max}$, and vertically by $-1 \le \mu \le +1$. This rectangle is itself divided into rectangular meshes. This introduces two kinds of unknowns: the fluxes at the intersections of the boundaries of the rectangles, and at their centres. In the 'diamond scheme' the unknown fluxes at the centres of the edges of the rectangles are also introduced.

In a planar geometry, the transport operator contains only a derivative with respect of x. To invert this operator, it is possible to keep only the unknowns at the centres of the meshes, and at the centres of the vertical edges. Indeed, when a mesh is treated,

- the source and the collision rates are considered at the mesh centres; and
- the derivative with respect of x is evaluated from the difference between two fluxes at neighbouring vertical edge centres.

The equations can be treated sequentially along x for the various discrete values of μ, following the direction of the neutrons, i.e.

- from the left and the entering flux (generally zero) when μ is positive; and
- from the right and the entering flux (also generally zero) when μ is negative.

N.B: an even value of N is always chosen for discrete ordinate calculations, to avoid the centres of the mesh from falling on the equator ($\mu = 0$).

In spherical geometry, the transport operator contains derivatives with respect to both r and μ. This is because some coordinate lines are curved while the neutrons travel in straight lines. To invert the transport operator, implies unknowns are needed at the mesh centres. These express the sources and the collision rates. Similarly, unknowns are needed at the vertical edge centres (to express the derivatives with respect of r), and at the horizontal edge centres (to express the derivatives with respect of μ). When a mesh is treated, the neutron balance equation has to be completed with two 'diamond' equations which permit these supplementary unknowns to be found, i.e.

- the half-sum of the fluxes on the horizontal edge centres = the flux at the mesh centre; and
- the half-sum of the fluxes on the vertical edge centres = the flux at the mesh centre.

As before, the equations can be treated sequentially along r, for each discrete value of μ, in the direction of the neutrons.

Note: in the 'diamond scheme', the fluxes at the mesh vertices are not introduced.

Exercise 14.16: maximum of the space mesh

For the discretised solution,

$$\Phi_i = \Phi_{i-1} \frac{1 - (h\Sigma)/(2\mu)}{1 + (h\Sigma)/(2\mu)} = \Phi_{i-1} \, e^{-\tilde{\kappa}h}.$$

If h is small, then $\tilde{\kappa} \to \kappa$. Clearly, h must not be greater than $2\mu/\Sigma$, otherwise some fluxes would be negative. This condition is the most restrictive for $\mu = \mu_1$. Using $h = \varepsilon\mu_1/\Sigma$, ε must be less than (preferably much less than) 2.

Example: the radius of the sphere: 228.5 mm. Using regular meshes according to the latitude, $\mu_1 = \sin \pi/(2N)$.

- $\mathbf{S_4}$: $\mu_1 = 0.38268$; $h = 0.012756$; 1 792 meshes;
- $\mathbf{S_8}$: $\mu_1 = 0.19509$; $h = 0.006503$; 3 514 meshes;
- $\mathbf{S_{16}}$: $\mu_1 = 0.09802$; $h = 0.003267$; 6 995 meshes.

Exercise 14.17: Milne's problem

a) In $\mathbf{P_1}$ and $\mathbf{P_3}$ approximations, the equations are

$$-\frac{1}{3}\varphi_1' = 0,$$

$$-\varphi_0' - \Sigma\varphi_1 = 0;$$

and

$$-\frac{1}{3}\varphi_1' = 0,$$

$$-\varphi_0' - \frac{2}{5}\varphi_2' - \Sigma\varphi_1 = 0,$$

$$-\frac{2}{3}\varphi_1' - \frac{3}{7}\varphi_3' - \Sigma\varphi_2 = 0,$$

$$-\frac{3}{5}\varphi_2' - \Sigma\varphi_3 = 0,$$

respectively.

b) In $\mathbf{P_1}$ approximation, the solution takes the form

$$\varphi_0 = a + bx, \qquad \varphi_1 = -\frac{b}{\Sigma},$$

$$\Phi(x,\mu) = a + bx - \frac{b\mu}{\Sigma}, \qquad \Phi(x) = 2(a + bx),$$

where a and b are constants.

The last relationship shows that the scalar flux goes to zero at the abscissa $x = d = -a/b$, known as the extrapolation distance.

The phase flux at the interface is

$$\Phi(0,\mu) = a - \frac{b\mu}{\Sigma}.$$

When the integral of this *phase flux* over the negative values of μ is zero, $b = -2a\Sigma$; therefore, the reduced extrapolation distance is $\Sigma d = 1/2$. When the integral over the negative values of μ of the *phase current*, $\mu\,\Phi(0,\mu)$ is zero, $b = -3a\Sigma/2$; therefore, the reduced extrapolation distance is $\Sigma d = 2/3$. This last value — which corresponds to the diffusion approximation — is based on a more physical criterion, namely a null total entering current. Hence, this implies that it is nearer to the exact value, 0.710446.

c) In $\mathbf{P_3}$ approximation, a fourth (and transitory) term is added to the previous expression of the phase flux:

$$c\left[1 - \frac{5}{2}P_2(\mu) + \frac{\sqrt{35}}{2}P_3(\mu)\right]\exp\left(\frac{\sqrt{35}}{3}\Sigma x\right).$$

When the moments of orders 0 and 1 of the flux, or the moments of orders 1 and 2 of the current, are zero,

$$\Sigma d = \frac{160 - 3\sqrt{35}}{195} = 0.7295 \qquad \text{and} \qquad \Sigma d = \frac{11}{3} - \frac{\sqrt{35}}{2} = 0.7086,$$

respectively. The second approximation is better: the error is about −0.26% instead of +2.68%.

Exercise 14.18: even-odd formulation of the Boltzmann equation

a) With the hypotheses, the equation to be solved is

$$\vec{\Omega}.\overrightarrow{\text{grad}}\Phi(\vec{r},\vec{\Omega}) + \Sigma_t(\vec{r})\,\Phi(\vec{r},\vec{\Omega}) =$$

$$\frac{\nu\Sigma_f(\vec{r})}{4\pi}\int_{(4\pi)}\Phi(\vec{r},\vec{\Omega}')\,d^2\Omega' + \int_{(4\pi)}\frac{\Sigma_{s0}(\vec{r}) + 3\Sigma_{s1}(\vec{r})\,\vec{\Omega}'\cdot\vec{\Omega}}{4\pi}\Phi(\vec{r},\vec{\Omega}')\,d^2\Omega'.$$

b) Substitute $\Phi = \psi + \chi$ into the equation, and express the even and odd parts as follows.

$$\vec{\Omega}\cdot\overrightarrow{\text{grad}}\chi(\vec{r},\vec{\Omega}) + \Sigma_t(\vec{r})\,\psi(\vec{r},\vec{\Omega}) =$$

$$\frac{\nu\Sigma_f(\vec{r})}{4\pi}\int_{(4\pi)}\psi(\vec{r},\vec{\Omega}')\,d^2\Omega' + \frac{\Sigma_{s0}(\vec{r})}{4\pi}\int_{(4\pi)}\psi(\vec{r},\vec{\Omega}')\,d^2\Omega';$$

$$\vec{\Omega}\cdot\overrightarrow{\text{grad}}\psi(\vec{r},\vec{\Omega}) + \Sigma_t(\vec{r})\,\chi(\vec{r},\vec{\Omega}) = \frac{3\Sigma_{s1}(\vec{r})}{4\pi}\vec{\Omega}\cdot\left[\int_{(4\pi)}\vec{\Omega}'\,\chi(\vec{r},\vec{\Omega}')\,d^2\Omega'\right].$$

c) When the scattering is isotropic, i.e. Σ_{s1} is null, the right hand side of the second equation is zero, and this equation gives explicitly

$$\chi(\vec{r},\vec{\Omega}) = -\frac{1}{\Sigma_t(\vec{r})}\vec{\Omega}\cdot\overrightarrow{\text{grad}}\psi(\vec{r},\vec{\Omega}).$$

Substituting this into the first equation, yields an equation governing only the unknown function ψ:

$$-\vec{\Omega}\cdot\overrightarrow{\text{grad}}\left[\frac{1}{\Sigma_t(\vec{r})}\vec{\Omega}\cdot\overrightarrow{\text{grad}}\psi(\vec{r},\vec{\Omega})\right] + \Sigma_t(\vec{r})\,\psi(\vec{r},\vec{\Omega}) =$$

$$\frac{\nu\Sigma_f(\vec{r})}{4\pi}\int_{(4\pi)}\psi(\vec{r},\vec{\Omega}')\,d^2\Omega' + \frac{\Sigma_{s0}(\vec{r})}{4\pi}\int_{(4\pi)}\psi(\vec{r},\vec{\Omega}')\,d^2\Omega'.$$

Notice that only the even flux need be calculated when only the reaction rates or associated quantities are wanted (power distribution, multiplication factor, etc.) This explains the purpose of eliminating χ.

The elimination of χ is similar to the elimination, in the diffusion approximation, of the current $\vec{J}$ between the balance equation and Fick's law, in order to get an equation containing only the flux Φ.

d) For a given and fixed value of $\vec{\Omega}$, the first term is a combination of second derivatives of ψ; hence, may be expressed as

$$-\sum_k \Omega_k \frac{\partial}{\partial k}\left[\frac{1}{\Sigma_t}\sum_\ell \Omega_\ell \frac{\partial \psi}{\partial \ell}\right],$$

where k and ℓ represent x, y, and z. This operator is very similar to the streaming operator in diffusion approximation:

$$-\text{div}\left[\frac{1}{3\Sigma_{tr}}\overrightarrow{\text{grad}}\,\Phi\right] = -\sum_k \frac{\partial}{\partial k}\left[\frac{1}{3\Sigma_{tr}}\frac{\partial \Phi}{\partial k}\right].$$

Except for the replacement of the scalar flux with the integral of the even phase flux, the three other terms are the same as the ones which appear in diffusion theory.

Finally, it appears that the algorithm needed to solve the equation for the even flux can be a simple adaptation of an existing code solving the diffusion equation. All the modules concerning the multigroup treatment, the iterations, the feedbacks, the evolution, etc. are indeed the same. Only the treatment of the phase variable $\vec{\Omega}$ must be added, and the treatment of the streaming operator slightly modified. The phase treatment can be made by one of the usual techniques: spherical harmonics, complete or simplified, discrete ordinates, etc. The following demonstrates that this conclusion remains true even when the anisotropy of the scattering is taken into account.

e) Compare the even-odd splitting to the spherical harmonic expansion, and notice that ψ is the sum of the harmonic terms of even orders n and χ, the sum of the harmonic terms of odd orders n. Therefore, the proposed approximation consists of keeping its main term $n = 1$ for χ only. Recall that the three first-order spherical harmonics can be replaced with the three components of the vector $\vec{\Omega}$; hence, the proposed expression.

With this hypothesis, the term between brackets in the second equation of part **b** is a vector with components

$$\int_{(4\pi)} \Omega'_k \sum_\ell u_\ell \,\Omega'_\ell \, d^2\Omega' = \frac{4\pi}{3} u_k,$$

since the integrals of the rectangle terms are equal to zero. The right hand side of this equation is, therefore,

$$\Sigma_{s1}\,\vec{\Omega}\cdot\vec{u} = \Sigma_{s1}\,\chi.$$

Notice again that χ can be expressed explicitly by simply replacing Σ_t with the transport cross-section:

$$\Sigma_{tr} = \Sigma_t - \Sigma_{s1},$$

taken from part **c**.

f) Consider again the equation of χ obtained in part **b**, then use

$$\vec{v}(\vec{r}) = \int_{(4\pi)} \vec{\Omega}'\,\chi(\vec{r},\vec{\Omega}')\,d^2\Omega'.$$

Hence,

$$\vec{\Omega}\cdot\overrightarrow{\text{grad}}\psi(\vec{r},\vec{\Omega}) + \Sigma_t(\vec{r})\,\chi(\vec{r},\vec{\Omega}) = \frac{3\Sigma_{s1}(\vec{r})}{4\pi}\,\vec{\Omega}\cdot\vec{v}(\vec{r}).$$

Multiply this by $\vec{\Omega}$ and integrate over all the directions $\vec{\Omega}$ in order to get $\vec{v}$ in the second term of the left hand side. This gives

$$\int_{(4\pi)} \vec{\Omega} \left[\vec{\Omega} \cdot \overrightarrow{\text{grad}}\psi(\vec{r}, \vec{\Omega}) \right] d^2\Omega + \Sigma_t(\vec{r})\, \vec{v}(\vec{r}) = \Sigma_{s1}(\vec{r})\, \vec{v}(\vec{r}).$$

The term on the right hand side of the equation is solved in a similar manner to before. It then allows $\vec{v}$ to be found. Hence, when substituted into the equation for χ, this gives $\chi(\vec{r}, \vec{\Omega})$. Finally, this leaves an equation for ψ only, when the expression for χ found in part **b** is substituted into the equation. Notice that this equation for ψ is exact when the scattering is assumed to be linearly anisotropic.

E. Fundamental mode

Exercise 14.19: elementary eigenfunctions of the Laplace operator

a) For a rectangular parallelepiped of edges equal to π/u, π/v and π/w, where u, v and w are the components of the vector $\vec{b}$,

$$f(x, y, z) = \sum_1^8 \exp\left[-i(\pm ux \pm vy \pm wz) \right] = 8 \cos ux \cos vy \cos wz.$$

b) For a cylinder of radius $j_{01}/\sqrt{u^2 + v^2}$ and of height π/w,

$$f(\rho, z) = \sum_1^2 \int_{(2\pi)} \exp\left[-i(\beta\rho \cos\varphi \pm wz) \right] d\varphi = 2\pi J_0(\beta\rho) \cos wz$$

$$(\beta^2 = u^2 + v^2).$$

c) For a sphere of radius π/b,

$$f(r) = \int_{(4\pi)} \exp(-ibr\cos\theta)\, \sin\theta\, d\theta\, d\varphi = 4\pi \frac{\sin br}{br}.$$

Exercise 14.20: diffusion coefficient in fundamental mode

a) The equations giving φ and s are

$$ib\mu\, \varphi(\mu) - \Sigma\, \varphi(\mu) + \int_{-1}^{+1} \Sigma_s(\mu' \longrightarrow \mu)\, \varphi(\mu')\, d\mu' + \frac{s}{2} = 0;$$

$$s = \nu\Sigma_f \int_{-1}^{+1} \varphi(\mu)\, d\mu.$$

b) Now notice that

$$\Phi(x) = \int_{-1}^{+1} \Phi(x, \mu)\, d\mu, \qquad J_x(x) = \int_{-1}^{+1} \Phi(x, \mu)\, \mu\, d\mu,$$

and that $P_0(\mu) = 1$ and $P_1(\mu) = \mu$; then, take into account the orthogonality and normalisation relationships of the Legendre polynomials.

c) Substituting the expansion into Legendre polynomials, gives

$$-(\Sigma - ib\mu)\sum_{n=0}^{\infty}\varphi_n P_n(\mu) + \sum_{n=0}^{\infty}\Sigma_{s,n}\varphi_n P_n(\mu) + \frac{s}{2}P_0(\mu) = 0.$$

d) After division by $\Sigma - ib\mu$, and projection on to each Legendre polynomial, the result is

$$-\frac{2}{2k+1}\varphi_k + \sum_{n=0}^{\infty}G_{kn}\Sigma_{s,n}\varphi_n + \frac{s}{2}G_{k0} = 0.$$

It more judicious to project to the Legendre polynomials after having divided by $\Sigma - ib\mu$ because it is possible to restrict the expansion of the differential scattering cross-section to only few terms, while the projection of the initial equation would give a $\mathbf{P_N}$ type system of equations which would require a very many terms for the flux expansion.

The G coefficients can finally be calculated, where the first ones are

$$G_{00} = \frac{2\xi}{\Sigma}; \qquad G_{01} = G_{10} = \frac{2i\left(1-\xi\right)}{b}; \qquad G_{11} = \frac{2\Sigma\left(1-\xi\right)}{b^2};$$

with

$$\xi = \frac{\Sigma}{b}\arctan\frac{b}{\Sigma}.$$

e) Noticing that $s = 2\nu\Sigma_f\varphi_0$ and using the first and the second equations to get φ_0 and φ_1, gives an equation expressing the neutron balance (production = absorption + leakage) and a formula giving the diffusion coefficient

$$D = \frac{1}{3\gamma\Sigma},$$

where

$$\gamma = \frac{\frac{b}{3\Sigma}\arctan\frac{b}{\Sigma}}{1-\frac{\Sigma}{b}\arctan\frac{b}{\Sigma}} \simeq 1 + \frac{4}{15}\left(\frac{b}{\Sigma}\right)^2.$$

f) Provided the scattering is assumed to be linearly anisotropic — i.e. only the two first moments $\Sigma_{s,0}$ and $\Sigma_{s,1} \equiv \bar{\mu}\,\Sigma_{s,0}$ of the scattering law are retained—then it is still possible to deduce the neutron balance and the diffusion coefficient from the two first equations. For this last one, the expression which is obtained—beyond the 'buckling correction' by the coefficient γ—shows also the transport correction:

$$D = \frac{1}{3\left(\gamma\Sigma - \bar{\mu}\Sigma_s\right)}.$$

At the limit $\gamma = 1$, the usual expression $1/3\Sigma_{tr}$ for the diffusion coefficient is obtained.

g) More generally, the so-called $\mathbf{B_N}$ approximation consists of keeping the first moments of the scattering law up to order N. The $N+1$ first equations constitute a system giving the $N+1$ first unknown coefficients $\varphi_0, \varphi_1, \cdots, \varphi_N$, and particularly the diffusion coefficient $D = \varphi_1/(3ib\varphi_0)$ for the fundamental mode.

Exercise 14.21: Behrens's correction

a) Per unit of time, the number of collisions (therefore of paths) is $V_m\Sigma_m\Phi$, and the number of entrances into a cavity is SJ with $J = \Phi/4$. The ratio of these rates is the fraction γ of the paths crossing a cavity. N.B. this 'γ' has no relation with the 'γ' of the previous exercise.

$$\gamma = \frac{S}{4V_m\Sigma_m}.$$

b) It was shown previously in exercise **3.2** that

$$\langle \rho_m \rangle = \frac{1}{\Sigma_m}; \qquad \langle \rho_m^2 \rangle = \frac{2}{\Sigma_m^2}.$$

c) The Cauchy theorem gives

$$\langle \rho_c \rangle = \frac{4V_c}{S}.$$

Then from the definition of the factor Q,

$$\langle \rho_c^2 \rangle = Q \langle \rho_c \rangle^2.$$

Therefore,

$$\langle (\vec{\rho}_{m1} + \vec{\rho}_c + \vec{\rho}_{m2})^2 \rangle = \frac{6}{\Sigma_m^2} + 4\frac{4V_c}{S\Sigma_m} + Q(\frac{4V_c}{S})^2.$$

d) The two last terms of the right hand side represent the *increase* of the mean square of the paths crossing a cavity. When it is multiplied by γ, the mean increase of the squared paths, either crossing or not crossing a cavity, is obtained. Finally, multiplying by the mean number of paths, $\langle n \rangle = \Sigma_m/\Sigma_{am}$, and dividing by six, gives the increase of the diffusion area:

$$\Delta L^2 = \frac{2V_c}{V_m}\left(1 + Q\frac{V_c\Sigma_m}{S}\right)\frac{1}{3\Sigma_m\Sigma_{am}} = \frac{2V_c}{V_m}\left(1 + Q\frac{V_c\Sigma_m}{S}\right)L_m^2.$$

By combining with the homogenisation formula for the absorption cross-section, the result for the diffusion coefficient is

$$D = (1 + h)\, D_m,$$

where D_m is the moderator diffusion coefficient, and where

$$h = \frac{V_c}{V_c + V_m}\left(1 + 2Q\frac{V_c\Sigma_m}{S}\right)$$

is the heterogeneity correction. This last correction is *not* a simple homogenisation formula, due to it being an average of *squared* quantities.

e) For a cylinder, $Q = 4/3$, the result is $h = 0.585$.

F. Monte Carlo method

Exercise 14.22: power law probability distribution

Since the n events are independent, the distribution function $F(x)$ of the maximum of the random values is x^n, i.e. the probability that the first selection gives a value smaller than x, multiplied by the probability that the second selection gives a value smaller than x, ..., multiplied by the probability that the n^{th} selection gives a value smaller than x. In other words, the appropriate probability law is $P(x)\,dx = dF = n\,x^{n-1}\,dx$, in the interval $[0, 1[$.

It is also possible to make the selection in one step by applying directly the function $y = x^n$, and then taking its n^{th} root; however, this is expected to require a greater amount of computer time.

Exercise 14.23: random point inside a circle

a) This method of selection is biased toward a greater probability of giving a point near the centre than near the periphery.

b) The distribution is uniform provided that $\rho^2 = \xi_1$, and $\varphi = 2\pi\xi_2$. For the radius, the calculation of the square root can be replaced with a double selection and subsequent search for the maximum—see the previous exercise.

c) This method gives a uniform distribution; however, $1 - \pi/4 = 21.5\%$ of the double selections will give a point outside the circle, which will be rejected.

Exercise 14.24: Buffon's needle problem

a) This probability is $2/\pi$.

b) Let X be the random variable which value is zero when the needle rests on one strip, and one when it lies across two slats. The mathematical expectation of X is $2/\pi$, and the standard deviation is

$$\sigma = \sqrt{2/\pi - 4/\pi^2} = 0.481.$$

After n trials, this standard deviation is reduced by a factor $\sqrt{n}$; for example, when $n = 10\,000$, $\sigma = 0.5\%$.

Exercise 14.25: evaluation of a resonance escape probability

A suitable algorithm is as follows.

- `repeat;`
  - `select a neutron possessing lethargy` u' `chosen uniformly at random within a length` ε `before the trap;`
  - `increment the lethargy by a random amount chosen according to the formula`

$$P(u)\,du = \frac{e^{-(u-u')}}{1-\alpha}\,du, \qquad 0 < u - u' < \varepsilon;$$

```
    – if u is beyond the trap, then increment the counter
      'surviving-neutrons';
    – if u is inside the trap, then increment the counter
      'captured-neutrons';

      /* else u is still before the trap, so continue; */

  – until sufficient trials have been conducted;

  – calculate statistical parameters;

  – output the results;

  – stop.
```

Recall that the exact expression of the probability to escape the trap is

$$p = 1 - \frac{1 - e^{-\gamma} - \alpha\gamma}{\xi(1 - \alpha)}.$$

15 Theory of Resonant Absorption of Neutrons

Introduction

Chapter 8 ended with a discussion of the physical aspects of the resonant absorption of neutrons and listed some calculation and modelling problems, which were deliberately put aside for later. We now return to the subject of resonant absorption of neutrons in order to clarify these theoretical aspects (although we do not claim to be giving a detailed analysis of this difficult problem of neutron physics) to give the reader an overview of the types of problem that can be solved by codes such as APOLLO-2, and of the points that still create some difficulties.

The main assumption made from the beginning, which was already applied in Chapter 8 (§ 8.1) was that the resonant material was purely absorbent. By applying the approach used by Michel Livolant and his doctoral student Françoise Jeanpierre in the late 1960s, we saw how to allow for scattering and slowing down by the resonant material, which affect the aspects that we introduced (self-shielding factors, heterogeneous-homogeneous equivalence, Dancoff effect, Doppler effect). This theory was introduced at that time in the first version of APOLLO. With the new developments introduced in Version 2 of this code, there was renewed interest in the theory of resonant absorption of neutrons, because the inadequacies of Livolant and Jeanpierre's original theory had been clearly identified. We shall now present these developments.

15.1. Energy scales of different neutron physics problems

Broadly speaking, neutron physics problems need to be solved at three levels of precision with respect to the energy variable:

1/ In the epithermal domain, the many resonances of heavy nuclei such as uranium 238 typically require *a few tens of thousands of energy groups* in order to properly describe each of the resonances. It is not essential to handle the heterogeneities very precisely at this level; in fact, as we have seen, by using an equivalence we can relate the real geometry to a *homogeneous geometry*.

2/ Handling the spectrum requires about *a hundred energy groups*; this can be done at the assembly constituting the elementary "mesh" of the core of a nuclear reactor,

but it requires "microscopic" heterogeneity to be taken into account; this means on the scale of the fuel element or assembly.

3/ In practice, the multiplication factor of a core and the power distribution in it can be calculated to a few energy groups only, e.g. two groups for the usual calculations for pressurised water reactor cores. This calculation takes "macroscopic" heterogeneity into account, i.e. the differences between assemblies and axial variations.

These three types of calculation must be performed one after the other: when calculations have been carried out at a given level, the mean values in space (homogenisation) and energy (condensation) must be taken in order to prepare for the calculation at the next level[1].

Chapter 17 mentions the passage from level **2** to level **3**. Here we shall concentrate on the passage from the first to the second level.

15.2. The heterogeneous-homogeneous equivalence: choice of Bell factor

15.2.1. Principle of pre-tabulations (review)

In Chapter 8, three key points of the Livolant–Jeanpierre theory were presented:

1/ The passage from an actual situation to a "fine structure" situation characterised by a macroscopic flux that is constant in lethargy and uniform in space.

2/ A heterogeneous-homogeneous equivalence, which we are about to describe in greater detail.

3/ A continuous-multigroup equivalence, which has not yet been mentioned but will be presented in the next section.

The heterogeneous-homogeneous equivalence leads to the concept of pre-tabulation in a homogeneous medium which, when the resonant nucleus and its temperature have been defined, turns out to be characterised by a single parameter: the dilution cross-section σ_d. It can therefore easily be explored and tabulated once and for all.

This tabulation can concern the effective resonance integral I_{eff}, which characterises all resonances. With a view to the assembly calculation (Level **2**) that follows, using the APOLLO code, for example, it is preferable to tabulate by group. In this case, we refer to *"effective reaction rates"* rather than an *"effective integral",* but the idea remains the same, except for the limits of the integral used in the expression:

$$\int \sigma_{a,\text{eff}}(u)du \quad \text{with:} \quad \sigma_{a,\text{eff}}(u) = \varphi(u)\sigma_{a,0}(u). \tag{15.1}$$

We must now specify how the equivalence between the heterogeneous situation under consideration and a homogeneous situation can be established.

[1] More precisely, as we shall see, these are "equivalences" that aim to match the reaction rates as closely as possible, these being the only truly relevant physical parameters in this case because they can be measured.

15.2.2. Principle of heterogeneous-homogeneous equivalence

As we have seen (Figure 8.5, § 8.3.2), the equivalent section $\sigma_e(u)$ of the heterogeneous case is almost a constant. In practice, *a Bell factor b* must be chosen.

This is the ratio $\bar{\sigma}_e/\sigma_{e,\infty}$ between the unique value $\bar{\sigma}_e$ that will be adopted and the asymptotic value $\sigma_{e,\infty}$ of the equivalent section for an infinite cross-section of the resonant material.

The principle applied is very simple: the essential parameter of the problem must be observed. This is the effective integral:

$$I_{\text{eff, heterogeneous}} = I_{\text{eff, homogeneous}}. \tag{15.2}$$

The left-hand side has a given value, and the right-hand side is a function of the dilution cross-section σ_d which characterises the "equivalent" homogeneous medium. The equality (theoretically) defines the value of σ_d, and therefore this equivalent homogeneous medium. We say "theoretically" because the left-hand side is unknown; in fact, it is what we are looking for!

That is why this equation will be re-written in a simplified context: on the one hand, the exact equation for slowing down by the resonant material will be replaced by a simplified model, and on the other hand, the real problem will be replaced by another simplified problem, the **P** problem where the macroscopic flux Ψ is "flat" in lethargy and space. The equivalent cross-section $\bar{\sigma}_e$ or the associated Bell factor b is therefore defined by the following equation:

$$I_{\text{eff, heterogeneous, model, "P" problem}} = I_{\text{eff, homogeneous, model, "P" problem}}. \tag{15.3}$$

Note: This heterogeneous-homogeneous equivalence can apply to the entire resonant domain or to several macrogroups or all resonant groups in the intermediate (Level **2**) multigroup mesh.

15.2.3. Definition of the simplified problem

This "**P**" problem, where the macroscopic function Ψ is "flat" in space and lethargy, gives rise to the fine structure equation (§ 8.2.1 and 8.3.1):

$$r_0\varphi + \sigma_e = (\sigma_0 + \sigma_e)\varphi. \tag{15.4}$$

Its solution φ is interpreted physically as the flux that would exist if the non-resonant materials (moderator etc.) were replaced by purely absorbent materials without changing their total cross-section, and if a neutron source were added with intensity equal to the cross-section of these non-resonant materials.

15.2.4. Implementation with the "narrow resonance" model

If slowing down by resonant nuclei is dealt with using the "narrow resonance" assumption (§ 8.2.2):

$$r_0\varphi \simeq \sigma_{p,0}, \quad \varphi(u) \simeq \varphi_{NR}(u) = \frac{\sigma_{p,0} + \sigma_e(u)}{\sigma_0(u) + \sigma_e(u)}, \tag{15.5}$$

[$\sigma_e(u)$ is replaced by σ_d for the homogeneous case], the heterogeneous-homogeneous equivalence equation is written as:

$$\int \frac{\sigma_{p,0} + \sigma_e(u)}{\sigma_0(u) + \sigma_e(u)} \sigma_{a,0}(u) du = \int \frac{\sigma_{p,0} + \sigma_d}{\sigma_0(u) + \sigma_d} \sigma_{a,0}(u) du, \tag{15.6}$$

where σ_d is the unknown value to be determined, and the equivalent cross-section of the heterogeneous case must be calculated by its definition formula (§ 8.3.1):

$$\sigma_e(u) = \frac{\sigma_0(u)[1 - P_{00}(u)]}{P_{00}(u)}. \tag{15.7}$$

Note that P_{00} depends on the lethargy u because it is a function of σ_0 which, in turn, is dependent on u; similarly, σ_e is actually a function of σ_0. To calculate these integrals, it is therefore simpler to avoid using the lethargy u and instead to use the total cross-section σ_0 of the resonant nucleus as the integration variable[2]. The equivalence equation is written as:

$$\int \frac{\sigma_{p,0} + \sigma_e(\sigma_0)}{\sigma_0 + \sigma_e(\sigma_0)} \pi(\sigma_0) d\sigma_0 = \int \frac{\sigma_{p,0} + \sigma_d}{\sigma_0 + \sigma_d} \pi(\sigma_0) d\sigma_0. \tag{15.8}$$

The boundaries of the integrals are now the extreme values of the total cross-section σ_0 of the resonant nucleus; the equivalent cross-section σ_e is considered as a function of σ_0; the "weight function" π is defined as follows: $\pi(\sigma_0)d\sigma_0$ is the sum of all the elements $\sigma_{a,0}(u)du$ for all lethargy intervals du where the total cross-section of the resonant nucleus is between σ_0 and $\sigma_0 + d\sigma_0$. This density π is obviously rather difficult to calculate, because to do this would require listing all the resonances, but this calculation can be performed once and for all like the effective integral tabulations. This second form of the equivalence equation is far simpler to implement than the first, because some very complicated functions of the lethargy u are replaced by far more regular functions of the cross-section σ_0. In practice, it suffices to tabulate π for a small number of values of σ_0, and then to calculate P_{00} and σ_e for the σ_0 values of the table for each case and to evaluate the integrals using a quadrature formula.

15.2.5. Implementation with the "wide resonance" model

If we choose to use the "wide resonance" approximation (§ 8.2.2):

$$r_0\varphi \simeq \sigma_{s,0}\varphi, \quad \varphi(u) \simeq \varphi_{WR}(u) = \frac{\sigma_e(u)}{\sigma_{a,0}(u) + \sigma_e(u)}, \tag{15.9}$$

a similar equivalence procedure can be implemented. It is, however, slightly more complicated because a weight must be tabulated as a function of both variables: σ_0 and $\sigma_{a,0}$.

[2] This type of change of variable where the second variable is not a monotonic function of the first is called the "Lebesgue integration technique".

15.2.6. Examining the width of resonances: example of uranium 238

To decide which model is better in practice, we need to compare the width of the resonance at the energy interval that can be reached when scattering occurs. This interval can be estimated (in terms of energy) by the product $\varepsilon_0 \times E_0$ where E_0 is the energy at the resonance peak, i.e. approximately the energy of the neutrons concerned and where ε_0, the maximum lethargy gain during scattering by a resonant nucleus, is approximately the maximum relative change in energy. The nuclear width Γ is not the relevant parameter for evaluating the width of the resonance. Using the Breit-Wigner formula, we can see that it is the width at half the height of the peak, but half the cross-section at the peak is still practically infinite. The relevant width is therefore likely to be significantly greater than Γ. In general, we use the "practical width", defined as the energy interval where the resonant cross-section exceeds the potential cross-section, i.e. where the total cross-section is more than double the asymptotic value. Using the Breit-Wigner formula (§ 2.7.1), neglecting the interference term, and noting that the cross-section at the peak, σ_{max}, is much larger than the potential cross-section, σ_p, the following expression is found for this practical width (where the index "0" is understood):

$$\Gamma_p \simeq \Gamma \sqrt{\sigma_{max}/\sigma_p}. \tag{15.10}$$

By way of example, if we take the resonances of uranium 238 that we listed (Table 2.4), we can create Table 15.1, where energies are expressed in eV and the last column is $\Gamma_p/(\varepsilon_0 E_0)$.

Ignoring any irregularities, it seems that the resonances are wider at low energies. A simple empirical model that is sometimes used involves handling all resonances above 50 eV with the "narrow resonance" model, and all resonances below 50 eV with the "wide resonance" model.

15.2.7. Macrogroup-by-macrogroup equivalence

If we wish to examine more than these two energy domains, an equivalence, and therefore a determination of the Bell factor, could be performed for each of the groups used for the spectrum calculation, in the APOLLO calculation groups for example. The model for the equivalence can be chosen differently for each group. In any case, because the equivalence error is second-order with respect to the error of the model itself, the choice of best model is not very important.

15.3. Continuous-multigroup equivalence

15.3.1. Why calculate the real flux rather than the macroscopic flux?

After introducing the factorisation $\Phi = \varphi\Psi$ and applying the principle of pre-tabulating the microscopic aspect φ, it would seem logical to try to calculate the macroscopic flux Ψ. But this was not the recommendation of the authors of the theory, who suggested the opposite

Table 15.1. Estimation of the width of the first resonances of uranium 238 (σ_p = 8.9 barns; ε_0 = 0.0170).

Energy of peak	Nuclear width	Practical width	Slowing down interval	Ratio
6.674	0.024	1.27	0.11	11.3
20.871	0.033	2.19	0.35	6.3
36.682	0.057	3.96	0.62	6.4
66.032	0.048	2.30	1.11	2.1
80.749	0.025	0.41	1.36	0.30
102.56	0.095	4.43	1.72	2.6
116.902	0.048	1.77	1.97	0.90
145.66	0.024	0.20	2.45	0.08
165.29	0.026	0.40	2.78	0.14
189.67	0.196	7.26	3.19	2.3
208.51	0.075	2.33	3.50	0.66
237.38	0.052	1.32	3.99	0.33
273.66	0.048	1.15	4.60	0.25
291	0.039	0.82	4.89	0.17

approach of using the real flux Φ to avoid the approximation that was used to go from the real problem to the simplified "**P**" problem, i.e. the "flat macroscopic flux" approximation. (As seen in § 8.2.1, this approximation is expressed by: $R_0(\varphi\Psi) \cong \Psi R_0(\varphi)$, where R_0 is the operator for slowing down by the resonant material.)

We will obviously not try to calculate the real flux Φ in the ultra-fine lethargy mesh used to calculate all resonances (requiring around 20,000 groups to process the resonant domain), but in the usual multigroup mesh for the calculation of cells or assemblies (about twenty groups in this energy domain), which is far too coarse to describe the resonances. In fact, the whole purpose of resonant absorption theory is to avoid always having to perform the fine calculation. The remaining problem is therefore to be able to calculate the real flux Φ correctly on a coarse mesh.

15.3.2. Principle of continuous-multigroup equivalence

When we say "correctly" in neutron physics, we mean that the reaction rates —the only parameters that are actually measurable— are correct. It does not matter if the flux itself —a non-measurable parameter— is not accurate, as long as it leads to correct reaction rates. This assumes that the flux values are associated with cross-sections that lead to the right reaction rates.

Note also that, in neutron physics, flux values depend on cross-sections because they are obtained by solving the Boltzmann equation containing the cross-sections. In practice, version of this equation that has been simplified to some extent is always used. For example, for the present problem of calculating Φ, a wide multigroup approximation is used to handle a resonance problem that requires a practically continuous approach. The procedure applied to overcome this difficulty is known as "equivalence". This requires the approximate theory used (in this case, wide multigroup theory) to observe the reaction

rates. In this case, *multigroup cross-sections* will be sought that, in association with the multigroup flux values, will lead to correct reaction rates in each group.

Because there are obviously as many reaction rates as cross-sections[3], this criterion leads to an equal number of equations and unknowns (the multigroup cross-sections). Multigroup fluxes depend, via the Boltzmann equation, on the multigroup cross-sections to be determined, and so the equations defining these cross-sections are implicit. They must be solved by iteration[4].

This approach might appear reasonable, but unfortunately it is impossible to apply rigorously. Because it is based on the idea of observing the exact reaction rates, it assumes the rates to be known, which means assuming that we know the solution to the problem we are attempting to solve. That is why it will not be applied to the real problem, which has not yet been solved, by definition, but to a simplified problem. If the simplified problem is close to the real problem, we might hope that the multigroup cross-sections determined on the simplified problem and then used for the real problem will give, if not exact results to the real problem, then at least results that are very close to being exact.

In our example, we obviously choose the "**P**" problem as the simplified problem; on the one hand it is close to the real problem[5], and on the other hand, the reaction rates of this problem are known because we obtained them by interpolation in the effective reaction rate tables.

After being obtained by "continuous-multigroup equivalence" on the "**P**" problem, the multigroup cross-sections will be used to calculate the multigroup flux Φ of the real problem, and then the reaction rates.

We can conclude that the complete calculation of resonant absorption in a heterogeneous problem (cell, assembly, etc.) involves *two equivalences:*

– the "heterogeneous-homogeneous" equivalence, which is used to define the homogeneous situation that represents the heterogeneous situation under consideration, and then to determine the effective reaction rates by interpolation in the tables previously established for the homogeneous case;

– the "continuous-multigroup" equivalence, intended to establish the correct multigroup "averages" of the cross-sections which, when associated with the multigroup flux calculated with these cross-sections, will lead to the reaction rates just obtained as a result of the "heterogeneous-homogeneous" equivalence.

These two equivalences are applied to the same "**P**" problem (macroscopic flux that is absolutely "flat" in terms of space and lethargy), simplified with respect to the real problem, but representative of the self-shielding situation. With regard to the "lethargy" aspect, the first equivalence is also based on a model of slowing down by the resonant material.

Finally, with practically negligible errors, "Livolant-Jeanpierre" theory reduces the number of groups to be used by a factor of about 1000 (from 20,000 to 20), which greatly reduces the number of calculations to be performed.

[3] Capture, fission, scattering, etc. on the resonant material and non-resonant materials for each group.

[4] Note that the multigroup cross-sections thus determined are the "reasonable" averages of the true cross-sections; in particular, for a constant-lethargy cross-section, the multigroup cross-section is equal to this constant.

[5] The only difference between these two problems is the macroscopic function Ψ which varies slowly in the real problem, and is rigorously constant in the simplified problem.

15.4. "One-by-one" handling of situations with several resonant nuclei

15.4.1. The need to handle situations with several resonant nuclei

The theory discussed above, which was introduced into APOLLO code as soon as it had been put forward, applies to problems involving one and only one resonant material, since the other nuclei are considered to be non-resonant. In fact, we are always dealing with a mixture and/or juxtaposition of different types of resonant material:

– Initially, the fuel has at least two types of resonant nucleus, for example uranium isotopes 238 and 235; after irradiation, other resonant nuclei appear (isotopes of neptunium, plutonium, americium, etc.);

– Around the fuel there can be other materials with resonances (zirconium, hafnium, etc.);

– A single material, such as uranium, can be at different temperatures in different regions of space, and can therefore have resonances that are differently widened by the Doppler effect (for example, the uranium oxide in the fuel pellets of water reactors varies from a little over 300 °C at the surface to well over 1000 °C at the centre);

– A single resonant material can appear in elements with different characteristics (for example, the plutonium assemblies of water reactors have zones of fuel rods with different plutonium content), etc.

15.4.2. Principle of "one-by-one" handling

The only approach that is directly compatible with the assumptions sub-tending the Livolant-Jeanpierre theory is the "one-by-one" process: this is what the APOLLO code does. For the first resonant nucleus, all other nuclei, whether resonant or not, are considered to be non-resonant and are handled as such for the calculation of the equivalent dilution cross-section of the nucleus declared resonant. For the second resonant nucleus, the self-shielding calculation is repeated, with the assumption that all other nuclei, including the first resonant nucleus handled, are non-resonant. This proceeds until the last resonant nucleus.

In practice, for nuclei that are effectively resonant but considered as non-resonant at the stage of calculation reached, we adopt:

– Non-self-shielding average multigroup cross-sections (those found in the library) if the nucleus has not yet been processed.

– Self-shielding multigroup cross-sections (the ones from the continuous-multigroup equivalence) if the nucleus has been processed.

To reduce error as much as possible, the nuclei should be processed in decreasing order of resonant absorption rate (for example, for natural or slightly enriched uranium reactors: uranium 238 before uranium 235).

It would be possible to iterate this procedure in order to replace the cross-sections of all the nuclei that are actually resonant but considered to be non-resonant with self-shielding multigroup cross-sections, but this leads to results that are approximate in any case, and not necessarily better. In practice, this iteration is not performed, which saves on calculation time.

15.5. Extensions of the Livolant-Jeanpierre theory

With Version 2 of the APOLLO code, theoretical developments were carried out to try to extend the scope and accuracy of the self-shielding theory. An overview is presented below.

15.5.1. Allowing for capture in the moderator

In the energy domain of the resonances of uranium, capture by the true moderators is totally negligible (1/v rule for capture cross-sections): that is why its authors created the resonant absorption theory with the assumption that non-resonant nuclei had a purely scattering effect. Structural materials, such as the zirconium in the cladding of fuel rods in water reactors, are obviously chosen with their low capture in mind (amongst other criteria). To consider them as purely scattering does not therefore lead to a great error in the self-shielding calculation.

We have seen, however, that in the "one-by-one" procedure, at certain stages in the calculation resonant materials could be treated as moderator materials. Obviously, however, these materials cannot be treated as purely scattering materials.

That is why the formalism set out by the authors had to be modified to take into account any capture by materials that act as moderators. Using the arguments that led to the fine structure equation[6], we see that to take this capture into account, it is necessary to replace the fine structure equation previously obtained:

$$r_0\varphi + \sigma_e = (\sigma_0 + \sigma_e)\varphi,$$

with:

$$r_0\varphi + \gamma\sigma_e = (\sigma_0 + \sigma_e)\varphi, \tag{15.11}$$

where $\gamma = \Sigma_{s1}/\Sigma_{t1}$ is the probability that an impact on the moderator[7] is a scattering event. It then becomes evident[8] that the solution φ_γ with capture is simply the product $\gamma \times \varphi_1$ (the factor γ times the solution φ_1 without capture). To take the capture into account, we therefore merely need to multiply by γ the effective reaction rates obtained by interpolation in the tables drawn up without capture. No additional tabulation or calculation is required.

[6] In the context we studied, either homogeneous (§ 8.2.1) or heterogeneous with only one fuel zone and a moderator zone (§ 8.3.1); but, as we shall see, it is possible to generalise.

[7] For the energy group in which the self-shielding calculation concerned is performed.

[8] The neutron source in the "**P**" problem was multiplied by γ.

15.5.2. Self-shielding in the thermal domain

The creators of the APOLLO code chose a two-part multigroup subdivision; one for the fast and epithermal domain, and the other for the thermal domain, with the dividing line at an energy E_c (for example: 52 + 47 = 99 groups with the dividing line at 2.7 eV).

The subdivision in the epithermal domain clearly cannot "follow" the resonances. On the other hand, the subdivision in the thermal domain was constructed so that the main resonances, such as those of plutonium 239 and plutonium 241 at 0.3 eV and that of plutonium 240 at 1 eV, would be accurately described. This subdivision can however be a little bit "borderline" and, in particular, can be poorly suited to other resonances, such as that of plutonium 242, located slightly below the cutoff energy. That is why the self-shielding formalism and the associated tables were extended to the thermal domain in Version 2 of the code.

15.5.3. Other slowing-down models

We have seen (§ 15.2.2) that the heterogeneous-homogeneous equivalence could in practice be applied only in the context of a model of slowing-down by the resonant nucleus in order to explicitly obtain the solution φ of the fine structure equation.

The accuracy of this equivalence is clearly likely to increase with increasing accuracy of the slowing down model.

We have already examined two classic models: the NR (narrow resonance) model and the WR (wide resonance) model. There is another model of this type: the IR (intermediate resonance) model. This consists of using an intermediate formula between the first two, with a coefficient λ between 0 and 1 that weights them in a way[9]:

$$\varphi_{NR} = \frac{\sigma_{p0} + \sigma_d}{\sigma_0 + \sigma_d}, \quad \varphi_{WR} = \frac{\sigma_d}{\sigma_{a0} + \sigma_d}, \quad \varphi_{IR} = \frac{\lambda\sigma_{p0} + \sigma_d}{\sigma_{a0} + \lambda\sigma_{s0} + \sigma_d}. \tag{15.12}$$

This model involves a difficulty because it is purely empirical and it is difficult to know how to choose λ, and it has therefore fallen into disuse.

In the context of the developments associated with APOLLO 2, two new models were proposed:

– The *statistical model* ST is a generalisation of the NR model. It consists of approximating the slowing down $r_0\varphi$ with the resonant nucleus instead of with σ_{p0}, which assumes that there is no other resonance above the one being dealt with (therefore φ = 1), but with the lethargy average of the scattering rate $\sigma_{s0}\varphi$ in the current domain or group. If we substitute this approximation into the fine structure equation, we can see that this model only requires the tabulation of one additional parameter: the average by group or lethargy domain of $\sigma_{s0}/(\sigma_0 + \sigma_d)$;

– The *all-resonance model (*AR) is a generalisation of the previous model (ST). It consists of approximating the diffusion rate in each of the groups by its average value in the group and calculating the transfers $r_0\varphi$ using this assumption; for a given group, these transfers are then the average diffusion rates in this group and the few preceding groups weighted by transfer coefficients expressed with simple analytical formulae for elastic and isotropic slowing down in the centre of mass.

[9] Variant: $\varphi_{IR} = \lambda\varphi_{NR} + (1 - \lambda)\varphi_{WR}$. Here we present the formulae for the homogeneous case.

The tests performed tend to suggest that other models should be replaced by this AR model for all resonant nuclei and all resonances (hence its name "all resonance").

15.5.4. Handling geometries with several moderator zones

Following the study of the homogeneous case (§ 8.2.1), we presented the Livolant–Jeanpierre theory for the heterogeneous case for the simple example of a two-zone geometry, a fuel containing the resonant nucleus and a moderator (§ 8.3.1).

If we assume that there is always only one resonant zone but any number of non-resonant but moderator zones, the calculation will be almost as simple[10] and we end up with the fine structure equation with the same expression for the equivalent cross-section, i.e.:

$$\sigma_e = \frac{\sigma_0(1 - P_{00})}{P_{00}}. \tag{15.13}$$

With the Bell-Wigner approximation, we thus generalise the breakdown into a homogeneous term and a heterogeneous term (§ 8.3.3).

15.5.5. Handling of cases with several resonant zones

On the other hand, the treatment of cases with several resonant zones leads to additional problems. Such situations will be encountered whenever we wish to give details of the distribution of resonant absorptions within the zone concerned. For example, the very large cross-sections in the resonances mean that the captures of neutrons from the moderator by uranium 238 largely occurs in the immediate neighbourhood of the surface of the fuel and not very deep; the formation of plutonium is therefore fairly heterogeneous and it is necessary to divide the fuel into "rings" to take this into account (see Figure 15.1).

More heterogeneous cases can also be encountered: irregular lattices, fuel irradiated during dissolving for reprocessing[11], etc.

If the resonant zones are numbered by an index α or β and the concentration of resonant material in zone α is denoted $N_{0\alpha}$, the equations for the "**P**" problem can be established using the general assumptions of Livolant and Jeanpierre (macroscopic flux Ψ that is "flat" in space and lethargy):

$$\varphi_\alpha = \sum_\beta \frac{P_{\alpha\beta}}{\Sigma_\beta} N_{0\alpha} r_0 \varphi_\beta + \sum_\beta \frac{P_{\alpha\beta}}{\Sigma_\beta} \sum_{i \in \beta} N_{i\beta} \gamma_i \sigma_i. \tag{15.14}$$

There is now one fine structure function φ_α per resonant zone α. The index i denotes the non-resonant nuclei, and the $N_{i\beta}$ values denote the concentrations of the non-resonant nuclei mixed with the resonant nuclei in resonant zones. All other notation has the same meaning as before.

[10] The sum must be performed on the index m, applying the reciprocity and complementarity relationships to the first collision probabilities.

[11] The first stage of reprocessing fuel elements of water reactors is to cut them into segments a few centimetres long, and then to dissolve them in nitric acid (the fuel only, not the cladding, goes into solution). There is a risk of criticality during this dissolution. It is therefore necessary to be able to form an accurate evaluation of this neutron physics situation where some of the resonant nuclei are in solution in the liquid and others are in solid form.

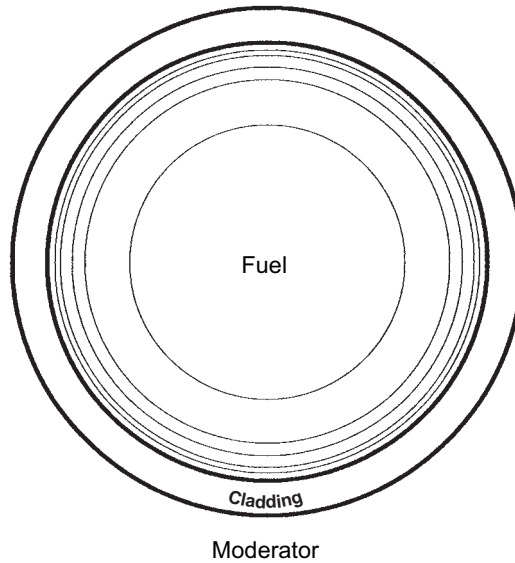


Figure 15.1. Example of the division of a water reactor fuel pellet into concentric crowns to take the "rim effect" into account in the formation of plutonium (from the centre to the edge, the ring volumes are 40%, 30%, 10%, 10%, 5% and 5% of the volume of the pellet).

Livolant and Jeanpierre suggested an additional approximation to simply decouple the equations of this system. This "Pic" approximation (name given by the authors to the probability here written as $P_{\alpha 0}$) consists of assuming that the incoming densities by slowing down on a resonant nucleus are the same in all resonant zones:

$$r_0\varphi_\alpha = r_0\varphi_\beta. \tag{15.15}$$

By replacing $r_0\varphi_\beta$ on the right-hand side with $r_0\varphi_\alpha$, we obtain independent fine structure equations that can be handled by the usual approach. This approximation is not completely arbitrary; it is correct in particular for the NR assumption, since in that case $r_0\varphi_\beta = \sigma_{p0}$ for any zone.

Livolant and Jeanpierre did not see that this additional approximation was not essential. In fact, it can be shown that the system of equations can be diagonalised, which means that it is possible to find a set of linear combinations $\psi_1, \psi_2 \ldots$ of the unknown functions φ_1, $\varphi_2 \ldots$ leading to independent equations for the new unknowns ψ_α. This was programmed in APOLLO 2 under the name of *dilution matrix method* (this matrix generalises the nearly-constant dilution cross-section).

In fact, it is simpler to implement the *"direct method",* which consists of inverting the order of the two calculation steps: 1/ diagonalising; 2/ using a slowing-down model. (We show that in the WR model, matrix inversions are necessary to handle the coupling in space, but with NR, ST, and AR models, there are only matrix × vector products to calculate.)