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THE MODERATION OF NEUTRONS IN NON-MULTIPLYING INFINITE HOMOGENEOUS MEDIA

by

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TABLE OF CONTENTS

LIST OF FIGURES

THE MODERATION OF NEUTRONS IN NON-MULTIPLYING INFINITE HOMOGENEOUS MEDIA

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CHAPTER I

THE NATURE OF THE PROBLEM

I-1. Introduction

The interaction of neutrons with a moderating medium is of great interest, not only for its practical importance as the underlying mechanism in the operation of nuclear reactors, but also as a purely scientific question concerning the dynamics of interacting systems of atomic and nuclear particles. The nature of the problem has been clarified greatly by the work of many authors during the last two decades, but its complexity is such that it can be studied only through the consideration of simplified models. Such models are necessarily much simplified in detail, and are apt to be misleading in important respects. For this reason, many points in the theory still await complete clarification.

Most of the early studies of neutron moderation dealt with the approximation known as slowing down theory. In this approach the nuclei of the moderator are considered to be free particles which are at rest before collision with the neutrons. Fermi and his collaborators,[1] Wick,[2] Placzek,[3] Marshak,[4] and many other authors have contributed to the development of the theory. The moderation of neutron energy over the higher part of the energy range is explained effectively by this model. However, in the range below a few electron volts it fails, since here the nuclei of the moderator no longer can be treated as being initially at rest. In the late 1940's, the theory underwent further refinement, stimulated by the additional experimental data of Sturm,[5] Zinn,[6] and others, in the low-energy region.

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[1] E. Fermi, Ricerca Scientifica VII-2, 13 (1936); English Translation: U.S. AEC Report NP-2385 (1951).
E. Amaldi, O. D'Agostino, E. Fermi et al., Proc. Roy. Soc. (London) A149, 522 (1935).

[2] G. C. Wick, Phys. Rev. 75, 738 (1949).

[3] G. Placzek, Phys. Rev. 69, 423 (1946).

[4] R. E. Marshak, Revs. Mod. Phys., 19, 3, 185 (1947).

[5] W. H. Sturm, Phys. Rev., 71, 757 (1947).

[6] W. J. Zinn, Phys. Rev., 71, 752 (1947).

The following phenomena lead to complications in the scattering process in the low-energy region:

(a) thermal motions of the moderator atoms;

(b) the binding of the moderator atoms in the lattice, with the appearance of quantized vibrational and rotational states; and

(c) interference effects arising from the wave nature of the neutron and of the moderator atoms.

When the neutron energy is large, these phenomena are not important in determining the interaction between the neutrons and the moderator. In this case the general result is a steady loss of energy by the neutrons. In the region of low energy, however, when the neutrons and the moderator come into equilibrium with each other, a neutron may gain (up-scattering) as well as lose (down-scattering) energy in collisions with the moderator atoms, so that the whole scattering process becomes much more complicated.

A somewhat different approach was introduced in 1944 by Wigner and Wilkins.[7] They treated the moderator nuclei as a monatomic Maxwellian gas, and ignored chemical binding and crystalline effects. With this model, in which neutrons and nuclei were considered as hard spheres, these authors were able to construct an integral equation valid over the whole range of neutron energies. The further study of this model, and of its relation to the slowing-down theory, is the major aim of the present study. A part of our analysis will be aimed also at prospective work on the inclusion of chemical binding effects in the theory.

I-2. Statement of the Problem

In a non-multiplying medium, neutrons are subject to the following general processes:

(a) scattering by atoms of the moderator;

(b) capture by atoms of the moderator; and

(c) leakage from the boundary surface of the moderator.

In a scattering process, a neutron may suffer no change in energy, or gain or lose energy. In any event, it is still available for further interaction with the moderator. In processes (b) and (c), on the other hand, the neutron is lost from the system.

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[7] E. P. Wigner and J. E. Wilkins, Jr., AECD-2275 (1944).

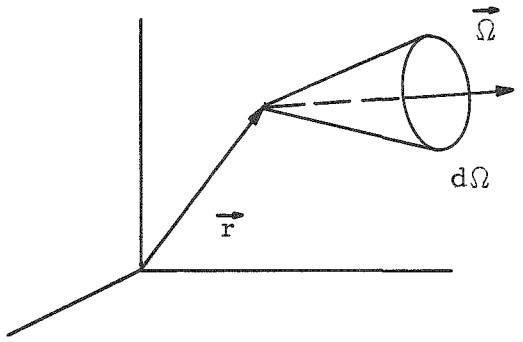

Fig. I-1. Geometrical Configuration of the Phase Space

The Boltzmann transport equation is usually adopted as the basis of the treatment of the development of the neutron distribution function in time. Let $n(\vec{r}, v, \vec{\Omega}, t)\, d\vec{r}\, dv\, d\Omega$ be the number of neutrons, at time t, per unit volume at the space point specified by the vector $\vec{r}$, with speeds in the range from v to v + dv, and with directions of motion lying in the elementary cone $d\Omega$ about the unit vector $\vec{\Omega}$. These geometrical conditions are shown in Fig. I.1. The Boltzmann equation then has the following form:

$$\frac{\partial n(\vec{r}, v, \vec{\Omega}, t)}{\partial t} = - v\vec{\Omega} \cdot \text{grad}\, n(\vec{r}, v, \vec{\Omega}, t) - [v\Sigma_s(\vec{r}, v) + v\Sigma_a(\vec{r}, v)]\, n(\vec{r}, v, \vec{\Omega}, t)$$
$$+ \iiint dv'\, d\Omega'\, v'\, \Sigma(\vec{r}; v'\vec{\Omega}' \rightarrow v\vec{\Omega})\, n(\vec{r}, v', \vec{\Omega}', t) + S(\vec{r}, v, \vec{\Omega}, t) \qquad (I\text{-}2\text{-}1)$$

Here $\Sigma_s(\vec{r}, v)$ and $\Sigma_a(\vec{r}, v)$ are the macroscopic scattering and absorption cross sections, respectively, and $\Sigma(\vec{r}; v'\vec{\Omega}' \rightarrow v\vec{\Omega})$ is the differential scattering cross section by which a neutron is scattered from velocity $v'\vec{\Omega}'$ into the velocity range $dv\, d\Omega$ about $v\vec{\Omega}$. All of these cross sections will depend on the space coordinates in an inhomogeneous medium.

The first member on the right-hand side of Eq. (I-2-1) represents the rate of loss of neutrons from the volume element $d\vec{r}\, dv\, d\Omega$ by virtue of their motion. The second member accounts for the rate of loss of neutrons by scattering and by absorption. The third member represents the rate at which neutrons are brought into the given volume element through scattering processes. The last member $S(\vec{r}, v, \vec{\Omega}, t)$ represents the rate of introduction of neutrons into $d\vec{r}\, dv\, d\Omega$ from an external source. Finally the left-hand side represents the rate of neutron increase in $d\vec{r}\, dv\, d\Omega$.

The Boltzmann Eq. (I-2-1) is too complex to solve in general, and it becomes necessary to reduce it to a simpler form by various means. One natural simplification is to consider first the case of a distribution which is independent of the spatial coordinates. This enables one to concentrate on the study of the velocity distribution of the neutrons. Our work will be confined to this case.

For this purpose we assume that the moderator is homogeneous and of infinite extent, and that the neutrons are introduced in a uniform manner throughout the whole assembly. It will be assumed further that the moderator is composed of a single nuclear species.

In this idealized situation, the transport Eq. (I-2-1) is simplified to the form

$$\frac{\partial n(v, t)}{\partial t} + v[\Sigma_s(v) + \Sigma_a(v)]\, n(v, t) = \int_0^\infty dv'\, v' \Sigma(v' \to v)\, n(v', t) + S(v, t) \quad , \tag{I-2-2}$$

where

$$\Sigma(v' \longrightarrow v) = \int\int d\Omega\, \Sigma(v'\vec{\Omega}' \to v\vec{\Omega}) \tag{I-2-3}$$

is the scattering cross section integrated over all directions of scattering.

Also, we set

$$S(v, t) = \int\int d\Omega S(v, \vec{\Omega}, t) \quad . \tag{I-2-4}$$

If we integrate both sides of Eq. (I-2-2) with respect to v, we have

$$\frac{\partial}{\partial t} \int_0^\infty n(v, t)\, dv = \int_0^\infty S(v, t)\, dv - \int_0^\infty v\Sigma_a(v)\, n(v, t)\, dv \quad . \tag{I-2-5}$$

Here we have defined

$$\Sigma_s(v') = \int_0^\infty \Sigma(v' \to v)\, dv \quad , \tag{I-2-6}$$

and so we obtain the formula

$$\int_0^\infty v\Sigma_s(v)\, n(v, t)\, dv = \int_0^\infty vdv\, n(v, t) \int_0^\infty \Sigma(v \to v')\, dv' \quad .$$

By an interchange of the symbols v and v' in the last integral,

$$\int_0^\infty v\Sigma_s(v)\, n(v, t)\, dv = \int_0^\infty dv \int_0^\infty dv'\, v' \Sigma(v' \to v)\, n(v', t) \quad . \tag{I-2-7}$$

The two scattering terms cancel each other when the integration with respect to v is performed in Eq. (I-2-2). This leads to Eq. (I-2-5).

Equation (I-2-5) shows that the distribution can be independent of time if, and only if,

$$\int_0^\infty S(v)\, dv = \int_0^\infty v\Sigma_a(v)\, n(v)\, dv \quad . \tag{I-2-8}$$

This equation states, in physical terms, that if the distribution is independent of time, the rate of absorption of neutrons per unit volume must be just equal to the total rate at which neutrons are introduced into the system per unit of volume by the external source.

We are led by these simplifying considerations to examine the special case of the steady-state velocity* distribution of neutrons in an infinite, homogeneous, non-multiplying moderator, for which the Boltzmann transport equation takes the following form:

$$v[\Sigma_s(v) + \Sigma_a(v)]\, n(v) = \int_0^\infty dv'\ v'\, \Sigma(v' \rightarrow v)\, n(v') + S(v) \quad . \quad \text{(I-2-9)}$$

Although this model clearly is a very specialized one, it is not trivial, since it still requires the determination of the velocity distribution of the neutrons under the influence of scattering collisions and absorption processes with the moderator atoms. This is the problem formulated originally by Wigner and Wilkins. It will be seen in the sequel that its analysis involves a number of somewhat subtle points.

In order to make the model correspond to practical neutron sources, we shall suppose that the neutrons are introduced at a very high energy by the external source. The neutron energies are then distributed over a wide range by collision processes, the distribution being modified at the same time by the absorption of neutrons.

I-3. Outline of the Analysis

Chapter II is devoted to a discussion of the theory of scattering cross sections for neutrons. The analysis is more detailed than would be strictly necessary for the consideration of the Wigner-Wilkins gas model, but the results are of interest for considerations on the effects of chemical binding and coherence effects at low neutron energies.

In Chapter III, the Wigner-Wilkins model is considered for moderator atoms of the same mass as the neutron. Although this corresponds to the idealized case of atomic hydrogen as a moderator, the discussion is particularly helpful in bringing out the nature of the moderation process.

Chapter IV extends the analysis to the case of a geseous moderator with atoms of general mass.

*In this study we shall follow the current practice of referring to the velocity distribution, although we have in mind only the magnitude of the velocity. Speed distribution might be better.

CHAPTER II

THE EVALUATION OF SCATTERING CROSS SECTIONS

II-1. Introduction

As a first step we shall review in Sections II-2 and II-3 the quantum mechanical theory of scattering cross sections in the Born approximation. The discussion in these sections is restricted to the case of two-body interactions, for the sake of simplicity, that is, we suppose that a neutron will interact with only one nucleus of the moderator at a time.

In Section II-4, this theory is applied to the evaluation of the cross sections which are needed in the monatomic gas model. In Section II-5, we shall examine the relationship between these results and those which are employed in the slowing-down theory. Our aim will be to examine the manner in which the cross sections used in the latter theory can be interpreted as limiting cases of those for the gas model.

II-2. Scattering Theory in the Born Approximation. The Two-body Fermi Pseudopotential

Let m and M be the masses of the neutron and the moderator nucleus, respectively. It will be supposed that the moderator nucleus is subject to a binding potential energy $V(\vec{r})$ which holds it in the lattice or molecule, while there is a potential energy $U(|\vec{r}-\vec{r}_n|)$ representing the interaction between the neutron and the nucleus. The Schrodinger equation for the system of two particles is

$$\left[-\frac{\hbar^2}{2m} \nabla_n^2 - \frac{\hbar^2}{2M} \nabla^2 + V(\vec{r}) + U(|\vec{r}_n - \vec{r}|) \right] \Psi(\vec{r}_n, \vec{r})$$

$$= (E_0 + W_0)\, \Psi(\vec{r}_n, \vec{r}) \quad , \qquad \text{(II-2-1)}$$

where E_0 is the kinetic energy of the incident neutron and W_0 is the energy of the nucleus in its initial state.

We seek a solution of this equation of the form

$$\Psi = \sum_{j=0}^{\infty} F_j(\vec{r}_n)\, \phi_j(\vec{r}) \quad , \qquad \text{(II-2-2)}$$

where the index j represents the various vibrational states of the bound nucleus in the moderator; the index value j = 0 represents the initial state, for convenience. We expect, further, that as $|\vec{r}_n| \to \infty$, the functions $F_j(\vec{r}_n)$ will have the asymptotic forms

$$F_0(\vec{r}_n) \sim e^{ik_0 z_n} + \frac{e^{ik_0 r_n}}{r_n} f_0(\theta_n, \varphi_n) \qquad \text{(II-2-3')}$$

and

$$F_j(\vec{r}_n) \sim \frac{e^{ik_j r_n}}{r_n} f_j(\theta_n, \varphi_n) \qquad (j \neq 0) \quad . \qquad \text{(II-2-3")}$$

The symbol F_0 thus represents the incident neutron wave together with the scattered neutron wave for which the nucleus is left in its initial state (elastic scattering of the neutron). Similarly, F_j $(j \neq 0)$ represents the scattered neutron wave when the nucleus is left in an excited state (inelastic scattering of the neutron). Correspondingly, $\phi_0(r)$ is the initial state wave function of the nucleus, with energy W_0, and $\phi_j(r)$ is its wave function in the final state, with energy W_j.

The wave function of the initial state of the nucleus satisfies the equation

$$\left[-\frac{\hbar^2}{2M} \nabla^2 + V(\vec{r}) \right] \phi_0(\vec{r}) = W_0 \phi_0(\vec{r}) \quad , \qquad \text{(II-2-4)}$$

and the wave functions of the excited states satisfy the equations

$$\left[-\frac{\hbar^2}{2M} \nabla^2 + V(\vec{r}) \right] \phi_j(\vec{r}) = W_j \phi_j(\vec{r})$$

$$(j = 1, 2, \ldots\ldots) \quad . \qquad \text{(II-2-5)}$$

The wave number vectors for the neutrons, corresponding to incident states of kinetic energy E_0 and final states of energies $E_0 + W_0 - W_j$, are

$$k_0^2 = 2mE_0/\hbar^2 \quad ; \quad k_j^2 = 2m(E_0 + W_0 - W_j)/\hbar^2 \quad . \qquad \text{(II-2-6)}$$

It will be assumed that the wave functions of the nucleus form a complete orthonormal set of functions for those final states which result from scattering processes. In particular, we will not consider inelastic processes in which the nucleus is knocked completely away from its original position in the lattice.

We next substitute Eq. (II-2-2) into (II-2-1), multiply both sides by $\phi_j^*(r)$, and integrate over the coordinates of the nucleus. If the assumed property of orthonormality of the nuclear wave functions is used, the following system of equations results:

$$(\nabla_n^2 + k_j^2) F_j(\vec{r}_n) = \frac{2m}{\hbar^2} \int d\vec{r}\, U(|\vec{r} - \vec{r}_n|)\, \Psi(\vec{r}_n, \vec{r})\, \phi_j^*(\vec{r})$$

$$(j = 0, 1, 2, \ldots.) \quad . \qquad \text{(II-2-7)}$$

Since the unknown functions F_j appear implicitly under the integral sign on the right-hand side of Eq. (II-2-6), we have, in reality, a system of integral equations for these functions. However, in the first Born approximation the function $\Psi(\vec{r}_n,\vec{r})$ is replaced by the approximate form

$$\Psi(\vec{r}_n,\vec{r}) \to e^{ik_0 z_n}\ \phi_0(\vec{r}) \quad , \tag{II-2-8}$$

representing the incident (undistorted) neutron wave, the nucleus being in its initial state. In this approximation, Eqs. (II-2-6) are to be used for the actual evaluation of the corresponding approximate expressions for the functions $F_j(\vec{r}_n)$, representing the scattered neutron waves.

When the right-hand side of Eq. (II-2-6) is regarded as a known function of the neutron coordinates, as it is in the Born approximation, Eq. (II-2-6) can be solved directly by making use of the known Green's function (source solution)

$$-\frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} \tag{II-2-8'}$$

of the Helmholtz equation

$$(\nabla^2 + k^2)\, F = 0 \quad . \tag{II-2-8''}$$

The result is the formula

$$F_j(\vec{r}_n) = -\frac{m}{2\pi\hbar^2}\int d\vec{r}_n' \int d\vec{r}\ \frac{e^{ik_j|\vec{r}_n-\vec{r}_n'|}}{|\vec{r}_n-\vec{r}_n'|}\cdot U(|\vec{r}-\vec{r}_n'|)\,\Psi(\vec{r}_n',\vec{r})\,\phi_j^*(\vec{r}) \quad . \tag{II-2-9}$$

On making the substitution (II-2-7), appropriate to the Born approximation, Eq. (II-2-9) assumes the form

$$F_j(\vec{r}_n) = -\frac{m}{2\pi\hbar^2}\int d\vec{r}_n' \int d\vec{r}\ \frac{e^{ik_j|r_n-r_n'|}}{|\vec{r}_n-\vec{r}_n'|}\cdot e^{ik_0 Z_n'}\cdot$$

$$U(|\vec{r}-\vec{r}_n'|)\ \phi_0(\vec{r})\phi_j^*(\vec{r}) \quad . \tag{II-2-10}$$

Fermi[1] has argued that in this problem the interaction potential $U(|\vec{r}-\vec{r}_n|)$, which is called the Fermi pseudopotential, between the neutron and the nucleus, can be taken to be

$$U(|\vec{r}-\vec{r}_n|) = \frac{2\pi\hbar^2}{m}(1+\mu)\, a' \cdot \delta(\vec{r}-\vec{r}_n) \quad , \tag{II-2-11}$$

where

$$(1 + \mu)\, a' = a_b \quad ; \quad \mu = m/M \quad , \tag{II-2-12}$$

and a_b is the Fermi scattering length for scattering of neutrons from the bound nucleus, when the latter is left in its ground state after the scattering process is completed. Breit[8] has given a further discussion of the Fermi pseudopotential and of the applicability of this modification of the Born approximation method.

If we insert Eq. (II-2-11) into (II-2-10), we obtain the formula

$$F_j(\vec{r_n}) = -a_b \int d\vec{r}\, \frac{e^{ik_j|\vec{r_n} - \vec{r}|}}{|\vec{r_n} - \vec{r}|}\, e^{ik_0 Z_n}\, t_0(\vec{r})\, \varphi_j^*(\vec{r}) \quad . \tag{II-2-13}$$

The asymptotic form of this expression, at large distances from the scattering nucleus, is readily evaluated. On comparison with expressions (II-2-3), it is found that

$$f_j = a_b \int \phi_0(\vec{r})\, e^{i(\vec{k_0} - \vec{k_j})\cdot\vec{r}}\, \varphi_j^*(\vec{r})\, d\vec{r} \quad , \tag{II-2-14}$$

where $\vec{k_0}$ and $\vec{k_j}$ are the (momentum) wave number vectors of the incident and scattered neutron waves, respectively. This formula holds also for the elastic scattering amplitude if we set $j = 0$; in this case $f_0 = a_b$, which follows directly from the definition of the Fermi scattering length a_b.

Since the scattering cross section is defined by the ratio of the scattered (outgoing) to the incident (incoming) current, it is given by the expression

$$I_j = \frac{k_j}{k_0} |f_j|^2 \quad . \tag{II-2-15}$$

On making use of the expression (II-2-14), we have

$$I_j(\theta, \varphi) = a_b^2 \frac{k_j}{k_0} \left| \int \phi_0(\vec{r})\, e^{i(\vec{k_0} - \vec{k_j})\cdot\vec{r}}\, \varphi_j^*(\vec{r})\, d\vec{r} \right|^2 \quad . \tag{II-2-16}$$

If this is expressed in Dirac's notation, it becomes

$$I_j(\theta, \varphi) = a_b^2 \frac{k_j}{k_0} \left\langle \phi_0 \left| e^{i(\vec{k_j} - \vec{k_0})\cdot\vec{r}} \right| \psi_j \right\rangle \left\langle \psi_j \left| e^{-i(\vec{k_j} - \vec{k_0})\cdot\vec{r}} \right| \phi_0 \right\rangle \quad . \tag{II-2-17}$$

Here θ is the angle of scattering of the neutron, that is, the angle between the wave number vectors $\vec{k_0}$ and $\vec{k_j}$.

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[8] G. Breit, Phys. Rev., 71, 215 (1947).

II-3. An Operator Formalism

It has been assumed up to this point that the moderator nucleus is in a specified initial state before its interaction with the neutron. In fact, however, not all of the nuclei will be initially in the same state; for example, they may have a distribution of energies appropriate to some given moderator temperature. It will be convenient, therefore, to specify the type of scattering process suffered by the neutron, and to recognize that this particular process may arise from transitions of the moderator nuclei from a variety of initial states to corresponding final states. The major criterion which must be satisfied by all possible combinations of initial and final states is that of conservation of energy.

Consider a process in which a neutron is scattered from a state of initial energy and momentum (direction of motion) $(E_0, \vec{\Omega}_0)$ into a state $(E, \vec{\Omega})$. We introduce the notation

$$\vec{\kappa} = \vec{k} - \vec{k}_0 \qquad \text{(II-3-1)}$$

$$\epsilon = E - E_0 = \hbar^2 (k^2 - k_0^2)/2m \quad . \qquad \text{(II-3-2)}$$

Since the final kinetic energy of the neutron cannot be negative, we must impose the restriction

$$\epsilon > \epsilon_0 = -E_0 = -\frac{\hbar^2}{2m} k_0^2 \quad . \qquad \text{(II-3-3)}$$

If this scattering process of the neutron is associated with a jump of the atom from a state of energy W_i to a state of energy W_f, then we must have

$$\epsilon = E - E_0 = W_i - W_f \quad . \qquad \text{(II-3-4)}$$

The differential scattering cross section can be written in the form

$$\sigma(E_0 \vec{\Omega}_0 \rightarrow E\vec{\Omega}) = a_b^2 \frac{k}{k_0} \sum_i \sum_f w_i \left\langle \phi_i \left| e^{i\vec{\kappa} \cdot \vec{r}} \right| \phi_f \right\rangle \left\langle \phi_f \left| e^{-i\vec{\kappa} \cdot \vec{r}} \right| \phi_i \right\rangle \cdot$$

$$\cdot \delta(\epsilon - W_i + W_f) \quad , \qquad \text{(II-3-5)}$$

where w_i is the (normalized) statistical weight of the initial state of the nucleus. The introduction of the delta function takes account formally of the energy conservation law of Eq. (II-3-4), and so allows us to extend the sums over the nuclear states to all combinations of initial and final states which are compatible with energy conservation.

Our next step is to replace the delta function by the (improper) integral function

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-ix\xi}\, d\xi \quad . \tag{II-3-6}$$

On inserting this expression into Eq. (II-3-5), we have the formula

$$\sigma(E_0\vec{\Omega}_0 \to E\vec{\Omega}) = \frac{a_b^2}{2\pi\hbar}\,\frac{k}{k_0}\int_{-\infty}^{+\infty} dt\, e^{-ict/\hbar} \sum_i \sum_f w_i\, e^{i(W_i - W_f)t/\hbar}$$

$$\left\langle \phi_i \middle| e^{i\vec{\kappa}\cdot\vec{r}} \middle| \phi_f \right\rangle \left\langle \phi_f \middle| e^{-i\vec{\kappa}\cdot\vec{r}} \middle| \phi_i \right\rangle \quad . \tag{II-3-7}$$

We note the following identities:

$$\left.\begin{aligned} e^{iW_i t/\hbar}\,\phi_i^* &= e^{-iHt/\hbar}\,\phi_i^* \\ e^{-iW_f t/\hbar}\,\phi_f^* &= e^{iHt/\hbar}\,\phi_f^* \end{aligned}\right\} \quad . \tag{II-3-8}$$

Since the Hamiltonian operator is Hermitian, by definition, the operators $\exp(\pm iHt/\hbar)$ are unitary, while $\exp(iHt/\hbar)$ and $\exp(-iHt/\hbar)$ are adjoint to each other. In the Dirac notation for matrix elements, which is equivalent to that for inner products involving operators, one has

$$\begin{aligned} \left\langle e^{-iHt/\hbar}\,\phi_i \middle| e^{i\vec{\kappa}\cdot\vec{r}} \middle| \phi_f \right\rangle &= \left\langle \phi_i \middle| e^{iHt/\hbar}\, e^{i\vec{\kappa}\cdot\vec{r}} \middle| \phi_f \right\rangle \\ \left\langle e^{iHt/\hbar}\,\phi_f \middle| e^{-i\vec{\kappa}\cdot\vec{r}} \middle| \phi_i \right\rangle &= \left\langle \phi_f \middle| e^{-iHt/\hbar}\, e^{-i\vec{\kappa}\cdot\vec{r}} \middle| \phi_i \right\rangle \quad . \end{aligned} \tag{II-3-9}$$

On making use of our assumption of completeness of the set of nuclear states, we see that, by the rules of matrix multiplication,

$$\begin{aligned} &\sum_f e^{i(W_i - W_f)t/\hbar} \left\langle \phi_i \middle| e^{i\vec{\kappa}\cdot\vec{r}} \middle| \phi_f \right\rangle \left\langle \phi_f \middle| e^{-i\vec{\kappa}\cdot\vec{r}} \middle| \phi_i \right\rangle \\ &= \sum_f \left\langle \phi_i \middle| e^{iHt/\hbar}\, e^{i\vec{\kappa}\cdot\vec{r}} \middle| \phi_f \right\rangle \left\langle \phi_f \middle| e^{-iHt/\hbar}\, e^{-i\vec{\kappa}\cdot\vec{r}} \middle| \phi_i \right\rangle \\ &= \left\langle \phi_i \middle| e^{iHt/\hbar}\, e^{i\vec{\kappa}\cdot\vec{r}}\, e^{-iHt/\hbar}\, e^{-i\vec{\kappa}\cdot\vec{r}} \middle| \phi_i \right\rangle \end{aligned} \tag{II-3-10}$$

This last expression is the expectation value of the indicated operator, and it will be convenient to indicate it by a special notation:

$$G_i(\vec{\kappa},t) = \left\langle \varphi_i \left| e^{iHt/\hbar}\ e^{i\vec{\kappa}\cdot\vec{r}}\ e^{-iHt/\hbar}\ e^{-i\vec{\kappa}\cdot\vec{r}} \right| \phi_i \right\rangle \quad . \qquad \text{(II-3-11)}$$

The average value of this quantity over the distribution of initial states of the nucleus will be written as

$$g(\vec{\kappa},\ t) = \sum_i w_i G_i\ (\vec{\kappa},t) \quad . \qquad \text{(II-3-12)}$$

This reduction allows us to write Eq. (II-3-7) in the form

$$\sigma(E_0\vec{\Omega}_0 \rightarrow E\vec{\Omega}) = \frac{a_b^2}{2\pi\hbar}\frac{k}{k_0}\int_{-\infty}^{+\infty} e^{-i\epsilon t/\hbar}\ g(\vec{\kappa},t)\ dt \quad . \qquad \text{(II-3-13)}$$

In the usual notation this differential cross section would be written as

$$\frac{d^2\sigma}{d\Omega d\epsilon} \quad , \qquad \text{(II-3-14)}$$

which shows explicitly that it is the differential scattering cross section per unit solid angle per unit energy range. The differential scattering cross section per unit solid angle, $d\sigma/d\Omega$, is readily calculable by integration of (II-3-13) over all possible energy changes of the neutron:

$$\frac{d\sigma}{d\Omega} = \int_{\epsilon_0}^{\infty} \frac{d^2\sigma}{d\Omega d\epsilon}\ d\epsilon \quad . \qquad \text{(II-3-15)}$$

The total scattering cross section is evaluated by a further integration of (II-3-15) over all scattering angles

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega}\ d\Omega = \int d\Omega \int_{\epsilon_0}^{\infty} d\epsilon\ \frac{d^2\sigma}{d\Omega d\epsilon} \quad . \qquad \text{(II-3-16)}$$

This work indicates that in the first Born approximation the evaluation of the scattering cross section is reducible to the evaluation of the expectation values $G_i(\vec{\kappa},t)$, and, finally, of the statistical average over all initial states, $g(\vec{\kappa},t)$. In carrying out these calculations the following formal relations are useful.

Making use of the fact that the solution of the Heisenberg equation of motion

$$i\hbar\ \frac{d\vec{r}(t)}{dt} = [\vec{r}(t),\ H] \qquad \text{(II-3-17)}$$

is

$$\vec{r}(t) = e^{iHt/\hbar}\, \vec{r}\, e^{-iHt/\hbar} \quad ,$$

we can write

$$e^{iHt/\hbar}\; e^{i\vec{\kappa}\cdot\vec{r}}\; e^{-iHt/\hbar} = e^{i\vec{\kappa}\cdot\vec{r}(t)} \quad . \tag{II-3-18}$$

This result allows us to write

$$G_i(\vec{\kappa},t) = \left\langle \phi_i \left| e^{i\vec{\kappa}\cdot\vec{r}(t)}\; e^{-i\vec{\kappa}\cdot\vec{r}(0)} \right| \phi_i \right\rangle \quad . \tag{II-3-19}$$

Another convenient formalism is the following. Since

$$e^{i\vec{\kappa}\cdot\vec{r}}\, \vec{p}\, e^{-i\vec{\kappa}\cdot\vec{r}} = \vec{p} - \hbar\vec{\kappa} \quad ,$$

we can write more generally

$$e^{i\vec{\kappa}\cdot\vec{r}}\, f(\vec{p})\, e^{-i\vec{\kappa}\cdot\vec{r}} = f(\vec{p} - \hbar\vec{\kappa}) \quad , \tag{II-3-20}$$

where f is a general algebraic function of its argument. This leads to the formula

$$e^{i\vec{\kappa}\cdot\vec{r}}\; e^{-iHt/\hbar}\; e^{-i\vec{\kappa}\cdot\vec{r}} = e^{-iH't/\hbar} \quad , \tag{II-3-21}$$

where H' denotes the Hamiltonian operator in which the momentum operator of the nucleus, $\vec{p}$, has been replaced by $\vec{p} - \hbar\vec{\kappa}$. Thus, if $H = H(\vec{p},\vec{r})$, then $H' = H(\vec{p} - \hbar\vec{\kappa}, \vec{r})$. We have, finally, from Eq. (II-3-19),

$$G_i(\vec{k},t) = \left\langle \varphi_i \left| e^{iHt/\hbar}\; e^{-iH't/\hbar} \right| \phi_i \right\rangle \quad . \tag{II-3-22}$$

Expressions (II-3-19) and (II-3-22) are both useful in applications, and either can be used where it gives the simpler formulation.

The function $g(\vec{\kappa},t)$ is to be evaluated after the expectation values $G_i(\vec{\kappa},t)$ have been found, by averaging over the assumed distribution of initial states of the nucleus.

This formalism will be applied in the next section to the simple case of a monatomic gas model, with omission of chemical biding effects, in which the initial distribution of nuclear states is supposed to be Maxwellian at the temperature of the moderator.

II-4. The Monatomic Gas Model

In the case of the monatomic gas model, Eq. (II-3-21) provides the most convenient form from which to evaluate the functions G_i. The Hamiltonian operator has the simple form

$$H = \vec{p}^2/2M \quad , \tag{II-4-1}$$

where $\vec{p}$ is the momentum operator of the nucleus. It follows that

$$H' = \frac{1}{2M}(\vec{p} - \hbar\vec{\kappa})^2 = \frac{1}{2M}(\vec{p}^2 - 2\hbar\vec{p}\cdot\vec{\kappa} + \hbar^2\vec{\kappa}^2) \quad . \tag{II-4-2}$$

Since the energy operators appearing in Eq. (II-3-21) are expressed directly in terms of the momentum operator of the nucleus, it will be most convenient to express the nuclear wave functions in momentum form. Equation (II-3-21) requires that we evaluate the expectation value of the operator

$$e^{it\vec{p}^2/2M\hbar}\ e^{-it(\vec{p}-\hbar\vec{\kappa})^2/2M\hbar} \quad .$$

If we take the initial atomic state as one in which the nucleus has momentum $\vec{p}_i$, the result is

$$G_i(\vec{\kappa},t) = e^{-it(\hbar\vec{\kappa}^2 - 2\vec{\kappa}\cdot\vec{p}_i)/2M} \quad . \tag{II-4-3}$$

In averaging over the momentum states of the nucleus, we must take account of the fact that they have a continuous distribution, so that expression (II-3-13) is to be interpreted as the integral

$$g(\vec{\kappa},t) = \int f(\vec{p})\, G_i(\vec{\kappa},t)\, d\vec{p} \quad , \tag{II-4-4}$$

where the function $f(\vec{p})$ expresses the statistical distribution of initial nuclear states.

If the moderator is assumed to be at a definite temperature T(°K), and that the nuclei of the moderator have a distribution of energies obeying the Maxwell-Boltzmann law, we have

$$f(\vec{p}) = (2\pi Mw)^{-3/2} \exp(-\vec{p}^2/2Mw) \quad , \tag{II-4-5}$$

where we use the temporary notation

$$w = kT \quad , \tag{II-4-6}$$

with k here as Boltzmann's constant.

We substitute Eq. (II-4-3) into Eq. (II-4-4) and find the following evaluation:

$$g(\vec{\kappa},t) = (2\pi Mw)^{-3/2} \int \vec{dp}\, \exp(-\vec{p}^2/2Mw)\exp[-it(\hbar\vec{\kappa}^2 - 2\vec{\kappa}\cdot\vec{p})/2M]$$

$$= \exp\left[-\left(it + \frac{wt^2}{\hbar}\right)\hbar\vec{\kappa}^2/2M\right] \qquad \text{(II-4-7)}$$

The differential scattering cross section can now be evaluated by substitution of Eq. (II-4-7) into Eq. (II-3-13). The results is

$$\sigma(E_0\vec{\Omega}_0 \rightarrow E\vec{\Omega}) = \frac{a_b^2 k}{2\pi\hbar k_0}\int_{-\infty}^{+\infty} \exp\left(-\frac{i\epsilon t}{\hbar}\right)\exp\left[-\frac{\hbar\vec{\kappa}^2}{2M}\left(it + \frac{wt^2}{\hbar}\right)\right]dt$$

$$= \frac{a_b^2 k}{\hbar\kappa k_0}\left(\frac{M}{2\pi w}\right)^{1/2} \exp\left[-\frac{M}{2w}\left(\frac{\epsilon}{\hbar\kappa} + \frac{\hbar\kappa}{2M}\right)^2\right] \quad . \qquad \text{(II-4-8)}$$

We express the wave numbers of the incident and scattered neutron states in terms of energies, make the replacement w = kT from Eq. (II-4-6), and eliminate the Fermi scattering length in terms of the scattering cross section. This gives the formula

$$\sigma(E_0\vec{\Omega}_0 \rightarrow E\vec{\Omega}) = \sigma_f \frac{(1+\mu)^2}{4\pi\hbar}\left(\frac{M}{2\pi kT}\right)^{1/2}\left(\frac{E}{E_0}\right)^{1/2}\frac{1}{\kappa}\exp\left[-\frac{M}{2kT}\left(\frac{\epsilon}{\hbar\kappa} + \frac{\hbar\kappa}{2M}\right)^2\right] \quad . \qquad \text{(II-4-9)}$$

It is to be remembered that in this formula k is Boltzmann's constant, $\mu = m/M = 1/A$, and σ_f is the scattering cross section of the free nucleus per unit energy range per steradian.

Up to this point, we have been concerned primarily with the evaluation of the microscopic scattering cross section. For our applications we need the macroscopic cross sections, which are, by definition,

$$\Sigma_f = N\sigma_f \quad ,$$

$$\Sigma(E_0\vec{\Omega}_0 \rightarrow E\vec{\Omega}) = N\sigma(E_0\vec{\Omega}_0 \rightarrow E\vec{\Omega}) \quad , \qquad \text{(II-4-10)}$$

where N is the number of nuclei per unit volume in the moderator.

Our primary application requires the evaluation of the scattering cross section per unit energy range, that is, the differential cross section integrated over all angles of scattering of the neutron. This is defined by the expression

$$\Sigma(E_0 \rightarrow E) = \int \Sigma(E_0\vec{\Omega}_0 \rightarrow E\vec{\Omega})\, d\Omega \quad . \qquad \text{(II-4-11)}$$

This also is known in the literature as the energy transfer cross section. To evaluate this integral we have the expressions

$$\Sigma(E_0 \rightarrow E) = \Sigma_f \frac{(1+\mu)^2}{4\pi\hbar} \left(\frac{M}{2\pi kT}\right)^{1/2} \left(\frac{E}{E_0}\right)^{1/2} \int \frac{1}{\kappa} \exp\left[-\frac{M}{2kT}\left(\frac{\epsilon}{\hbar\kappa} + \frac{\hbar\kappa}{2M}\right)^2\right] d\Omega$$

$$= \Sigma_f \frac{(1+\mu)^2}{4} \left(\frac{1}{\mu kT}\right)^{1/2} \left(\frac{E}{E_0}\right)^{1/2}$$

$$\int_{-1}^{+1} \frac{\exp\left\{-\frac{1}{4\mu kT}\left[\frac{E - E_0}{\sqrt{E + E_0 - 2\varphi\sqrt{EE_0}}} + \mu\sqrt{E + E_0 - 2\varphi\sqrt{EE_0}}\right]^2\right\}}{\sqrt{E + E_0 - 2\varphi\sqrt{EE_0}}} d\varphi \,, \tag{II-4-12}$$

where

$$\varphi = \cos(\vec{k}, \vec{k_0}) \quad . \tag{II-4-13}$$

It will be convenient to introduce a condensed notation as follows:

$$\theta = \frac{1+\mu}{2\sqrt{\mu}} = \frac{A+1}{2\sqrt{A}} \quad ; \quad \zeta = \frac{1-\mu}{2\sqrt{\mu}} = \frac{A-1}{2\sqrt{A}} \quad ; \quad \beta^2 = \frac{1}{2kT} \tag{II-4-14}$$

and

$$\left.\begin{aligned} \epsilon &= m\beta^2 v^2 = mv^2/2kT = E/kT \\ \epsilon_0 &= m\beta^2 v_0^2 = mv_0^2/2kT = E_0/kT \end{aligned}\right\} \quad . \tag{II-4-15}$$

With this notation, the final evaluation of the energy transfer cross section is given by the following formula:

$$\Sigma(\epsilon_0 \rightarrow \epsilon) = \Sigma_f \frac{\theta^2}{2\epsilon_0} \cdot$$

$$\begin{cases} e^{-(\epsilon - \epsilon_0)} \left\{\Theta\left(\theta\sqrt{\epsilon_0} - \zeta\sqrt{\epsilon}\right) + \Theta\left(\theta\sqrt{\epsilon_0} + \zeta\sqrt{\epsilon}\right)\right\} + \Theta\left(\theta\sqrt{\epsilon} - \zeta\sqrt{\epsilon_0}\right) \\ \qquad - \Theta\left(\theta\sqrt{\epsilon} + \zeta\sqrt{\epsilon_0}\right) \qquad \epsilon_0 \ \epsilon \\ e^{-(\epsilon - \epsilon_0)} \left\{\Theta\left(\theta\sqrt{\epsilon_0} - \zeta\sqrt{\epsilon}\right) - \Theta\left(\theta\sqrt{\epsilon_0} + \zeta\sqrt{\epsilon}\right)\right\} + \Theta\left(\theta\sqrt{\epsilon} - \zeta\sqrt{\epsilon_0}\right) \\ \qquad + \Theta\left(\theta\sqrt{\epsilon} + \zeta\sqrt{\epsilon_0}\right) \qquad \epsilon_0 > \epsilon \end{cases} \quad . \tag{II-4-16}$$

Here

$$\Theta(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-u^2}\, du \quad . \tag{II-4-17}$$

The total scattering cross section is evaluated by integration over the final energy of the neutron. The calculation yields the result

$$\Sigma_s(\epsilon_0) = \int_0^\infty \Sigma(\epsilon_0 \rightarrow \epsilon)\, d\epsilon$$

$$= \Sigma_f \frac{1}{2A\epsilon_0} \left[(2A\epsilon_0 + 1)\ \Theta(\sqrt{A\epsilon_0}) + \frac{2}{\sqrt{\pi}} \sqrt{A\epsilon_0}\ e^{-A\epsilon_0} \right] \quad . \tag{II-4-18}$$

Another quantity of interest is the mean energy change of the neutron, per collision, for a given incident neutron energy E_0. This is found to be

$$\left\langle \epsilon - \epsilon_0 \right\rangle_{Av} = \frac{\int_0^\infty (\epsilon - \epsilon_0)\ \Sigma(\epsilon_0 \rightarrow \epsilon)\, d\epsilon}{\int_0^\infty \Sigma(\epsilon_0 \rightarrow \epsilon)\, d\epsilon}$$

$$= kT \left[\frac{5}{(A+1)^2} - \frac{4}{(A+1)} + \frac{2A}{(A+1)^2}\ \epsilon_0 - \frac{2}{(A+1)^2}\ \frac{\Theta(\sqrt{A\epsilon_0})}{\Theta(\sqrt{A\epsilon_0})(2A\epsilon_0 + 1) + \frac{2}{\sqrt{\pi}}\ A\epsilon_0\, e^{-A\epsilon_0}} \right] \tag{II-4-19}$$

The dependence of this quantity on the incident neutron energy provides useful information on the moderation process.

For the purposes of practical calculation, it is convenient to express these formulas in terms of a new notation, with the variables

$$x = \sqrt{\epsilon} = \sqrt{E/kT}$$
$$x_0 = \sqrt{\epsilon_0} = \sqrt{E_0/kT} \quad . \tag{II-4-20}$$

In this notation we have the formulas, corresponding to Eqs. (II-4-16) and (II-4-18),

$$\Sigma(x_0 \rightarrow x) = \Sigma_f\ \theta^2\ (x/x_0^2)$$

$$\begin{cases} e^{-(x^2 - x_0^2)} \left\{ \Theta(\theta x_0 - \zeta x) + \Theta(\theta x_0 + \zeta x) \right\} + \Theta(\theta x - \zeta x_0) - \Theta(\theta x + \zeta x_0) & \\ & x_0 < x \\ e^{-(x^2 - x_0^2)} \left\{ \Theta(\theta x_0 - \zeta x) - \Theta(\theta x_0 + \zeta x) \right\} + \Theta(\theta x - \zeta x_0) + \Theta(\theta x + \zeta x_0) & \\ & x_0 > x \end{cases} \tag{II-4-21}$$

$$\Sigma_s(x_0) = \Sigma_f \frac{1}{x_0}\left[\left(x_0 + \frac{1}{2Ax_0}\right)\left(\sqrt{A}x_0\right) + \frac{1}{\sqrt{A\pi}} e^{-Ax_0^2}\right] \quad . \qquad \text{(II-4-22)}$$

The following quantities are sometimes useful in the consideration of the scattering of a neutron of given initial energy:

$$\Sigma_u(x_0) = \int_{x_0+0}^{\infty} \Sigma(x_0 \to x)\, dx \qquad \text{(II-4-23)}$$

$$\Sigma_d(x_0) = \int_{0}^{x_0-0} \Sigma(x_0 \to x)\, dx \quad . \qquad \text{(II-4-24)}$$

Here Σ_u measures the portion of scattering processes in which the neutron gains energy (up-scattering), and Σ_d similarly measures the scattering processes in which the neutron gives up energy (down-scattering) to the nuclei of the moderator. The quantities can be evaluated from our formulas, with the results

$$\Sigma_u(x_0) = \Sigma_f \frac{1}{x_0^2}\left\{\Theta\left(\frac{x_0}{\sqrt{A}}\right)\left[\left(\frac{A}{4}+\frac{1}{2}\right) - \frac{x_0^2}{2}\right] + \Theta\left(\sqrt{A}x_0\right)\left(\frac{x_0^2}{2}+\frac{1}{4A}\right) + \frac{x_0}{\sqrt{\pi}}\left[\frac{1}{2\sqrt{A}} e^{-Ax_0^2} - \frac{\sqrt{A}}{2} e^{-x_0^2/A}\right]\right\} \qquad \text{(II-4-25)}$$

$$\Sigma_d(x_0) = \Sigma_f \frac{1}{x_0^2}\left\{\Theta\left(\frac{x_0}{\sqrt{A}}\right)\left[\frac{x_0^2}{2} - \left(\frac{A}{4}+\frac{1}{2}\right)\right] + \Theta\left(\sqrt{A}x_0\right)\left(\frac{x_0^2}{2}+\frac{1}{4A}\right) + \frac{x_0}{\sqrt{\pi}}\left[\frac{1}{2\sqrt{A}} e^{-Ax_0^2} + \frac{\sqrt{A}}{2} e^{-x_0^2/A}\right]\right\} \quad . \qquad \text{(II-4-26)}$$

If one wishes to express his results in terms of the neutron density, rather than the neutron flux, it is convenient to make use of quantities expressing the scattering rate per neutron, rather than the cross section. The following expressions for the scattering rates, in unit of Σ_f, are convenient for our purposes:

$$P(x_0 \to x) = x_0\, \Sigma(x_0 \to x)/\Sigma_f \qquad \text{(II-4-27)}$$

$$V(x_0) = x_0\, \Sigma_s(x_0)/\Sigma_f \qquad \text{(II-4-28)}$$

$$V_u(x_0) = x_0\, \Sigma_u(x_0)/\Sigma_f \qquad \text{(II-4-29)}$$

$$V_d(x_0) = x_0\, \Sigma_d(x_0)/\Sigma_f \quad . \qquad \text{(II-4-30)}$$

The quantity $P(x_0 \to x)$ is often referred to as Wigner-Wilkins kernel.[7]

For the sake of future reference, we observe that the Wigner-Wilkins kernel satisfies the principle of detailed balancing for a Maxwellian distribution $M(x) = \text{const. } x^2 e^{-x^2}$; that is,

$$P(x_0 \to x)\, M(x_0) = P(x \to x_0)\, M(x) \quad . \qquad \text{(II-4-31)}$$

This can be verified readily by direct calculation using Eq. (II-4-27).

Graphs showing the behavior of these quantities are given in Figs. II-1 through II-4 for comparison with the conventional slowing-down theory.

II-5. The Relationship between Cross Sections in the Monatomic Gas Model and the Slowing-down Theory

We investigate in this section the manner in which the cross sections appropriate to the conventional slowing-down theory are interpreted as limits of those for the monatomic gas model. In the following formulas the superscript SD will be used for all quantities appropriate to the slowing-down theory.

In a straightforward way we can show that the scattering cross section $\Sigma^{SD}(E_0 \rightarrow E)$ in the slowing-down model is obtained as a limit of the monatomic gas model by requiring all moderator nuclei to be initially at rest, or, which is equivalent, by requiring the temperature in the moderator Maxwellian distribution to be zero. With the moderator nuclei initially at rest, the distribution function in Eq. (II-4-5) becomes

$$f(\vec{p}) = \delta(\vec{p}) \quad . \tag{II-5-1}$$

Equation (II-4-4) then takes the form

$$g(\vec{\kappa},t) = \int \vec{dp}\ \delta(\vec{p})\ e^{-(it/2M)\,(\hbar\kappa^2 - 2\vec{p}\cdot\vec{\kappa})} = \exp\left(-i\,\frac{\hbar\kappa^2}{2M}\,t\right) \quad . \tag{II-5-2}$$

Substitution of Eq. (II-5-2) into Eq. (II-3-13) yields the result

$$\sigma^{SD}(E_0\vec{\Omega}_0 \rightarrow E\vec{\Omega}) = \frac{a_b^2}{2\pi\hbar}\,\frac{k}{k_0}\int_{-\infty}^{+\infty} e^{-i\epsilon t/\hbar}\ e^{-i(\hbar\kappa^2/2M)\,t}\ dt$$

$$= \frac{a_b^2}{\hbar}\,\frac{k}{k_0}\ \delta\left(\frac{E-E_0}{\hbar} + \frac{\hbar(\vec{k}-\vec{k}_0)^2}{2M}\right) \quad . \tag{II-5-3}$$

Multiply both sides of this expression by N, the number density of moderator nuclei, and integrate over all scattering angles. This yields the macroscopic cross section for energy transfer:

$$\Sigma^{SD}(E_0 \rightarrow E) = \Sigma_f\,\frac{\theta^2}{E_0}\begin{cases} 1 & \text{if } [(A-1)/(A+1)]^2 E_0 < E < E_0 \\ 0 & \text{otherwise,} \end{cases} \tag{II-5-4}$$

with

$$\theta = \frac{A+1}{2\sqrt{A}} = \frac{1}{\sqrt{1-\alpha^2}} \quad ; \quad \alpha = \frac{A-1}{A+1} \quad . \tag{II-5-5}$$

It will be convenient for purposes of comparison to express energies in units of kT, as we have done in the monatomic gas theory, although in the slowing-down theory this unit is purely formal. With $\epsilon = E/kT$, we have, from Eq. (II-5-4),

$$\Sigma^{SD}(\epsilon_0 \to \epsilon) = \Sigma_f \frac{\vartheta^2}{\epsilon_0} \begin{cases} 1 & \text{if } \alpha^2\epsilon_0 < \epsilon < \epsilon_0 \\ 0 & \text{otherwise} \end{cases} \quad . \tag{II-5-6}$$

Furthermore,

$$\Sigma_s^{SD}(\epsilon_0) = \int_0^\infty \Sigma^{SD}(\epsilon_0 \to \epsilon)\, d\epsilon = \Sigma_f \quad . \tag{II-5-7}$$

When expressed in terms of the variable $x = \sqrt{\epsilon} = \sqrt{E/kT}$, the scattering rates, corresponding to Eqs. (II-4-27) and (II-4-28), are

$$P^{SD}(x_0 \to x) = \frac{\theta^2 x}{x_0} \begin{cases} 2 & \text{if } \alpha x_0 < x < x_0 \\ 0 & \text{otherwise} \end{cases} \tag{II-5-8}$$

$$V^{SD}(x_0) = x_0 \quad . \tag{II-5-9}$$

The main physical differences between the two models are easily expressed. In the slowing-down model, the moderator nuclei are assumed to be initially all at rest. Consequently, the incident neutrons can only lose energy to the nuclei (down-scattering), and there is a lower limit to the possible energy loss, which is fixed by the mass ratio $A = M/m$. In the gas model, both up- and down-scattering processes are possible, and all energy exchanges are allowed.

The gas model thus degenerates into the slowing-down model in the limit $T \to 0$. Furthermore, in the region of high neutron energies, in which the neutron energy greatly exceeds the mean kinetic energy of the nuclei at the given moderator temperature, the two models give quite similar results, which can be examined in greater detail from our formulas of Section II-4 for the gas model by considering the asymptotic behavior for $\epsilon \gg 1$.

Figure II-1 illustrates the degeneration of the gas model into the slowing-down model for two different high incident neutron energies in moderators of masses 1 and 12.

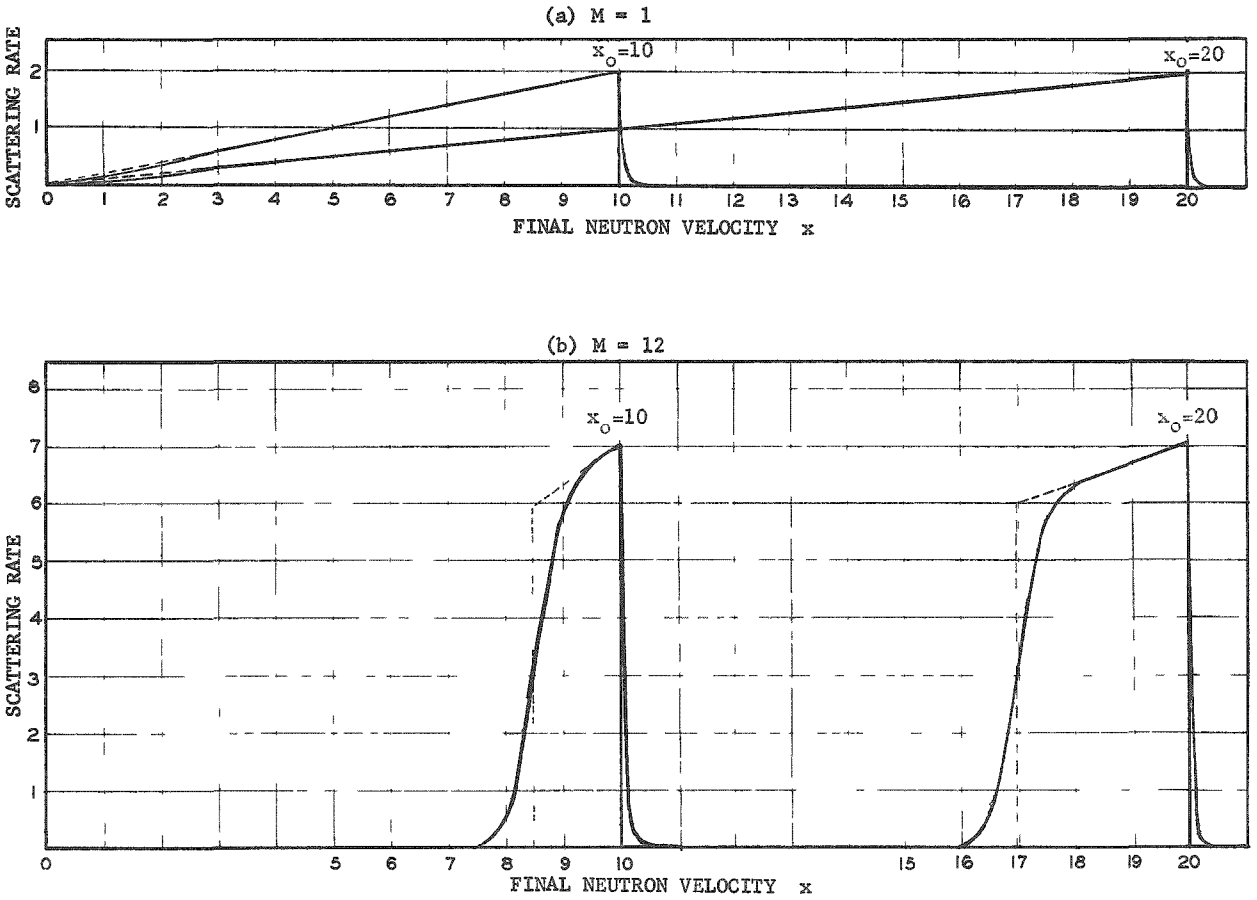

Fig. II-1. High-velocity Incident Neutron Scattering Rate $P(x_0 \rightarrow x)$

– – – – – – Slowing-down Model ———— Gas Model

Figure II-2 illustrates the two models for the same two moderator masses, but for two different low incident neutron energies, where low and high incident energies are referred to the peak of the moderator distribution taken as x = 1. This figure shows the marked difference between the two models, which lies in the fact that the gas model includes the up-scattering of low-energy neutrons whereas the slowing-down model ignores it.

Figure II-3 is a plot of the scattering rate V versus neutron speed for three moderator masses, together with the up-scattering rate V_u and the down-scattering rate V_d at each speed, that shows that, as the moderator mass increases, the scattering rate approaches the straight line of the slowing-down model at lower and lower energy. Figure II-4 is a replot of Figure II-3 that shows the down scattering rate as a fraction of the total scattering for several moderator masses. From this figure one can determine, for different moderator masses, the energies above which the slowing-down model may be used.

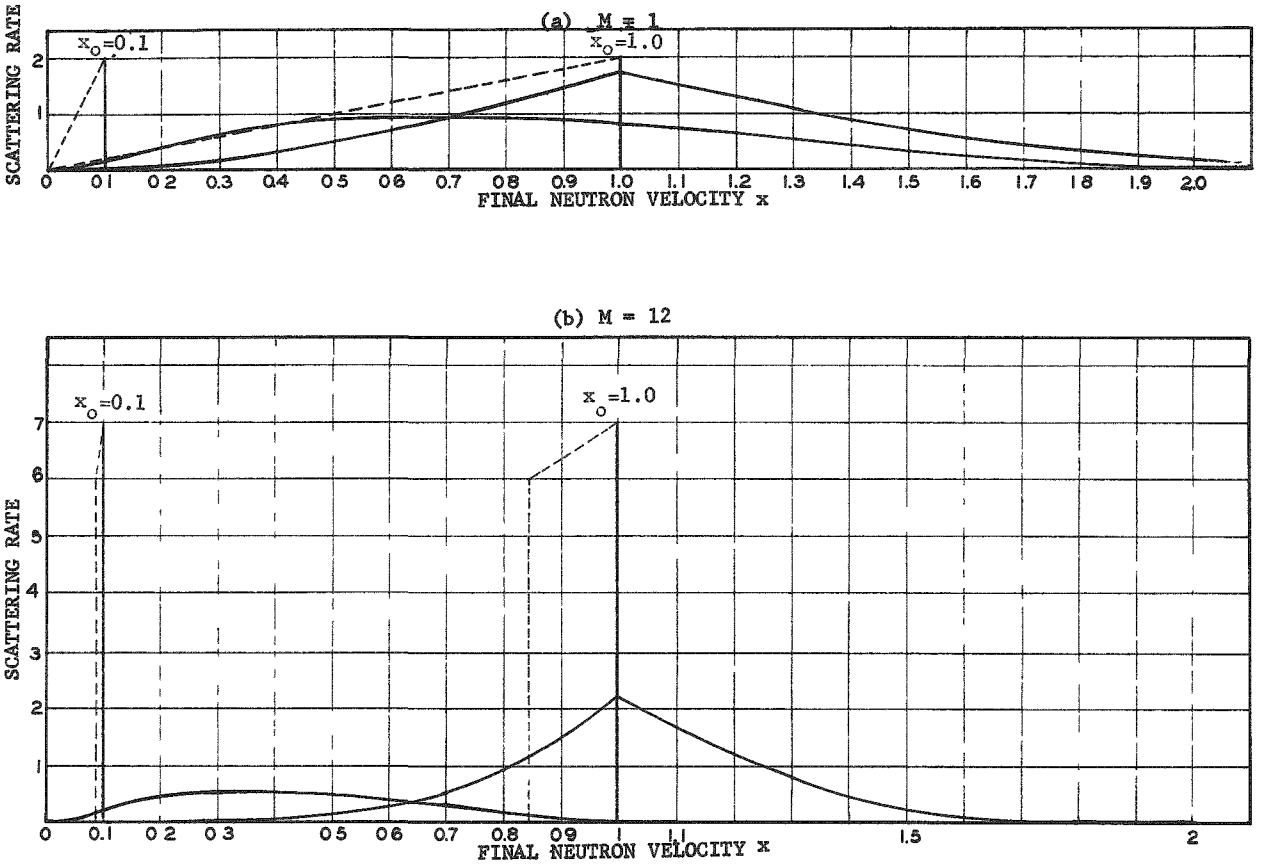

Fig. II-2. Low-Velocity Incident Neutron Scattering Rate $P(x_0 \rightarrow x)$

– – – – – Slowing-down Model ——— Gas Model

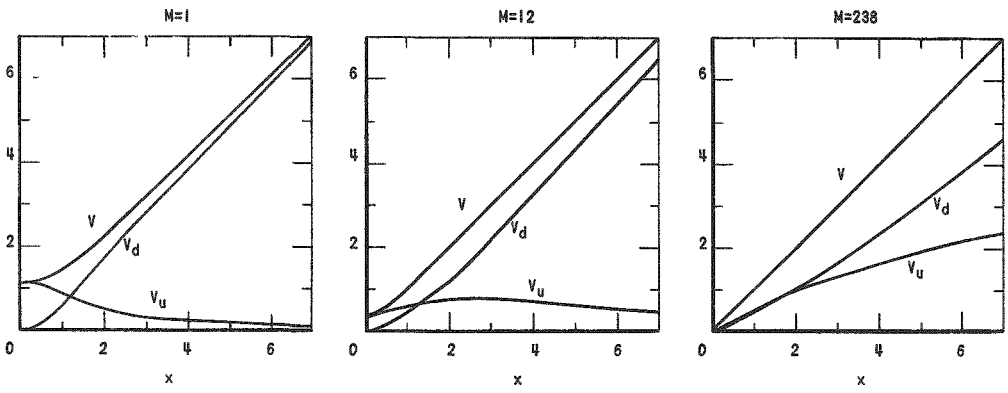

Fig. II-3. Scattering Rates vs. Incident Neutron Velocity

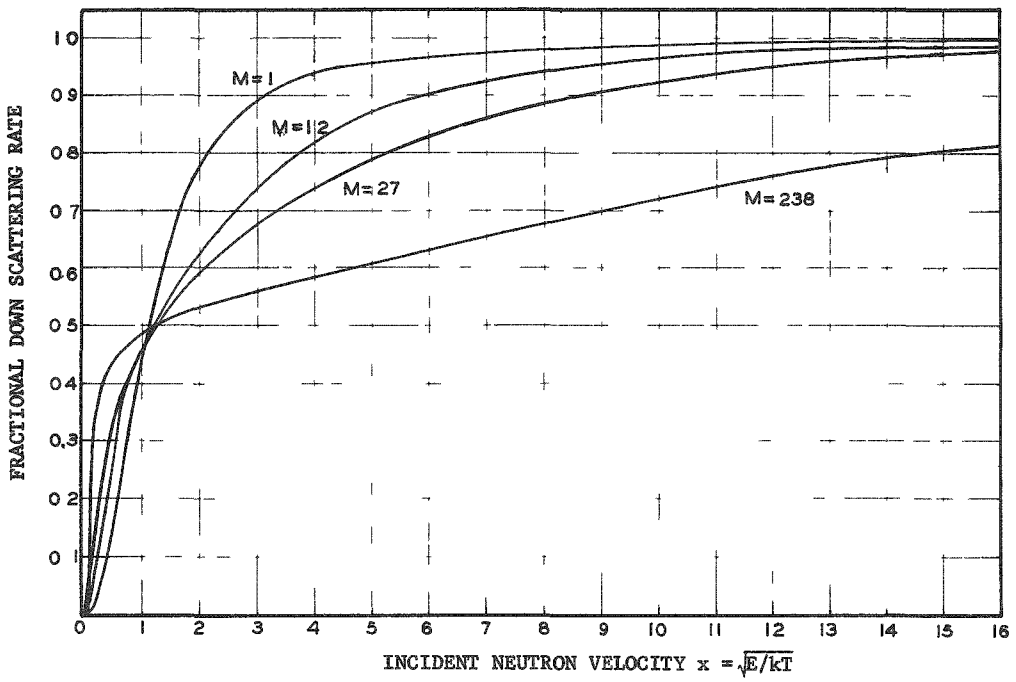

Fig. II-4. Fractional Down-scattering Rates vs. Incident Neutron Velocity

CHAPTER III

MODERATION OF NEUTRONS IN MODERATORS OF UNIT ATOMIC MASS

III-1. Introduction

In the slowing-down model, with the moderator at rest, an exact analytical solution can be found for nuclei of unit atomic mass. This case is usually called the monatomic hydrogen gas moderator, even though hydrogen gas is actually diatomic. In the present treatment, with the moderator in motion, no exact solution is known, even for the case of moderator nuclei of unit mass, much less for the case of a general mass. It is necessary, therefore, to develop approximation procedures for testing the formulas of the theory.

It will be convenient for practical reasons, and also for gaining a better insight into the nature of the results, to treat the case of moderator atoms of unit mass in this chapter, reserving the case of general mass for the following chapter. The qualitative nature of the solution is discussed in Section III-2. The slowing-down theory for this case is found as an asymptotic form of our solution in Section III-3. Section III-4 will treat the direct numerical solution of our integral equation. An alternative method which is available for this special case is discussed in Section III-5, in conjunction with a discussion of the work of Wigner and Wilkins.[7] Finally, Section III-6 will be devoted to a comparison of some of the existing work and miscellaneous considerations.

III-2. Qualitative Considerations on the Solution

It was shown in Chapter I that the condition that the total rate of absorption of neutrons is just equal to the rate at which neutrons are introduced into the system provides a relation governing the stationary distribution. This equation is the following:

$$[v\Sigma_s(v) + v\Sigma_a(v)]n(v) = \int_0^\infty dv'\, v'\Sigma(v' \to v)\, n(v') + S(v) \quad . \text{(III-2-1)}$$

When the scattering and absorption cross sections are known, this is an integral equation for the neutron density function $n(v)$.

The most reasonable interpretation to be made is that the neutrons are introduced into the system at a relatively high energy, of the order of 1 Mev. We will be interested in the velocity distribution of the neutrons over the whole velocity range below this value. For the sake of simplicity, the initial neutron source is supposed to be monoenergetic.

Immediately after their introduction, neutrons with high initial energy will undergo scattering, with large energy losses, with the moderator atoms. Since we impose an absorption law varying as $1/v$, the absorption rate will be small for the high-energy neutrons. The mean energy loss per collision will be large in this region, and most of the neutrons which survive the very small probability of capture will pass through this stage quickly. This will be referred to as region 1.

As the neutrons descend the energy scale, the energy loss per collision will decrease and the rate at which slowing-down occurs will diminish. At the same time, the possibility of capture will increase, and absorption becomes appreciable. This will be referred to as region 2.

Neutrons which come down the energy scale to a point at which their kinetic energies are of the order of the kinetic energy of the moderator atoms will exchange only a small amount of energy per collision, and may even gain energy from the moderator atoms (up-scattering). The mean energy loss per collision of the neutrons will be very small in this case, whereas absorption will play a more significant role. This will be referred to as region 3.

Neutrons which have passed through period 3 will tend to gain energy on scattering, whereas absorption will be very strong. This will be referred to as region 4.

If there were no capture of neutrons, and we introduced a burst of high-energy neutrons at a particular instant and then isolated the system, the neutrons would be degraded in energy by collisions and would ultimately come into equilibrium with the moderator atoms at the stated temperature of the moderator. When capture (absorption) processes are present, and neutrons are introduced continually to produce a stationary distribution of neutrons, the neutron energy spectrum will be appreciably hardened over the first case. This follows from the simple fact that neutrons are introduced at high energies, whereas absorption is most effective in removing neutrons of low energy.

In the monatomic gas model of the moderator which we are using, the distribution of energies of the moderator atoms should be of Maxwellian form at the temperature of the moderator. The argument just given shows that the stationary neutron energy distribution will contain a higher proportion of high-energy neutrons than the Maxwell law, i.e., the neutron energy spectrum will be harder than the Maxwellian distribution at the given temperature.

The direct analytical solution of Eq. (III-2-1) is not known. In our study, we make use of numerical calculation methods, with the aim in mind of extending them later to moderator atoms of arbitrary mass. Further considerations of an analytical nature will be given in Section III-5.

The first difficulty which we encounter in the numerical work is the fact that the upper limit of the integral in the left hand side of Eq. (III-2-1) is infinite. We avoid this by the following considerations.

It has been shown in Chapter II that, in the high-energy region, the cross sections which we shall use reduce to those employed in the conventional slowing-down theory. If we assume at first that all of the neutrons are in the regions of higher energy (regions 1 and 2), with energies well above the energies of the moderator atoms, we can determine a type of distribution. The thermal motions of the moderator atoms and the up-scattering of low-energy neutrons will not affect this distribution very much. We can therefore determine the solution in the high-energy region as a type of asymptotic solution of Eq. (III-2-1). This asymptotic solution will be determined in the next section, and when found it will be used as a kind of normalization condition in the numerical work extending into the low-energy region.

III-3. The Asymptotic Solution for Large Neutron Energies

We use the symbol T for the temperature of the moderator, as in Chapter II, and use the variable $x = (E/kT)^{1/2}$, where k is Boltzmann's constant. In terms of this independent variable, Eq. (III-2-1) becomes

$$[x\Sigma_s(x) + x\Sigma_a(x)]\,n(x) = \int_0^\infty dx_0 x_0 \Sigma(x_0 \rightarrow x)\,n(x_0) + S(x_0) \quad . \text{(III-3-1)}$$

On dividing both sides by the scattering cross section of the free atom, Σ_f, which will be assumed to be constant (i.e., independent of neutron energy), we have the equation

$$[V(x) + \Gamma]\,n(x) = \int_0^\infty dx_0 P(x_0 \rightarrow x)\,n(x_0) + X(x) \quad , \qquad \text{(III-3-2)}$$

with the notation

$$\Gamma = x\Sigma_a(x)/\Sigma_f \quad ; \qquad \text{(III-3-3)}$$

$$P(x_0 \rightarrow x) = (1/\Sigma_f)\, x_0 \Sigma(x_0 \rightarrow x) \quad ; \qquad \text{(III-3-4)}$$

$$V(x) = x\Sigma_s(x)/\Sigma_f \quad ; \qquad \text{(III-3-5)}$$

and $X(x) = S(x)/\Sigma_f$. It is to be noticed that, with the 1/v law of absorption, the quantity Γ is independent of neutron energy.

Using the results of Chapter II for moderator nuclei of unit mass, we have

$$P(x_0 \to x) = \frac{2x}{x_0} \begin{cases} \Theta(x_0) \exp(x_0^2 - x^2) & , \quad x_0 < x \\ \Theta(x) & , \quad x_0 > x \end{cases} \tag{III-3-6}$$

$$V(x) = \left(x + \frac{1}{2x}\right) \Theta(x) + \frac{1}{\sqrt{\pi}} \exp(-x^2) \tag{III-3-7}$$

with

$$\Theta(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} \, dy \tag{III-3-8}$$

It will be well at this point to introduce a discussion of the nature of the source function to be used. In the physical problem, neutrons are introduced into the system by the fission process, most of the neutrons having kinetic energies of the order of 1 to 2 Mev. Every practical source yields neutrons of energy well above thermal. The part of the neutron energy spectrum which is of major concern is that in the low-energy range, say of the order of 1 ev. It is evident that the actual initial energies of the neutrons cannot have a determinative influence on the low-energy spectrum when a stationary distribution is being considered. It will, therefore, be a considerable mathematical simplification for us to assume that the neutrons are introduced at an indefinitely high energy. This idealization of the source as being at infinite energy will not prevent our normalization of the neutron density function through the requirement that the total rate of absorption of neutrons per cm^3 per sec is just equal to the rate of introduction of neutrons. Since our solution will be found to yield a finite total number of neutrons per cm^3, this criterion makes physical as well as mathematical sense.

With this interpretation to be assigned to the neutron source, we can formally drop the second member on the right-hand side of Eq. (III-3-2) and write the integral equation in the form

$$[V(x) + \Gamma] N(x) = \int_0^\infty dx_0 \, P(x_0 \to x) \, N(x_0) \quad . \tag{III-3-9}$$

Here we have introduced the new notation

$$N(x) = n(x) \qquad 0 \leq x \quad \infty \tag{III-3-10}$$

for the neutron density function, to emphasize the fact that N(x) represents the density function for those neutrons which have suffered one or more collisions, and so does not include the initial virgin neutrons which have not yet suffered a collision.

This equation can be written in a somewhat simplified form for large values of x by substitution of the asymptotic expressions

$$P(x_0 \rightarrow x) = \frac{2x}{x_0} \begin{cases} 0 \text{ if } x_0 < x \\ 1 \text{ if } x_0 > x \end{cases} \qquad \text{(III-3-11)}$$

$$V(x) = x \quad . \qquad \text{(III-3-12)}$$

Thereby we obtain the integral equation of $N_{as}(x)$ as

$$(x + \Gamma)\, N_{as}(x) = 2x \int_x^\infty \frac{N_{as}(x_0)}{x_0}\, dx_0 \quad . \qquad \text{(III-3-13)}$$

Although Eq. (III-3-13) has been found as the asymptotic form of Eq. (III-3-9), it has a wider significance. It was shown in Chapter II that the asymptotic forms of the cross sections used in the gas model are equivalent to those employed in the slowing-down theory. It is to be expected, therefore, that the asymptotic form of the neutron distribution function of the gas model should be the exact solution for the slowing-down model, and hence Eq. (III-3-13) should be the exact integral equation for the latter model. This is, in fact, the case, as is shown by the fact that the solution of Eq. (III-3-13) given below was found by Placzek[3] from the slowing-down theory by a different process, whereas Wigner and Wilkins[7] showed that their series solution takes this same form approximately in the asymptotic energy range. We can therefore consider Eq. (III-3-13) to apply to the slowing-down model, for all values of x. This remark will be of use to us in the next section.

In order to solve Eq. (III-3-13) we make the substitution

$$\Phi_{as}(x) = \frac{x + \Gamma}{x} N_{as}(x) \quad . \qquad \text{(III-3-14)}$$

Differentiation of both sides of Eq. (III-3-13) with respect to x yields the following first-order differential equation:

$$\frac{d\Phi_{as}}{dx} = -\frac{2}{x + \Gamma}\, \Phi_{as} \quad , \qquad \text{(III-3-15)}$$

which has the solution

$$\Phi_{as}(x) = C/(x + \Gamma)^2 \quad , \qquad \text{(III-3-16)}$$

where C is a constant of integration which will be determined shortly. On using Eq. (III-3-14), we find at once the following solution of Eq. (III-3-13):

$$N_{as}(x) = Cx/(x + \Gamma)^3 \quad . \tag{III-3-17}$$

Formula (III-3-17) shows that $N_{as}(x)$ has a maximum at $x = \Gamma/2$. Consideration of the motions of the moderator atoms indicates that in the gas model this maximum should come at a somewhat higher value of x. The low value predicted by the slowing-down theory comes about by the fact that it ignores the rapid decrease in the differential scattering cross section for low energies, and the existence of up-scattering which is particularly significant in the low-energy region.

The determination of the integration constant C in Eq. (III-3-17) can be made by equating the rate of absorption of neutrons to the rate of injection by the source. This will be done in a particular way for the purposes of numerical integration in the next section.

III-4. Numerical Integration for N(x)

In order to carry out the numerical integration of Eq. (III-3-9) for N(x) we introduce a certain energy value, x_c, chosen sufficiently large that for $x > x_c$ we can require $N(x) = N_{as}(x)$, where the latter quantity is given by Eq. (III-3-17). It will be necessary also to neglect the up-scattering from the energy range $x < x_c$ into the range $x > x_c$. This approximation is not so serious for the case of moderator atoms of unit mass as it is for heavier moderators.

In the energy range $x < x_c$, the second member of the right-hand side of Eq. (III-3-9) will be small, according to the discussion of the last section, and will be neglected. With these reductions, Eq. (III-3-9) takes the form

$$[V(x) + \Gamma]\, N(x) = \left(\int_0^x + \int_x^{x_c} \right) dx_0 P(x_0 \rightarrow x)\, N(x_0) + \int_{x_c}^{\infty} dx_0 P(x_0 \rightarrow x)\, N_{as}(x_0) \quad . \tag{III-4-1}$$

The functional forms of the quantities $V(x)$ and $P(x_0 \rightarrow x)$ as found in the last section are

$$V(x) = \left(x + \frac{1}{2x} \right) \Theta(x) + \frac{\exp(-x^2)}{\sqrt{\pi}} \tag{III-4-2}$$

and

$$P(x_0 \rightarrow x) = \frac{2x}{x_0} \begin{cases} \Theta(x_0) \exp(x_0^2 - x^2) & \text{if} \quad x_0 < x \\ \Theta(x) & \text{if} \quad x_0 > x \end{cases} . \qquad \text{(III-4-3)}$$

The functional form of $P(x_0 \rightarrow x)$ allows us to evaluate the third member on the right-hand side of Eq. (III-4-1) explicitly. On substitution of Eq. (III-3-17) for $N_{as}(x)$, we find that

$$\int_{x_0}^{\infty} dx_0 P(x_0 \rightarrow x)\, N_{as}(x_0) = 2x\,\Theta(x) \int_{x_c}^{\infty} \frac{C x_0}{x_0(x_0 + \Gamma)^3}\, dx_0$$

$$= x\,\Theta(x)\, \frac{C}{(x_c + \Gamma)^2} = Rx\,\Theta(x) \quad , \qquad \text{(III-4-4)}$$

with $R = C/(x_c + \Gamma)^2$. The explicit integrability of this expression is characteristic of the case of moderator atoms of unit mass. For the case of moderator atoms of general mass, to be treated in the next chapter, a much rougher approximation will have to suffice at this point.

We divide the finite interval $(0, x_c)$ into M subintervals, the lengths of which are not necessarily equal. Employing the simplest trapezoidal rule, Eq. (III-4-1) is replaced by the approximate expression

$$\sum_{j=1}^{i-1} P(x_j \rightarrow x_i)\, N(x_j)\, H_j + [P(x_i \rightarrow x_i)\, H_i - V(x_i) - \Gamma]\, N(x_i)$$

$$+ \sum_{j=i+1}^{M} P(x_j \rightarrow x_i)\, H_j N(x_j) = -2\, x_i\, \Theta(x_i)\, R \qquad (i = 1, 2, \ldots, M)$$

(III-4-5)

where H_j denotes the size of the j-th mesh and includes the fractions in the trapezoidal rule. Since $N(0) = 0$, the number of equations in the system (III-4-5) is just M.

A straightforward solution of this set of simultaneous linear equations was first tried for M = 100, employing the subroutine for matrix inversion for the IBM 704 computer at the Argonne National Laboratory.[9]

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[9] Argonne National Laboratory, AMD Subroutine AN F403.

The result was quite satisfactory with this program, but had the disadvantage that a relatively long machine time of about 11 or 12 min was required for the inversion of the 100 x 100 matrix. Furthermore, the accuracy of the calculation could not be controlled. Since the machine time required for matrix inversion is proportional to the cube of M, an increase in the number of mesh points quickly raises the required machine time.

These considerations led to a revised program based on an iteration process instead of matrix inversion. Taking into account the capacity of IBM 704, which has a total memory space of 32,000, a maximum number of mesh points M = 150 was possible for this process. Various degrees of accuracy can be achieved by adjustment of the convergence criteria. The computer requires the rather long time of 1.5 to 2 min for the evaluation of the cross sections. By fixing the choice of mesh sizes and points, these cross sections could be used repeatedly for different values of the absorption parameter Γ. The machine time required for the iteration process, using M = 100, with the increment on successive iterations less than 10^{-4}, was less than 2 min.

For the iteration process Eq. (III-4-5) was rewritten in the form

$$N(x_i) = \frac{1}{V(x_i) + \Gamma} \left[\sum_{j=1}^{M} P(x_j \rightarrow x_i) H_j N(x_j) + 2R x_i \Theta(x_i) \right] \quad . \quad \text{(III-4-6)}$$

The asymptotic solution $N_{as}(x)$ from Eq. (III-3-18) was used as the initial trial function to start the process.

The normalization procedure requires some consideration. For this purpose we first set

$$\int_0^\infty N_{as}(x)\, dx = 1 \quad , \qquad \text{(III-4-7)}$$

from which we find, using Eq. (III-3-18), that

$$C = 2\Gamma \quad . \qquad \text{(III-4-8)}$$

At this point we have taken advantage of the fact that $N_{as}(x)$ is the correct neutron distribution function for the slowing-down model for all values of the neutron energy. This normalization condition fixes the strength of the external source of neutrons to be $Q = \Gamma$.

Suppose that the total source strength of the neutron source is given. Then, regardless of the nature of the model used, or of any other conditions, the existence of a stationary state implies that the total rate of absorption of neutrons must just equal the rate of input. If this condition is expressed in terms of the density functions on the neutron velocity scale, as was done in Eq. (I-2-8), we have the following conditions:

$$\int_0^\infty v\Sigma_a(v)\,N(v)\,dv = \int_0^\infty v\Sigma_a(v)\,N_{as}(v)\,dv = \int_0^\infty S(v)\,dv. \quad \text{(III-4-9)}$$

However, since we assume throughout this thesis the usual "1/v law" of absorption, $\Sigma_a(v) \propto 1/v$, so that $v\Sigma_a(v)$ is independent of neutron velocity; i.e., the probability of absorption of a neutron per unit time is independent of its velocity or energy. In this case, Eq. (III-4-9) takes the simpler form

$$\int_0^\infty N(v)\,dv = \int_0^\infty N_{as}(v)\,dv = \frac{1}{v\Sigma_a(v)} \int_0^\infty S(v)\,dv \quad , \quad \text{(III-4-10)}$$

from which it follows that

$$\int_0^\infty [N(v) - N_{as}(v)]\,dv = 0 \quad . \quad \text{(III-4-11)}$$

From this point on it will be convenient to express our density functions on the scale of neutron energy, rather than velocity, that is, we use the variable x instead of v. In these terms Eq. (III-4-11) will be

$$\int_0^\infty [N(x) - N_{as}(x)]\,dx = 0 \quad . \quad \text{(III-4-12)}$$

This relation shows that the function

$$g(x) = N(x) - N_{as}(x) \quad \text{(III-4-13)}$$

must not be one-signed over the whole energy range. The argument given at the end of Section III-3 shows that g(x) is positive for large energies, and negative for low energies, for the case of a moderator with atoms of unit mass.

Since we have required that $N(x) = N_{as}(x)$ when $x > x_c$, Eq. (III-4-12) requires that

$$\int_0^{x_c} N(x)\,dx = \int_0^{x_c} N_{as}(x)\,dx = \left(\frac{x_c}{x_c + \Gamma}\right)^2 \quad \text{(III-4-14)}$$

when we make use of Eq. (III-3-17) for the evaluation of the second integral. In a similar way, the strength of the external neutron source can be evaluated from formula (III-4-10). Since this evaluation is of no further interest to us, we do not write it out explicitly.

The graphs given in Figs. III-1 through III-4 show clearly the point mentioned in Section III-4 concerning the low value of energy at which the maximum of the distribution function $N_{as}(x)$ is reached. The maximum in N(x) moves to higher energies with increase of the absorption constant.

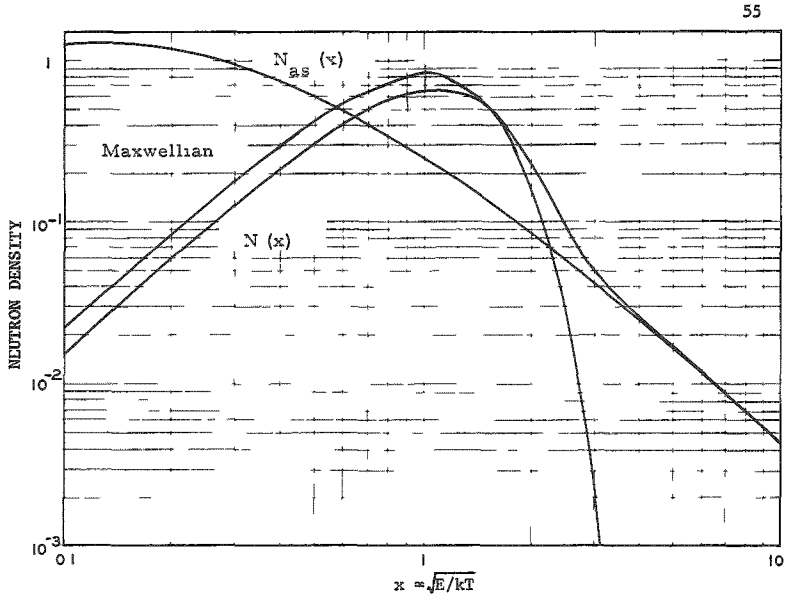

Fig. III-1. Neutron Density in Moderator of Unit Atomic Mass for $\Gamma = 0.226$.

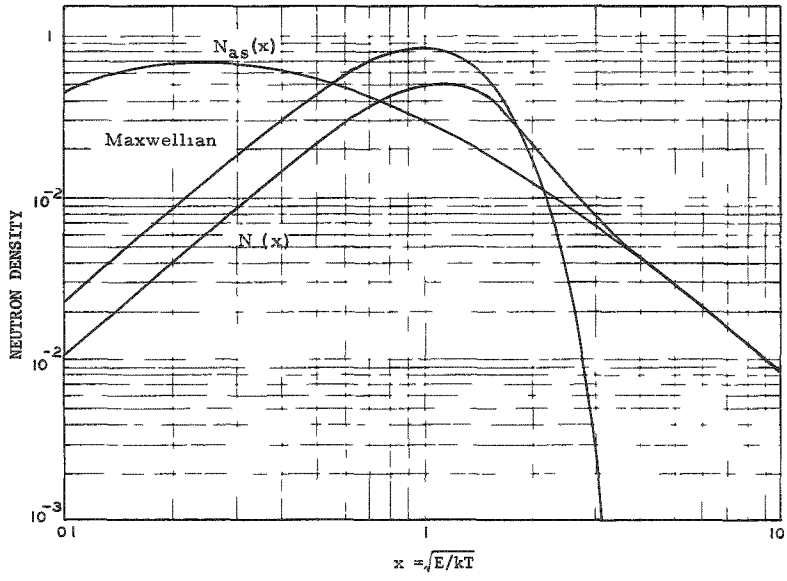

Fig. III-2. Neutron Density in Moderator of Unit Atomic Mass for $\Gamma = 0.451$.

In the low-energy region, in which the neutrons have about the same mean kinetic energies as the gas atoms, the distribution resembles the Maxwellian in form, but in the high-energy region, well above the value $kT(x >> 1)$ it takes on the form of $N_{as}(x)$.

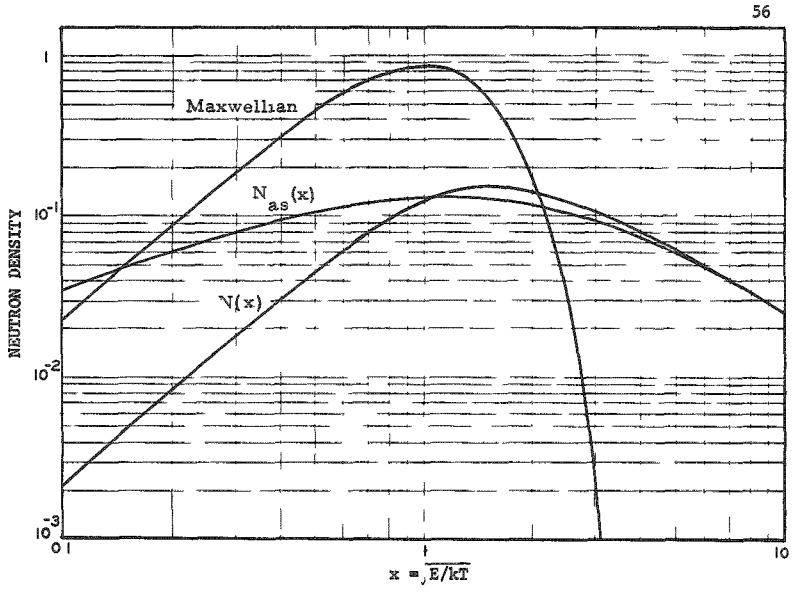

Fig. III-3. Neutron Density in Moderator of Unit Atomic Mass for $\Gamma = 2\ 257$

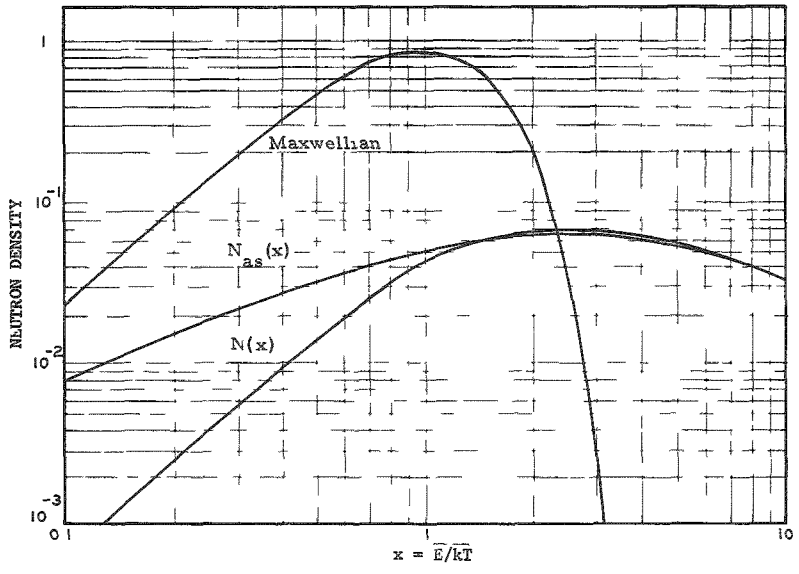

Fig. III-4 Neutron Density in Moderator of Unit Atomic Mass for $\Gamma = 5.0$

III-5. Reduction to the Wigner- Wilkins Differential Equation

It was shown by Wigner and Wilkins[7] that for moderator nuclei of unit mass it is possible to replace the integral equation of the gas model by a second-order differential equation. This results from the factorization of the kernel $P(x_0 \rightarrow x)$ into a product of two functions, each depending on only one of the variables, as is shown explicitly in Eq. (III-3-6). This factorization does not hold for moderator nuclei of other masses.

Wigner and Wilkins make the reduction of their differential equation after symmetrizing the kernel by use of the condition of detailed balancing (cf. Section II-4):

$$P(x_0 \rightarrow x)\, M(x_0) = P(x \rightarrow x_0)\, M(x) \quad , \tag{III-5-1}$$

where $M(x)$ is the Maxwellian distribution function. This condition holds for our density function $N(x)$ if no absorption occurs and no external source is present, in which case $N(x)$ takes the Maxwellian form.

It is of some importance to observe that so far as reduction of the integral equation to a differential equation is concerned, the Wigner-Wilkins symmetrization procedure is unnecessary. For this purpose, we first rewrite Eq. (III-3-9) in the form

$$[V(x) + \Gamma]\, N(x) = 2xe^{-x^2} \int_0^x e^{x_0^2}\, \Theta(x_0)\, \frac{N(x_0)}{x_0}\, dx_0 + 2x\, \Theta(x) \int_x^\infty \frac{N(x_0)}{x_0}\, dx_0 \quad . \tag{III-5-2}$$

Next, we introduce the definition

$$\Phi(x) = \frac{V(x) + \Gamma}{x}\, N(x) \quad . \tag{III-5-3}$$

This transformation brings Eq. (III-5-2) to the form

$$e^{x^2} \Phi(x) = 2 \int_0^x e^{x_0^2}\, \Theta(x_0)\, \frac{\Phi(x_0)}{V(x_0) + \Gamma}\, dx_0 + 2e^{x^2}\, \Theta(x) \int_x^\infty \frac{\Phi(x_0)}{V(x_0) + \Gamma}\, dx_0 \quad . \tag{III-5-4}$$

The differential equation satisfied by $\Phi(x)$ which we are seeking can be found by differentiation of Eq. (III-5-4) twice with respect to x, and reduction of the resulting formulas. We introduce the abbreviation

$$P(x) = x\Theta(x) + \frac{1}{\sqrt{\pi}}\exp(-x^2) \quad , \qquad \text{(III-5-5)}$$

and the differential equation is found to be

$$\frac{d^2\Phi}{dx^2} + \left[2x - \frac{\Theta(x)}{P(x)}\right]\frac{d\Phi}{dx} + \left[\frac{(2/\sqrt{\pi})e^{-x^2}}{P(x)} + \frac{4P(x)}{V(x) + \Gamma}\right]\Phi = 0 \qquad \text{(III-5-6)}$$

This equation is equivalent to that found by Wigner and Wilkins. Once the solution of this equation is known, the neutron density function N(x) can be calculated from Eq. (III-5-3).

Unfortunately, no analytical solution is known for Eq. (III-5-6), or for the equivalent equation given by Wigner and Wilkins, and so one is forced to make use of numerical integration, just as was the case for original integral equation.

In order to make a comparison with our numerical results for the integral equation, a numerical solution of Eq. (III-5-6) was made on the IBM 650 computer at the Argonne National Laboratory. The results of higher quality could have been made by use of the IBM 704, but the extra effort did not seem to be justified by the nature of the problem.

III-6. Concluding Comments

In summary, it was found that the numerical solutions of the integral and differential equations for the gas model, with moderator atoms of unit mass, agreed well among themselves and also with the numerical work published by Wigner and Wilkins. This in itself is not surprising, since the reduction from the integral to the differential equation in this particular case is exact. It is, in fact, more a check on the reasonable compatibility of the various approximations used by the different authors. It may be remarked that Coveyou, Bate, and Osborn[10] have carried out a Monte Carlo calculation with results comparable with those of Wigner and Wilkins.

The favorable character of the results for the particular case of moderator atoms of unit mass cannot be expected to hold for atoms of higher mass, as will be seen in the next chapter. In this case there is no known exact reduction of the integral equation to a differential equation, and the various approximation methods become less accurate.

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[10] R. R. Coveyou, R. R. Bate, and R. K. Osborn, J. Nuclear Energy, 2, 153 (1956).

CHAPTER IV

THE GAS MODEL FOR MODERATOR ATOMS OF GENERAL MASS

IV-1. Introduction

We saw in Chapter III that for moderator nuclei of unit mass (atomic hydrogen as a moderator), the Wigner-Wilkins integral equation of the gas model can be reduced to a differential equation of the second order. For moderators with masses greater than unity, this reduction is not possible, except as an approximation, and one is obliged to depend upon numerical calculations entirely for the study of the integral equation. The difficulties of the problem in this case are quite severe. The corrections to the differential cross sections due to the thermal motions of the moderator atoms are more complex than for unit mass, and are strongly mass dependent. The larger the mass of the moderator nuclei, the more difficult it is to obtain a numerical solution of the integral equation for a given accuracy.

In Section IV-2 we shall consider some qualitative features of the solution. Section IV-3 is devoted to the asymptotic solution (slowing-down theory) and the approximations involved in it. In Section IV-4 we describe a direct numerical solution of the integral equation. Section IV-5 will be devoted to a discussion of some of the approximate solutions which have appeared in the literature. Section IV-6 contains a comparison of all results, and Section IV-7 summarizes the results of this study.

IV-2. Some Qualitative Considerations

The general features of the moderation of high-energy neutrons are similar to those described in Chapter III for moderation by nuclei of unit mass. However, as the moderator mass increases, the energy distribution of the moderator nuclei changes over the entire energy range affecting both scattering and absorption of neutrons. The scattering is affected because, as the moderator mass is increased, more momentum is available at every energy for scattering neutrons. This can be seen from the expression for the moderator Maxwellian distribution in momentum: $4\pi^{-1/2} M^{-3/2} \beta^3 p^2 \exp(-\beta^2 p^2/M)$, where $p = Mv$. As M is increased, the peak and the entire distribution is shifted to higher values of p. Thus the effect of moderator motion is felt at higher energies for greater moderator masses, and the energy range over which the numerical integration must be performed is extended (cf. figures in Chapter II).

The absorption is affected because, as the moderator mass is increased, the energy lost per collision is decreased, thereby requiring a greater number of neutron collisions for a given reduction in neutron energy. By requiring more collisions for a given energy reduction, the probability of absorption is increased, and so the effect of absorption extends higher in energy with increased moderator mass.

IV-3. The Asymptotic Solution (Slowing-down Model).

Our aim is again to use the neutron distribution of the slowing-down model as the asymptotic form of the solution for the gas model at high energy. As was indicated in Chapter II, this connection is based on the fact that the cross sections for the gas model degenerate into those for the slowing-down model at high energy for arbitrary moderator mass.

However, for a general mass the determination of a suitable analytic approximation for the distribution function of the slowing-down model is difficult, and the approximation procedure used in Chapter III is no longer adequate. The form of the integral equation for the slowing-down model with the external source placed at infinite energy was discussed in Section III-3, and is

$$(x + \Gamma)\, N_{as}(x) = 2\theta^2 x \int_x^{x/\alpha} \frac{N_{as}(x_0)}{x_0}\, dx_0 \quad , \qquad \text{(IV-3-1)}$$

with $\alpha = (A - 1)/(A + 1)$, $A = 1/\mu = M/m$, $\theta^2 = 1/(1 - \alpha^2)$.

If we set $A = 1$, for which $\alpha = 0$, and $\theta = 1$, Eq. (IV-3-1) reverts to the form (III-3-13), with the known solution (III-3-17) for the case of hydrogen as a moderator. When $A > 1$, the exact solution of the integral Eq. (IV-3-1) is not known in closed form. For this reason it is not profitable to attempt to determine $N_{as}(x)$ from Eq. (IV-3-1). Instead, we start from a different argument, given by Weinberg and Wigner,[11] which gives an approximate evaluation of $N_{as}(x)$ which is adequate for our purposes.

According to these authors, if we use the neutron energy E as the independent variable, the slowing-down density in the slowing-down model should be expressible (approximately) in the form

$$q(E) = \Sigma(E)\, E\, \xi\, \Phi(E) \quad , \qquad \text{(IV-3-2)}$$

where $q(E)$ is the number of neutrons crossing energy E per second per unit volume toward lower energies; $\Sigma(E)$ is the total (scattering plus absorption) cross section; $\Phi(E)$ is the neutron flux; and

$$\xi = 1 + \frac{(A-1)^2}{2A} \ln\left(\frac{A-1}{A+1}\right) \qquad \text{(IV-3-3)}$$

is the average logarithmic energy loss in the slowing-down theory.

If the distribution is stationary, as we are supposing it to be, the number of neutrons absorbed per unit volume per second below the energy E must be just equal to the slowing-down density $q(E)$. This equality

[11] A. M. Weinberg and E. P. Wigner, The Physical Theory of Reactors, The University of Chicago Press (1958), p. 316.

provides the following equation for the neutron flux $\Phi(E)$:

$$\Sigma_s(E)\,\xi E\Phi(E) = \int_0^E \Sigma_a(E_0)\Phi(E_0)\,dE_0 \quad . \tag{IV-3-4}$$

If the absorption follows the $1/v$ law, as we assume, Eq. (IV-3-4) reduces to the following simpler form:

$$\frac{\xi}{2}x(x+\Gamma)N_{as}(x) = \Gamma\int_0^x N_{as}(x_0)\,dx_0 \quad . \tag{IV-3-5}$$

On differentiation of both sides of Eq. (IV-3-5) with respect to x, we find the following differential equation:

$$\frac{dN_{as}(x)}{dx} + \left(\frac{1+\frac{2}{\xi}}{x+\Gamma} + \frac{1-\frac{2}{\xi}}{x}\right)N_{as}(x) = 0 \quad , \tag{IV-3-6}$$

which has the solution

$$N_{as}(x) = \frac{C}{x^2}\left(\frac{x}{x+\Gamma}\right)^{(2/\xi)+1} \quad , \tag{IV-3-7}$$

where C is a normalization constant.

We observe, as a check, that if we set $A = 1$ ($\xi = 1$), Eq. (IV-3-7) reduces to Eq. (III-3-17) of Chapter III, which we found by a different argument for the case of moderator nuclei of unit mass. Also in Chapter III we found the maximum of the asymptotic neutron distribution to be located at $x = \Gamma/2$, and Eq. (IV-3-7) gives a maximum at $x = A\Gamma/2$, using $\xi \cong 2/(A - \frac{2}{3})$ for large A.

As a further check on the validity of Eq. (IV-3-7), we shall consider the exact integral Eq. (IV-3-1) satisfied by $N_{as}(x)$, taking the ratio of the two terms:

$$\Psi(x) = \frac{2\theta^2 x}{N_{as}(x)(x+\Gamma)}\int_0^{x/\alpha} N_{as}(x_0)\,\frac{1}{x_0}\,dx_0 - 1 \quad . \tag{IV-3-8}$$

Substitution of Eq. (IV-3-7) into Eq. (IV-3-8) yields, upon integration,

$$\Psi(x) = x^2\frac{2\theta^2}{\Gamma^2}\left\{\frac{1}{\frac{2}{\xi}-1}\,\frac{x+\Gamma}{x}\left[\left(\frac{x+\Gamma}{x+\alpha\Gamma}\right)^{(2/\xi)-1} - 1\right] - \frac{\xi}{2}\left[\left(\frac{x+\Gamma}{x+\alpha\Gamma}\right)^{2/\xi} - 1\right]\right\} \quad . \tag{IV-3-9}$$

We now expand the exponential terms in the binomial expansion and retain only the first two terms, since x is large and α nearly unity:

$$\Psi(x) \cong \frac{2}{1+\alpha} \quad \frac{1}{1+\alpha\frac{\Gamma}{x}} \quad . \tag{IV-3-10}$$

For A larger than 9 and Γ/x much less than unity, α is close to unity, and $\Psi(x) \cong 1$.

Formula (IV-3-7) is also in reasonable agreement with one derived by Corngold[12] by a different method. Corngold gives the asymptotic expansion for large x:

$$N_{as}(x) \approx \frac{C}{x^2}\left[1 - \frac{\Delta}{2}\left(1 + \frac{4}{3A}\right)\frac{1}{x} + - - -\right] \quad , \tag{IV-3-11}$$

whereas from Eq. (IV-3-7) we find the expansion

$$N_{as}(x) \approx \frac{C}{x^2}\left[1 - \frac{\Delta}{2}\left(1 + \frac{5}{3A}\right)\frac{1}{x} + - - -\right] \quad , \tag{IV-3-12}$$

where $\Delta = 2A\Gamma$. The argeement between these two expressions is quite satisfactory for present purposes, and gives further confidence in the use of the closed form (IV-3-7) as the appropriate asymptotic density function at large energies for the gas model.

IV-4. Numerical Solution of the Integral Equation

The integral equation for a moderator of mass greater than unity is of the same form as Eq. (III-3-9) of Chapter III:

$$[V(x) + \Gamma]N(x) = \int_0^\infty dx_0\, x_0\, P(x_0 \rightarrow x)\, N(x_0) \quad , \tag{IV-4-1}$$

where now we must use the expressions for V(x) and $P(x_0 \rightarrow x)$ derived in Chapter II for a moderator mass greater than unity, namely:

$$V(x) = \left(x + \frac{1}{2Ax}\right)\Theta\left(\sqrt{A}x\right) + \frac{1}{\sqrt{A\pi}}\, e^{-Ax^2} \tag{IV-4-2}$$

$$P(x_0 \rightarrow x) = \frac{2x}{x_0}\left[e^{x_0^2 - x^2}\left\{\Theta(\quad x_0 - \quad x) + \Theta(\quad x_0 + \quad x)\right\} + \Theta(\quad x - \quad x_0) - \Theta(\quad x + \quad x_0) \text{ if } x_0 < x\right. \tag{IV-4-3'}$$

$$\left.e^{x_0^2 - x^2}\left\{\Theta(\quad x_0 - \quad x) - \Theta(\quad x_0 + \quad x)\right\} + \Theta(\quad x - \quad x_0) + \Theta(\quad x + \quad x_0) \text{ if } x_0 > x\right] \tag{IV-4-3''}$$

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[12] N. Corngold, Ann. Phys., 6, 368 (1959).

and

$$\Gamma = x\Sigma_a(x)/\Sigma_f \quad . \tag{IV-4-4}$$

The numerical solution of Eq. (IV-4-1) will be undertaken by the same general procedures as were used in Section III-4. The first point is that above a sufficiently high value, x_c, we assume that $N(x) = N_{as}(x)$, where the latter function is given in Eq. (IV-3-7). Unfortunately, the choice of a suitable numerical value for x_c gives some trouble for large moderator masses, since it must be chosen as high as is reasonable, still being compatible with a suitable choice of range over which the numerical work must be extended.

We replace Eq. (IV-4-1) by the equation

$$(V(x) + \Gamma)\, N(x) = \int_0^x dx_0\, P(x_0 \rightarrow x)\, N(x_0) + \int_x^{x_c} dx_0\, P(x_0 \rightarrow x)\, N(x_0)$$

$$+ \int_{x_c}^{\infty} dx_0\, P(x_0 \rightarrow x)\, N_{as}(x_0) \quad , \tag{IV-4-5}$$

where

$$N_{as}(x) = \frac{C}{x^2}\left(\frac{x}{x+\Gamma}\right)^{(2/\xi)+1} \quad . \tag{IV-4-6}$$

For general moderator mass, the last integral of (IV-4-5) is not immediately calculable, and must be treated by approximation methods. We assume that x_c has been chosen so large that in this integral we can replace the function $P(x_0 \rightarrow x)$ by its asymptotic form

$$P(x_0 \rightarrow x) \sim \theta^2 \frac{x}{x_0} \begin{cases} 2 & \text{if } \alpha x_0 < x < x_0 \\ 0 & \text{otherwise} \end{cases} \tag{IV-4-7}$$

$$(V(x) + \Gamma)\, N(x) = \int_0^{x_c} dx_0\, P(x_0 \rightarrow x)\, N(x_0) + 2\,\theta^2 x \int_{x_c}^{x/\alpha} \frac{C x_0^{(2/\xi)-2}}{(x_0+\Gamma)^{(2/\xi)+1}}\, dx_0$$

$$\text{if } x > \alpha x_c \tag{IV-4-8}$$

$$(V(x) + \Gamma)\, N(x) = \int_0^{x_c} dx_0\, P(x_0 \rightarrow x)\, N(x_0) \quad \text{if } x < \alpha x_c \quad . \tag{IV-4-9}$$

The analysis will be developed along the lines of that of Section III-4. Equations (IV-4-8) and (IV-4-9) are written in approximate form by means of the trapezoidal rule for integrals:

$$N(x_i) = \frac{1}{V(x_i) + \Gamma}\left[\sum_{j=1}^{M} P(x_j \rightarrow x_i)\, N(x_j)\, H_j + 2\theta^2 x_i f(x_i)\right] , \qquad \text{(IV-4-10)}$$

where H_j is the mesh size of the j-th interval and

$$f(x_i) = \begin{cases} 0 & , \text{ if } x_i < \alpha x_c \\ \displaystyle\int_{x_c}^{x_i/\alpha} dx_0 \frac{C x_0^{(2/\xi)} - 2}{(x_0 + \Gamma)^{(2/\xi)+1}} & , \text{ if } x_i > \alpha x_c \end{cases} . \qquad \text{(IV-4-11)}$$

The total number of mesh points is M. The mesh sizes H_j need not be the same over the whole range of the independent variable. The principal difference from Eq. (III-4-6) of Section III-4 is in that equation R is a constant, whereas in Eq. (IV-4-10) we have a function f(x) which vanishes over a certain portion of the energy range.

Equation (IV-4-10) was solved by a successive iteration method, using the asymptotic solution (IV-4-6) as the first trial function.

The normalization requirement was determined in the same way as in Section III-4, that is, we require the condition

$$\int_0^{x_c} N_{as}(x)\, dx = \int_0^{x_c} N(x)\, dx = \left(\frac{x_c}{x_c + \Gamma}\right)^{2/\xi} , \qquad \text{(IV-4-12)}$$

which reduces to Eq. (III-4-10) of Section III-4 upon setting $\xi = 1$.

It is necessary to take the value of x_c larger than for the calculation in Chapter III, and the value chosen must increase monotonically with the moderator mass if one is to retain a certain accuracy in the solution. This procedure is limited by the memory capacity of the computing machine.

The numerical evaluation of Eq. (IV-4-10) was carried out on the IBM 704 computor at the Argonne National Laboratory. With 150 mesh points, each iteration process required about 10 sec. The number of iterations required to achieve a given degree of convergence increases with the moderator mass. Renormalization of the neutron density is carried out after each iteration to prevent accumulation of errors.

Examples of numerical solutions for various values of the moderator mass and the absorption coefficient are shown in Figs. IV-1 through IV-8 (see pp. 53,54) along with solutions we computed from the Wilkins and Corngold expressions given in the following section. In addition, we have reproduced graphs of the Monte Carlo solution of Coveyou, Bate and Osborn.[10] The deviations from the Maxwellian distribution are of the same character as those found for hydrogen moderator (unit mass) shown in Figs. III-1 through III-4. The major point which shows up is that since neutron absorption becomes more effective as the moderator mass is increased, the peak of the distribution curve shifts to higher energies with an increase of both moderator mass and absorption coefficient.

IV-5. The Heavy Moderator Approximation

Wilkins[13] gave a reduction of the Wigner-Wilkins integral equation for a moderator gas of mass much greater than unity. The major analytical difficulty one encounters stems from the fact that for a general moderator mass the kernel of the integral equation is not separable.

The procedure used by Wilkins was to expand the integral in a power series in the inverse mass ratio μ. He proposed a formal theory of summability[14] for the expansion as a justification for its use. In fact, by retaining only terms of the first order in μ, he was able to replace the integral equation by a second-order differential equation, which is usually known as the Wilkins equation. This process can be extended formally. By retaining only powers of μ of successive degrees, one can replace the resulting integral equation by ordinary differential equations of successively increasing degrees.

Hurwitz, Nelkin, and Habetler[15] used a somewhat different approach by expanding the Wigner-Wilkins integral in terms of the energy transfer moments of the differential scattering cross section. However, they also used an expansion in powers of μ, so that the ambiguity in the neglect of terms of higher order in this parameter remains as it does in Wilkins' formulation.

In order to discuss this work, we consider first Wilkins' method. When attention is restricted to the region of lower energy, below the energy at which neutrons are introduced into the system, the Wigner-Wilkins integral equation has the form

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[13] J. E. Wilkins, Jr., CP-2481 (1944).

[14] J. E. Wilkins, Jr., Annals of Mathematics, 49, 189 (1948).

[15] H. Hurwitz, M. S. Nelkin, and G. J. Habetler, Nuclear Science and Engineering, 1, 280 (1956).

$$(V(x) + \Gamma)\, N(x) = \int_0^\infty P(x_0 \rightarrow x)\, N(x_0)\, dx_0 \quad . \tag{IV-5-1}$$

The function $P(x_0 \rightarrow x)$ satisfies the principle of detailed balancing in the form (cf. Section II-4)

$$M(x_0)\, P(x_0 \rightarrow x) = M(x)\, P(x \rightarrow x_0) \quad , \tag{IV-5-2}$$

where $M(x) = x^2 e^{-x^2}$ is the Maxwellian distribution function. We define a new function, $\nu(x)$, by the formula

$$N(x) = \sqrt{M(x)}\ \nu(x) = x e^{-x^2/2}\, \nu(x) \quad , \tag{IV-5-3}$$

which yields from (IV-5-1), on use of (IV-5-3),

$$(V(x) + \Gamma)\, \nu(x) = \int_0^\infty S(x, x_0; \mu)\, \nu(x_0)\, dx_0 \quad , \tag{IV-5-4}$$

where the kernel of this integral equation is the symmetrized function

$$S(x, x_0; \mu) = \theta^2 \quad .$$

$$\begin{cases} e^{1/2(x^2 - x_0^2)} \left[\Theta(\theta x - \zeta x_0) + \Theta(\theta x + \zeta x_0)\right] \\ \qquad + e^{-1/2(x^2 - x_0^2)} \left[\Theta(\theta x_0 - \zeta x) - \Theta(\theta x_0 + \zeta x)\right] \text{ if } x < x_0 \end{cases} \tag{IV-5-5'}$$

$$\begin{cases} e^{1/2(x^2 - x_0^2)} \left[\Theta(\theta x - \zeta x_0) - \Theta(\theta x + \zeta x_0)\right] \\ \qquad + e^{-1/2(x^2 - x_0^2)} \left[\Theta(\theta x_0 - \zeta x) + \Theta(\theta x_0 + \zeta x)\right] \text{ if } x > x_0 \end{cases} \tag{IV-5-5"}$$

Wilkins argued from his theory of summability that the right-hand side of (IV-5-4) can be expanded in the following series form:

$$\int_0^\infty S(x, x_0; \mu)\, \nu(x_0)\, dx_0 = x\nu(x) + \frac{\mu}{2}\left[(4x - x^2)\nu + \nu'(x) + x\nu''(x)\right] + \frac{\mu^2}{6}\left[(x^5 - 6x^3 + 3x)\nu(x) + 6(1 - x^2)\nu'(x)\right. \tag{IV-5-6}$$

$$\left. + 2(3x - x^3)\nu''(x) + 2\nu'''(x) + x\nu^{(IV)}(x)\right] + 0(\mu^3) \quad .$$

It may be noted that, in this expansion, the condition $\sqrt{A}\,x >> 2$ is not actually needed, contrary to a statement given in Ref. 10.

Using this expansion in Eq. (IV-5-4), we have the following relation:

$$(V(x) + \Gamma)\,\nu(x) = x\nu(x) + \frac{\mu}{2}\left[(4x - x^2)\,\nu(x) + \nu'(x) + x\,\nu''(x)\right] + 0(\mu^2) \quad , \tag{IV-5-7}$$

which is equivalent to the relation

$$(V(x) + \Gamma)\,N(x) = xN(x) + \frac{\mu}{2}\left[\left(\frac{1}{x} + 4x\right)N + (2x^2 - 1)\,N' + xN''\right] + 0(\mu^2) \quad . \tag{IV-5-8}$$

In the energy region $x >> 2\sqrt{\mu}$,

$$V(x) \approx x + \frac{1}{2Ax} + 0(e^{-Ax^2}) \quad . \tag{IV-5-9}$$

If we keep only the first two members on the right-hand side of Eq. (IV-5-9) and drop all members of the form $0(\mu^2)$ in Eq. (IV-5-8), we obtain the following differential equation:

$$xN'' + (2x^2 - 1)\,N' + (4x - \Delta)\,N = 0 \quad , \tag{IV-5-10}$$

where

$$\Delta = 2A\Gamma \quad . \tag{IV-5-11}$$

Wilkins has obtained a solution of Eq. (IV-5-10) in the form of a series. The results predicted from this solution are of reasonable physical character, the distribution function being Maxwellian for lower energies and behaving like $1/E$ at higher energies.

On the other hand, the nature of the approximation procedure used by Wilkins is unusual, and at first seems to be quite unclear on mathematical grounds. As has been indicated, the formal solution of Eq. (IV-5-4) by expansion of the right-hand side in powers of μ, with omission of successively higher powers of μ, leads to the consideration of a sequence of differential equations of increasing orders. Although no general theory is known to the author, the approximation of functions by solutions of differential equations of increasing orders would seem to be closely related to the Weierstrass theorem concerning the approximation of continuous functions by polynomials. In the present case the differential equations involved are so complicated that the convergence of the process could be tested only by extensive numerical calculations, which would not have been justified in this work. In the last analysis, the fact that the distribution function has

a quite simple form may be a strong contributing factor in the convergence of the various methods of approximation.

A comparison of the results obtained by numerical evaluation of the Wigner-Wilkins integral equation with similar calculations made for the Wilkins differential Eq. (IV-5-10) will be given in Section IV-6. It need only be said here that the agreement is so good that it increases confidence that the convergence of the approximation procedure is actually quite good in this problem, even though we have no detailed proof of this fact.

It is of interest to compare Wilkins' reduction of the Wigner-Wilkins integral equation with that developed by Hurwitz, Nelkin and Habetler.[15] Let $\phi(\epsilon)$ be the neutron flux per unit energy range, with $\Sigma_s(\epsilon)$ and $\Sigma_a(\epsilon)$ the macroscopic scattering and absorption cross sections, respectively. The neutron energy will be measured in the reduced units $\epsilon = E/kT$. In these variables the Wigner-Wilkins integral Eq. (IV-5-1) takes the form

$$[\Sigma_s(\epsilon) + \Sigma_a(\epsilon)]\,\phi(\epsilon) = \int_0^\infty \Sigma_s(\epsilon_0 \rightarrow \epsilon)\phi(\epsilon_0)\,d\epsilon_0 \quad . \qquad \text{(IV-5-12)}$$

The total and differential scattering cross sections, $\Sigma_s(\epsilon)$ and $\Sigma(\epsilon_0 \rightarrow \epsilon)$, are given by Eqs. (II-4-18) and (II-4-16), respectively, of Chapter II. They are related by the formula

$$\Sigma_s(\epsilon) = \int_0^\infty \Sigma(\epsilon \rightarrow \epsilon_0)\,d\epsilon_0 \quad . \qquad \text{(IV-5-13)}$$

The absorption cross section will be assumed to be proportional to $1/\sqrt{\epsilon}$, as is done throughout this work.

We will set

$$\phi(\epsilon) = M(\epsilon)\,g(\epsilon) = \epsilon e^{-\epsilon} g(\epsilon) \quad , \qquad \text{(IV-5-14)}$$

so that the deviation of the function $g(\epsilon)$ from the constant value unity measures the deviation of the distribution from the Maxwellian form $M(\epsilon)$.

By means of the principle of detailed balancing,

$$\Sigma(\epsilon_0 \rightarrow \epsilon)\,M(\epsilon_0) = \Sigma(\epsilon \rightarrow \epsilon_0)\,M(\epsilon) \quad ,$$

and the relation (IV-5-14), we get

$$\Sigma(\epsilon_0 \rightarrow \epsilon)\,\phi(\epsilon_0) = \Sigma(\epsilon \rightarrow \epsilon_0)\,g(\epsilon_0)\,M(\epsilon) \quad . \qquad \text{(IV-5-15)}$$

Substitution of this into Eq. (IV-5-12), gives, after a little manipulation,

$$\frac{\Sigma_a(\epsilon)}{\Sigma_s(\epsilon)}\, g(\epsilon) = \overline{\Delta\epsilon}\ \frac{dg}{d\epsilon} + \frac{1}{2}\ \overline{\Delta\epsilon^2}\ \frac{d^2g}{d\epsilon^2} + \cdots + \frac{1}{n!}\ \overline{\Delta\epsilon^n}\ \frac{d^ng}{d\epsilon^n} + \cdots \quad .$$

(IV-5-16)

The $\overline{\Delta\epsilon^n}$'s are the energy change moments of the differential scattering cross section, defined by the formula

$$\overline{\Delta\epsilon^n} = \frac{1}{\Sigma_s(\epsilon)} \int_0^\infty d\epsilon_0 (\epsilon_0 - \epsilon)^n\, \Sigma(\epsilon \rightarrow \epsilon_0)\ (n = 1,2,3,\cdots) \quad .$$

(IV-5-17)

Straightforward evaluations of these quantities can be made to give full expressions without use of the formalism of Hurwitz et al.[15]

The first few of these quantities are as follows:

$$\overline{\Delta\epsilon} = \frac{4}{A+1} - \frac{2A}{(A+1)^2}\epsilon - \frac{5}{(A+1)^2} + \frac{2}{(A+1)^2}\, R_1\left(\sqrt{A\epsilon}\right)$$

$$\overline{\Delta\epsilon^2} = \frac{16}{3}\ \frac{A^2}{(A+1)^2}\,\epsilon^2 + \left(\frac{4A}{(A+1)^2} - \frac{32A}{(A+1)^2} + \frac{112}{3}\ \frac{A}{(A+1)^4}\right)\epsilon$$
$$+ \left(\frac{34}{(A+1)^2} - \frac{80}{(A+1)^3} + \frac{124}{3}\ \frac{1}{(A+1)^4}\right)$$
$$+ \left(\frac{-22}{3(A+1)^2} + \frac{32}{(A+1)^3} - \frac{6}{(A+1)^4}\right) R_1\left(\sqrt{A\epsilon}\right) - \frac{8}{3}\ \frac{1}{(A+1)^4}\, R_2\left(\sqrt{A\epsilon}\right)$$

$$\overline{\Delta\epsilon^3} = \frac{-16A^3}{(A+1)^6}\ \epsilon^3 - \left[\frac{32A^2}{(A+1)^4} - \frac{192A^2}{(A+1)^5} + \frac{216A^2}{(A+1)^6}\right]\epsilon^2$$
$$+ \left[\frac{96A}{(A+1)^3} - \frac{704A}{(A+1)^4} + \frac{1344A}{(A+1)^5}\right]\epsilon$$
$$- \left[\frac{732}{(A+1)^6} - \frac{432}{(A+1)^3} + \frac{1448}{(A+1)^4} - \frac{1488}{(A+1)^5}\right]$$
$$+ \left[\frac{-96}{(A+1)^3} + \frac{608}{(A+1)^4} - \frac{888}{(A+1)^5} + \frac{522}{(A+1)^6}\right] R_1\left(\sqrt{A\epsilon}\right)$$
$$+ \left(\frac{300}{(A+1)^3} - \frac{16}{(A+1)^4} + \frac{96}{(A+1)^5} - \frac{174}{(A+1)^6}\right) R_2\left(\sqrt{A\epsilon}\right) - \frac{8}{(A+1)^6}\, R_3\left(\sqrt{A\epsilon}\right)$$

(IV-5-18)

The three functions appearing in the above expressions have the definitions

$$R_1(\sqrt{A\epsilon}) = \frac{\Theta(\sqrt{A\epsilon})}{\Theta(\sqrt{A\epsilon})(2A\epsilon + 1) + \frac{2}{\sqrt{\pi}}\sqrt{A\epsilon}\, e^{-A\epsilon}}$$

$$R_2(\sqrt{A\epsilon}) = \frac{2}{\sqrt{\pi}} \frac{\sqrt{A\epsilon}\, e^{-A\epsilon}}{\Theta(\sqrt{A\epsilon})(2A\epsilon + 1) + \frac{2}{\sqrt{\pi}}\sqrt{A\epsilon}\, e^{-A\epsilon}}$$

$$R_3(\sqrt{A\epsilon}) = A\epsilon\, R_2(\sqrt{A\epsilon}) \quad . \qquad \text{(IV-5-19)}$$

These functions are all bounded, varying from 0 to 0.5. In the evaluation of the higher moments, we need functions of the form of $(A\epsilon)^{\kappa} R_2(\sqrt{A\epsilon})$ ($\kappa = 2,3\cdots$), but each of these is also bounded.

Though in Hurwitz' formalism the condition $\mu T/E < 1$ was necessary to guarantee the convergence of the expression, we do not require any condition in this straightforward evaluation.

Upon looking at expression (IV-5-18), we realize the situation is similar to that we have faced in (IV-5-6), i.e., we have to be careful in the treatment of higher order in $1/A = \mu$. The first term in $\overline{\Delta\epsilon^2}$ varies as $(\epsilon/A)^3$, and the first and the second terms in $\overline{\Delta\epsilon^3}$ vary as $(\epsilon/A)^3$ and $(\epsilon/A)^2$, respectively. As in Eq. (IV-5-6), the simple assumption of $1/A << 1$ is not enough to justify one omission of these terms in $\overline{\Delta\epsilon^3}$; rather, we require $(\epsilon/A) << 1$ in addition to $\mu = 1/A << 1$.

With the condition that $(\epsilon/A) << 1$, the $\overline{\Delta\epsilon^n}$'s are approximated by retaining only first-order terms in μ:

$$\overline{\Delta\epsilon} \simeq 2\mu(2-\epsilon)$$

$$\overline{\Delta\epsilon^2} \simeq 4\mu\epsilon$$

$$\overline{\Delta\epsilon^n} = 0[\mu^2, (\mu\epsilon)^2] \qquad n \geq 3 \quad . \qquad \text{(IV-5-20)}$$

Here $1/(A+1)$ is treated as $1/(A+1) \simeq 1/A = \mu$ by virtue of the condition $\mu << 1$.

By substituting these approximate expressions into Eq. (IV-5-16) and assuming that the role of the derivatives of higher order are insignificant if their coefficients are small, we get the following approximate second-order differential equation:

$$\frac{d^2g}{d\epsilon^2} + (2 - \epsilon)\frac{dg}{d\epsilon} = \frac{A}{2}\frac{\Sigma_a(\epsilon)}{\Sigma_s(\epsilon)}\, g(\epsilon) \quad . \qquad \text{(IV-5-21)}$$

We remind ourselves that this equation may be valid in the energy range $0 \leq \epsilon \ll A$ provided $1/A \ll 1$.

This equation is sometimes referred to as the Hurwitz equation, and has been the point of departure for numerous studies[16] of the space- or time-dependent thermalization problem.

Hurwitz et al., remarked further that, if one approximates $\Sigma_s(\epsilon)$ by Σ_f, Eq. (IV-5-21) reduces to the Wilkins Eq. (IV-5-10) on changing the independent variable from ϵ to x and transforming to neutron density. It appears, therefore, that apart from minor differences, the reduction procedures followed by Wilkins and by Hurwitz et al., for the Wigner-Wilkins integral equation are effectively equivalent. Both involve the following assumptions:

(1) The moderator nuclei are very massive;

(2) The total scattering cross section is approximated by free nuclear scattering cross section; and

(3) The contributions of the higher-order derivative terms in the expansions are small.

As concerns item (2), we note more specifically that Wilkins used the approximation $\Sigma_s(x) \approx \Sigma_f \left(1 + \frac{1}{2Ax^2}\right)$, whereas Hurwitz et al., used $\Sigma_s(x) \approx \Sigma_f$. Clearly, there is an insignificant difference between them for large values of $\sqrt{A}x$.

Corngold[12] has used another formalism employing an extensive expansion of the scattering cross sections. After expanding N(x) in powers of μ, i.e.,

$$N(x) = \sum_{k=0}^{\infty} N^{(k)}(x)\mu^k \quad , \qquad \text{(IV-5-22)}$$

he has shown that the Wilkins Eq. (IV-5-10) is deducible from his formalism as a first approximation. He also gives the next-order approximation, which comes directly from Eq. (IV-5-6) by retaining second-order terms in μ.

Wilkins' equation,

$$xN_0'' + (2x^2 - 1)N_0' + (4x - \Delta)N_0 = 0$$

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[16] M. V. Kazanovskii, A. V. Stepanov, and F. L. Shapiro, Proceedings of the International Conference on Peaceful Uses of Atomic Energy, Geneva, 1958, United Nations, 16, p. 279.

and the second-order equation proposed by Corngold as the next order of approximation,

$$xN_1'' + \left[2x^2 - 1 - \frac{1}{A}\left(\frac{2}{x^2} + \frac{2\Delta}{3}\,\frac{1}{x}\right)\right]N_1' + \left[4x - \Delta + \frac{1}{A}\left(\frac{4}{x^3} + \frac{2\Delta}{x^2} + \frac{\Delta^2}{3} - 4\right)\frac{1}{x} - \frac{4\Delta}{3}\right]N_1 = 0 \quad , \quad \text{(IV-5-23)}$$

were solved numerically by employing the IBM 704 at the Argonne National Laboratory. In both equations, the normalization condition

$$\int_0^\infty N_0(x)\,dx = \int_0^\infty N_1(x)\,dx = \int_0^\infty N(x)\,dx = 1 \qquad \text{(IV-5-24)}$$

was imposed for easy comparison with our solution N(x) of the integral equation. These solutions are compared in the next section.

IV-6. Comparison of Results

The solutions of the integral equation for different moderator masses and absorptions computed from Eq. (IV-4-10) are shown in Figs. IV-1 through IV-8, and are denoted by N(x). For reference we have plotted a neutron Maxwellian distribution at the moderator temperature on all graphs. In addition, on each graph we have plotted the asymptotic solution $N_{as}(x)$ for the moderator at rest but with absorption present. In each case, N(x) approaches $N_{as}(x)$ at higher energies, as it should, since at higher neutron energies, the influence of moderator motion becomes negligible. At lower neutron energies, all graphs show the effect of moderator motion on the neutron distribution, namely, the up-scattering of neutrons by the moderator.

There are two other effects to be observed in the graphs. One is the influence of the mass of the moderator, which shifts the peak of the neutron distribution to higher energies as the moderator mass increases. This arises from the up-scattering caused by a heavier moderator mass, which has more momentum to impart to a neutron upon collision. The second effect is the influence of absorption, which also shifts the peak of the neutron distribution to higher energies as the absorption increases. Throughout our calculations we have assumed $1/v$ absorption, which means a constant absorption rate for neutrons of all energies; fewer neutrons are left at the lower energies. Thus, the neutron distribution is hardened by absorption and also by a heavier moderator.

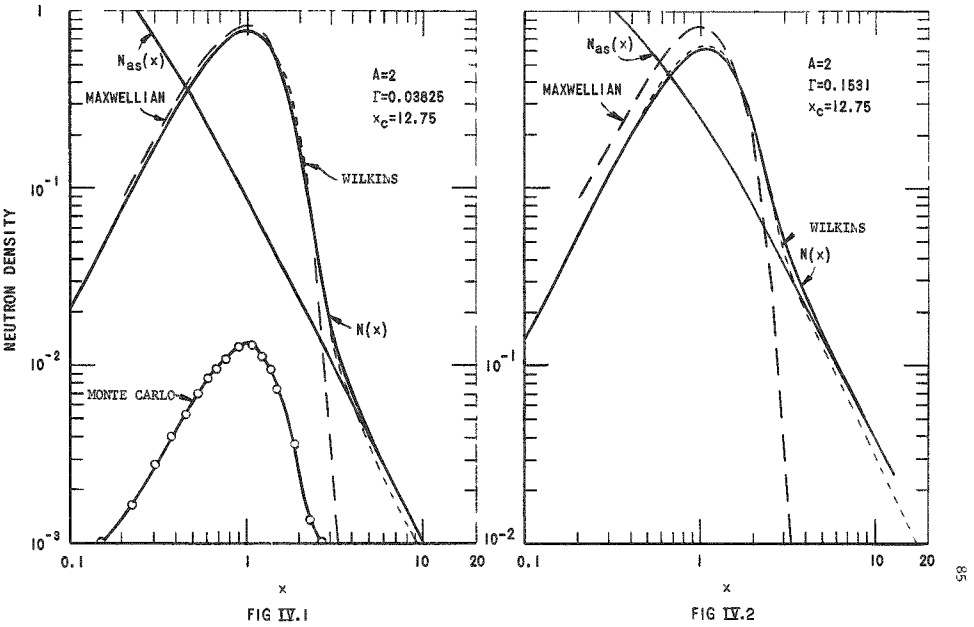


FIG IV.1

(A = 2 and Γ = 0.03825)

FIG IV.2

(A = 2 and Γ = 0.1531)

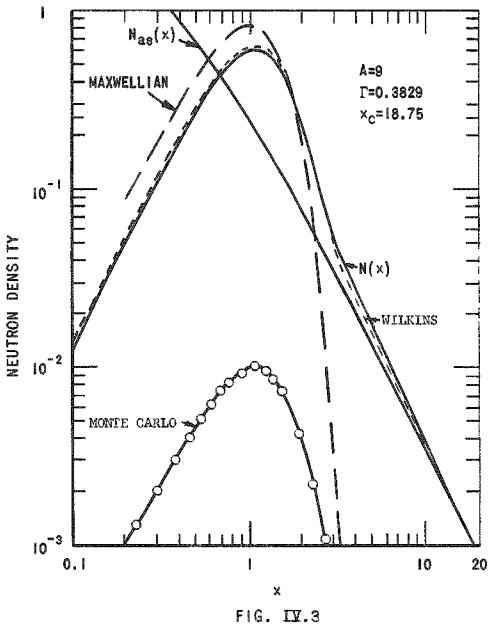


FIG. IV.3

(A = 9 and Γ = 0.03829)

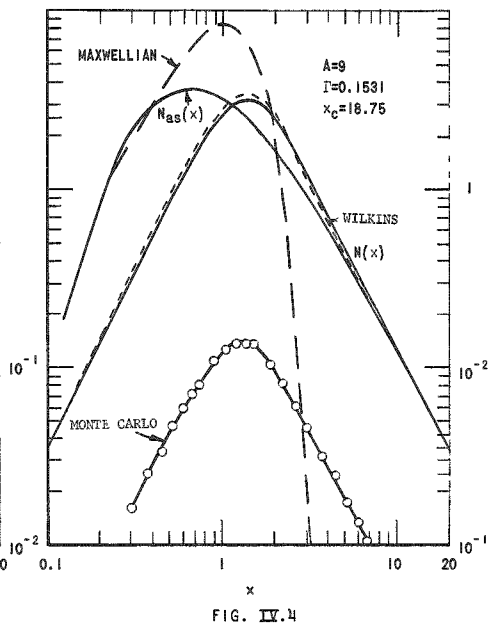


FIG. IV.4

(A = 9 and Γ = 0.1531)

Figs. IV-1 thru IV-4

Neutron Density in Moderator of General Mass

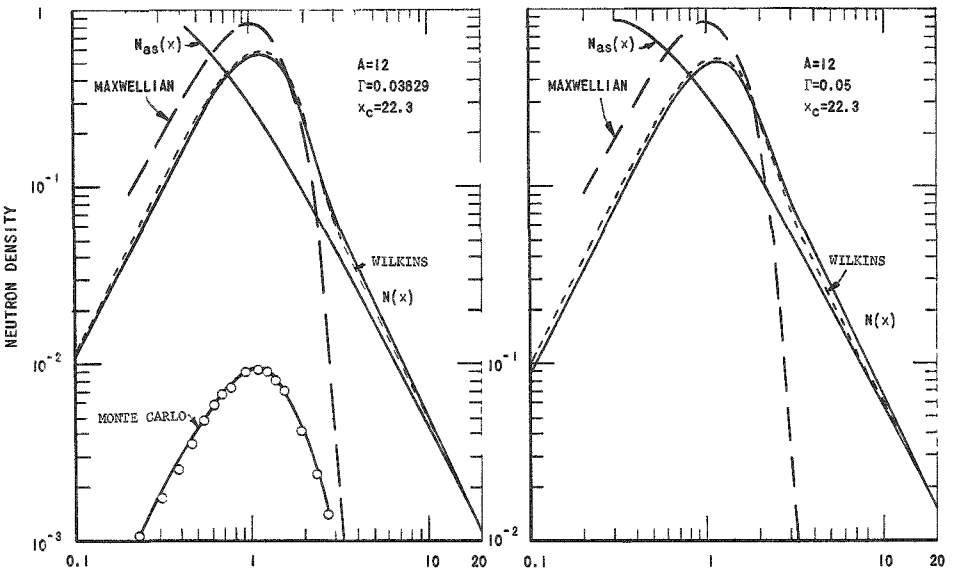


FIG. IV.5

(A = 12 and Γ = 0.03829)

FIG. IV.6

(A = 12 and Γ = 0.05)

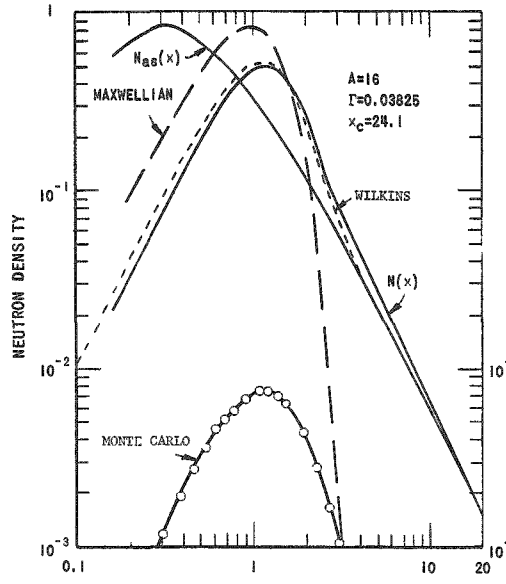


FIG. IV.7

(A = 16)

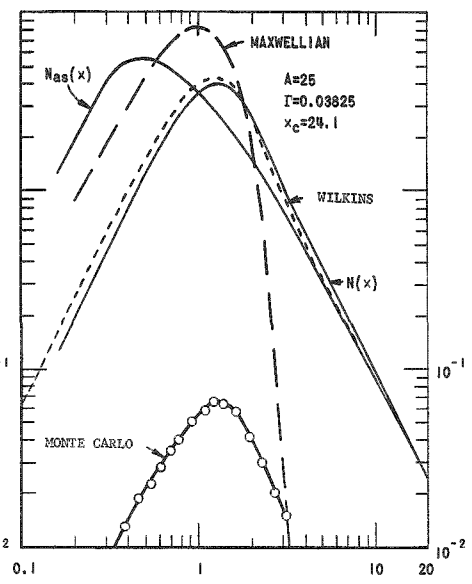


FIG. IV.8

(A = 25)

Figs. IV-5 thru IV-8

Neutron Density in Moderator of General Mass

In six of the graphs we have reproduced the Monte Carlo results of Coveyou, Bate, and Osborn.[10] The Monte Carlo curves appear lower than ours because of a different choice of normalization by these authors, and with renormalization, their curves are coincident with ours. We have converted their absorption and abscissa units into ours for these plots. Thus our solution N(x) is in excellent agreement with this Monte Carlo calculation, which is a totally different way of calculating the neutron distribution. Ordinates for the Monte Carlo curves are given on the right-hand side of the figures.

On each of the graphs we have shown as a dotted curve our solution of Wilkins' equation. We have chosen the normalization of our N(x) and Wilkins' solution so that the area under each curve is unity. We observe that there is a consistent slight difference between the solution to Wilkins' equation and our N(x), and the surprising thing is that this difference is approximately the same regardless of the moderator mass or absorption. However, in the region of greatest interest, from the peak of the neutron distribution to the asymptotic range, our solution is a slightly harder neutron distribution than that of Wilkins'.

Corngold's solution, although not shown in our graphs, lies between Wilkins' solution and our N(x) from the peak to the asymptotic region, but at very low energies drops markedly below N(x).

To bring out the difference between solutions of the Wigner-Wilkins integral equation and the heavy moderator approximations, namely, Wilkins' equation and Corngold's equations, we computed the activation of $_{70}Yb^{168}$. This isotope has a resonance absorption peak at 0.597 ev, which is approximately in the energy region where these solutions show marked differences Furthermore, the differences are magnified by covering of Yb with a 0.01-in.-thick layer of cadmium to eliminate the contribution of the thermal portion of the spectra. Numerical estimates of foil activations were made for moderators of masses 2, 9, and 12, and flux depressions caused by the presence of the indicator were ignored. We have also estimated the response of other detectors, such as of Lu^{176}, U^{235} and Pu^{239}, for the same moderator masses and tabulated the results in Table IV-1 along with ones for Yb^{168}. Activation or fission is given in unit of N (number of atoms) x 10^{-24}.

We observe that the Yb^{168} response and the Pu^{239}/U^{235} fission ratio are sensitive indicators. The former shows more than 10% difference, and this is even further magnified by using a cadmium layer. On the other hand, the responses of Lu^{176} and U^{235} are insensitive.

It is noticeable that the lightest moderator (mass 2) shows the greatest difference, although the order of the magnitude is about the same for all three of them. The Corngold solution gives a correction to the Wilkins solution in the direction of the solution of the Wigner-Wilkins integral equation, but it is still closer to the Wilkins solution rather than to the Wigner-Wilkins solution.

Table IV-1

	Yb^{168} Activation (Unit N x 10^{-24})			Lu^{176} Activation	Pu^{239} and U^{235} Fission		
	Bare	0.01" Cd-Shielded	(Cd Ratio)$^{-1}$	Bare (Unit N x 10^{-24})	U^{235} (Unit N_{25} x 10^{-24})	Pu^{239} (Unit N_{29} x 10^{-24})	Ratio Unit $\frac{N_{25}}{N_{29}}$
Mass 2, Γ 0.15310							
Wigner-Wilkins	10971	5071	0.4622	4538	8249	16021	0.5149
Wilkins	9431	3957	0.4195	4441	8348	15343	0.5441
Ratio $\left(\frac{W.W.-W.}{W.W.}\right)$	0.1404	0.2196	0.0924	0.0213	(-)0.0120	0.0423	(-)0.0567
Mass 9, Γ 0.03829							
Wigner-Wilkins	11389	5319	0.4670	4693	8273	16376	0.5052
Wilkins	10142	4431	0.4369	4556	8339	16054	0.5194
Ratio $\left(\frac{W.W.-W.}{W.W.}\right)$	0.1095	0.1667	0.0644	0.0292	(-)0.0078	0.0197	(-)0.0281
Mass 12, Γ 0.03829							
Wigner-Wilkins	13508	6868	0.5084	4912	8057	17508	0.4602
Wilkins	11922	5746	0.4820	4748	8108	16629	0.4876
Corngold	12242	5981	0.4885	4751	8082	16737	0.4829
Ratio $\left(\frac{W.W.-W.}{W.W.}\right)$	0.1174	0.1633	0.0519	0.0334	(-)0.0063	0.0502	(-)0.0556
Ratio $\left(\frac{W.W.-C.}{W.W.}\right)$	0.0937	0.1291	0.0391	0.0328	(-)0.0031	0.0440	(-)0.0493

IV-7 Summary and Concluding Remarks

It has been the purpose of this thesis to examine the gas model of neutron thermalization for a general moderator mass. To do this, we have formulated the thermalization process as an integral equation. This integral equation, with a nonseparable kernel, cannot be solved in closed form, nor can its asymptotic solution, the slowing-down model solution, be given in closed form, except for unit moderator mass. Wigner and Wilkins have solved the integral equation for unit moderator mass, the one case for which the kernel is separable, by converting to a differential equation and then solving the differential equation numerically.

For moderators of general mass, however, the integral equation cannot be converted into a differential equation because of the nonseparability of the kernel. As a result, different authors have expanded the kernel or replaced the integral by a power series in the inverse mass ratio, and finally solved these abbreviated forms numerically. The mathematical and physical implications of these procedures are not entirely clear.

Because numerical solutions had to be resorted to in all cases anyway, even for the simplest, unit-mass moderator, we have undertaken a numerical solution of the original integral equation. This procedure has the drawback that for even the slightest change in one parameter the entire numerical solution must be repeated. However, we are able to give a solution for any desired set of parameters without first altering the integral equation before applying numerical methods.

It is interesting to note that the solutions to some of the approximations made by other authors are surprisingly close to our numerical solutions. This closeness suggests that the integral equation has some character of stability of its solution that merits further investigation.

The work developed here is by no means a complete study of neutron moderation. But it is hoped that the means we have provided for obtaining specific numerical solutions, together with the comparison to other works, will be of help in the construction of a really satisfactory theory of thermalization.

ACKNOWLEDGMENTS

The author wishes to express his appreciation for guidance in this study to Dr. B. I. Spinrad and Mr. F. G. Prohammer of the Argonne National Laboratory, and for guidance in a more general sense to his advisers Professors E. L. Hill and H. S. Isbin of the University of Minnesota. Dr. R. H. Land provided invaluable guidance in the development of codes for the computer work. Conversations with Dr. C. Kelber were very helpful in the clarification of important points in neutron moderation.

Finally, the author is very appreciative of the support received from the International Cooperation Administration (ICA), the University of Minnesota, and the Argonne National Laboratory during his period of graduate work.

APPENDIX

IBM 704 PROGRAM FOR SOLUTION OF WIGNER-WILKINS INTEGRAL EQUATION FOR MODERATOR OF GENERAL MASS

Equation (IV-4-5) on page 43 is solved by successive iteration method by putting in the asymptotic solution (IV-4-6) on the same page as the first trial function.

After reducing to the form (IV-4-10) on page 44, a simple change of independent variable gives the explicit expression for the second member inside of the bracket:

$$B(x_i) = 2\theta^2 x_i f(x_i)$$

$$= \begin{cases} 0 & \text{if } x \leq \alpha x_c \\ S x_i \left[\dfrac{Z(x_i)^R}{R} - \dfrac{Z(x_i)^P}{P} + Q \right] & \text{if } x > \alpha x_c \end{cases} ,$$

where

$$S = 2\theta^2 P/\Gamma = \text{constant}$$

$$P = 2/\xi$$

$$R = P-1$$

$$Y = x_c/(x_c + \Gamma)$$

$$Z(x_i) = x_i/(x_i + \alpha\Gamma)$$

and

$$Q = (Y^P/P) - (Y^R/R) = \text{constant} .$$

By setting $RM(x_i) = V(x_i) + \Gamma$, Eq. (IV-4-10) on page 44 is written as

$$N(x_i) = \frac{1}{RM(x_i)} \left[\sum_{j=1}^{M} P(x_j \rightarrow x_i)\, H_j\, N(x_j) + B(x_i) \right] , \qquad (A-1)$$

where $(M + 1)$ is the total number of mesh points under consideration $[N(0) \equiv 0]$.

The set of equations (A-1) is to be solved by successive iteration process.

The normalization is taken such that

$$\int_0^{x_c} N(x)\,dx = \int_0^{x_c} N_{as}(x)\,dx = \left(\frac{x_c}{x_c + \Gamma}\right)^{2/\xi} \qquad (A\text{-}2)$$

is to be satisfied, as was mentioned in the text [Section IV-4, Eq. (IV-4-12)].

As was also mentioned in the text, the program was written in such a manner that the computer did not need to repeat the evaluation of the quantities $P(x_0 \rightarrow x)$ and $V(x)$ so long as the moderator mass and arrangement of mesh points were kept fixed.

The program was written to make use of a maximum of 150 mesh divisions. For a given arrangement of mesh points, the energy scale was divided into three regions: (0, M1), (M1, M2), (M2, M). It was convenient to have αx_c fall on one of the mesh points in the region M2 by proper choice of x_c.

The program could be written to operate in different ways by the use of sense switches. It could furnish evaluations of the scattering rates (both differential and total) if desired. It was possible also to write out values of $ABCR(I) = |D^{(n)}(I) - D^{(n-1)}(I)|$ or of

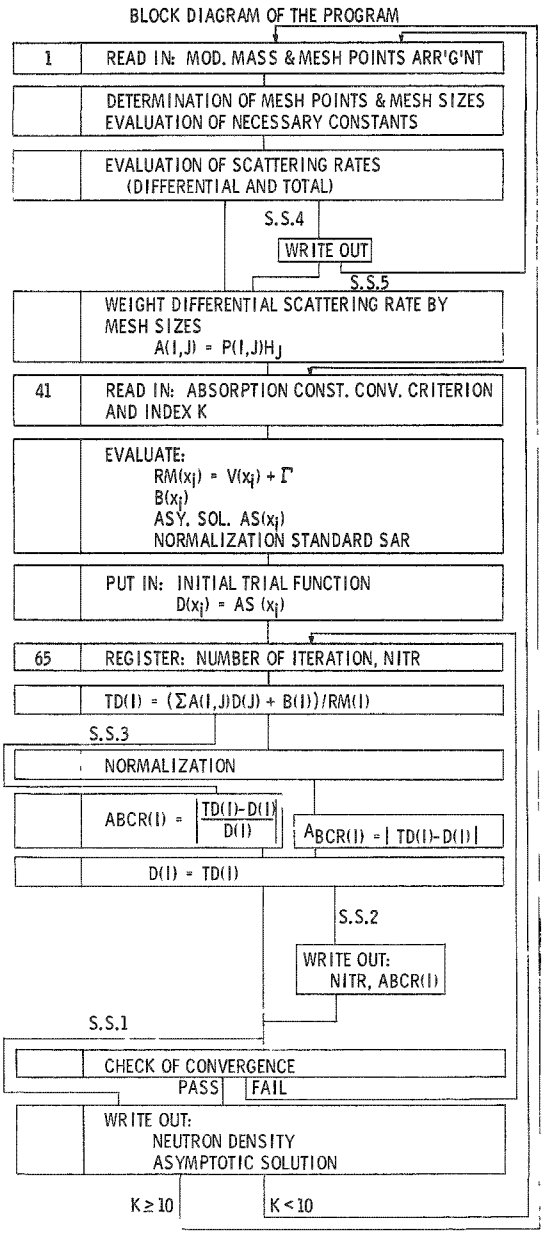
$$ABCR(I) = \left| \frac{D^{(n)}(I) - D^{(n-1)}(I)}{D^{(n-1)}(I)} \right|$$

after any number of iterations. Sense switch 1 provided a write out of the neutron density after any desired iteration and stops the progress.

The output data were the values of x, with the values of the asymptotic solution and of the neutron density at each such point.

The input data were read in with two cards. The first provided the mesh arrangements and the moderator mass. The second care provided the absorption constant, convergence criterion, and the index K which gave the order to the machine as to whether it should read in new first input data and start the problem with new moderator and mesh point arrangements, or to carry another iteration process but for a new value of the absorption coefficient ($K > 10$ leads back to command 1).

A block diagram of the program is shown below and a write-up of the program is attached.


BLOCK DIAGRAM OF THE PROGRAM
1
READ IN: MOD. MASS & MESH POINTS ARR'G'NT
DETERMINATION OF MESH POINTS & MESH SIZES
EVALUATION OF NECESSARY CONSTANTS
EVALUATION OF SCATTERING RATES
(DIFFERENTIAL AND TOTAL)
S.S.4
WRITE OUT
S.S.5
WEIGHT DIFFERENTIAL SCATTERING RATE BY
MESH SIZES
A(I,J) = P(I,J)H_J
41
READ IN: ABSORPTION CONST. CONV. CRITERION
AND INDEX K
EVALUATE:
RM(x_I) = V(x_I) + Γ
B(x_I)
ASY. SOL. AS(x_I)
NORMALIZATION STANDARD SAR
PUT IN: INITIAL TRIAL FUNCTION
D(x_I) = AS (x_I)
65
REGISTER: NUMBER OF ITERATION, NITR
TD(I) = (ΣA(I,J)D(J) + B(I))/RM(I)
S.S.3
NORMALIZATION
ABCR(I) = |TD(I)-D(I)| / D(I)
A_BCR(I) = | TD(I)-D(I)|
D(I) = TD(I)
S.S.2
WRITE OUT:
NITR, ABCR(I)
S.S.1
CHECK OF CONVERGENCE
PASS
FAIL
WRITE OUT:
NEUTRON DENSITY
ASYMPTOTIC SOLUTION
K≥10
K<10

```
      Q=(Y**P)/P-(Y**R)/R
      S=THETAS*2.0*P/GAMMA
      DO50I=M2,M
      Z=X(I)/(X(I)+ALPHA*GAMMA)
   50 B(I)=X(I)*S*((Z**R)/R-(Z**P)/P+Q)
      G=P*GAMMA
      T=P+1.0
      DO55I=1,M
      U=X(I)/(X(I)+GAMMA)
   55 AS(I)=G*((U**T)/(X(I)**2))
      SAR=Y**P
      DO60I=1,M
   60 D(I)=AS(I)
   65 NITR=NITR+1
      DO67I=1,M
      TD(I)=B(I)
      DO66J=1,M
   66 TD(I)=TD(I)+A(I,J)*D(J)
   67 TD(I)=TD(I)/RM(I)
      IF(SENSE SWITCH 3) 74,70
   70 AR=TD(1)*H1
      DO71I=2,M11
   71 AR=AR+TD(I)*H1
      AR=AR+TD(M1)*HM1
      DO72I=M12,M21
   72 AR=AR+TD(I)*H2
      AR=AR+TD(M2)*HM2
      DO73I=M22,M3
   73 AR=AR+TD(I)*H3
      AR=AR+TD(M)*HM
      RNC=SAR/AR
      DO88I=1,M
      TD(I)=TD(I)*RNC
   88 ABCR(I)=ABSF(TD(I)-D(I))
      GOTO 75
   74 DO99I=1,M
   99 ABCR(I)=ABSF((TD(I)-D(I))/D(I))
```

```
      DO31I=2,M
      J1=I-1
      DO31J=1,J1
   31 A(I,J)=(THETAS*X(I)/X(J))*(EXPF(X(J)**2-X(I)**2)
     X*(ERRORF(THETX(J)-ZETAX(I))+ERRORF(THETX(J)+ZETAX(I)))
     X+ERRORF(THETX(I)-ZETAX(J))-ERRORF(THETX(I)+ZETAX(J)))
      IF(SENSESWITCH4)32,35
   32 WRITEOUTPUTTAPE2,800
      WRITEOUTPUTTAPE2,810,AMASS
      DO33I=1,M
      WRITEOUTPUTTAPE2,820,X(I)
      WRITEOUTPUTTAPE2,830
   33 WRITEOUTPUTTAPE2,840,(J,X(J),A(I,J),J=1,M)
      WRITEOUTPUTTAPE2,850
      WRITEOUTPUTTAPE2,860
      WRITEOUTPUTTAPE2,840,(I,X(I),V(I),I=1,M)
      IF(SENSESWITCH5)1,35
   35 HM1=(H1+H2)/2.0
      HM2=(H2+H3)/2.0
      HM=H3/2.0
      DO40I=1,M
      DO36J=1,M11
   36 A(I,J)=A(I,J)*H1
      DO37J=M12,M21
   37 A(I,J)=A(I,J)*H2
      DO38J=M22,M3
   38 A(I,J)=A(I,J)*H3
      A(I,M1)=A(I,M1)*HM1
      A(I,M2)=A(I,M2)*HM2
   40 A(I,M)=A(I,M)*HM
   41 READ150,N,K,CRTM,GAMMA
      NITR=0
      DO42I=1,M
   42 RM(I)=V(I)+GAMMA
      DO45I=1,M21
   45 B(I)=0.0
      Y=XC/(XC+GAMMA)
```

```
      NEUTRON THERMALIZATION (ITERATION)   6-14
      DIMENSIONFP(150),X(150),THETX(150),ZETAX(150),AS(150),
     XD(150),TD(150),ABCR(150),A(150,150),RM(150),B(150),V(150)
    1 READ100,M1,M2,M,H1,H2,AMASS
      AMS=SQRTF(AMASS)
      ALPHA=(AMASS-1.0)/(AMASS+1.0)
      THETA=(AMASS+1.0)/(2.0*AMS)
      ZETA=(AMASS-1.0)/(2.0*AMS)
      THETAS=THETA*THETA
      GSI=1.0+(((AMASS-1.0)**2)/(AMASS*2.0))*LOGF(ALPHA)
      P=2.0/GSI
      R=P-1.0
      M11=M1-1
      M12=M1+1
      M21=M2-1
      M22=M2+1
      M3=M-1
      DO5I=1,M
    5 FP(I)=FLOATF(I)
      DO10I=1,M1
   10 X(I)=FP(I)*H1
      DO15I=M12,M2
   15 X(I)=X(M1)+(FP(I)-FP(M1))*H2
      XC=X(M2)/ALPHA
      H3=(XC-X(M2))/(FP(M)-FP(M2))
      DO20I=M22,M
   20 X(I)=X(M2)+(FP(I)-FP(M2))*H3
      DO25I=1,M
      THETX(I)=THETA*X(I)
      ZETAX(I)=ZETA*X(I)
   25 V(I)=(X(I)+1.0/(2.0*AMASS*X(I)))*ERRORF(AMS*X(I))
     X+(0.56418958/AMS)*EXPF(-AMASS*X(I)**2)
      DO30I=1,M
      DO30J=I,M
   30 A(I,J)=(THETAS*X(I)/X(J))*(EXPF(X(J)**2-X(I)**2)
     X*(ERRORF(THETX(J)-ZETAX(I))-ERRORF(THETX(J)+ZETAX(I)))
     X+ERRORF(THETX(I)-ZETAX(J))+ERRORF(THETX(I)+ZETAX(J)))
```

```
 75 DO76I=1,M
 76 D(I)=TD(I)
    IF(SENSESWITCH2)77,78
 77 WRITEOUTPUTTAPE2,300,N,M1,M2,M,H1,H2,AMASS,GAMMA,XC,CRTM
    WRITEOUTPUTTAPE2,400,NITR
    WRITEOUTPUTTAPE2,500,(I,ABCR(I),I=1,M)
 78 IF(SENSESWITCH1)85,79
 79 DO80I=1,M
    IF(CRTM-ABCR(I))65,80,80
 80 CONTINUE
 85 WRITEOUTPUTTAPE2,200
    WRITEOUTPUTTAPE2,300,N,M1,M2,M,H1,H2,AMASS,GAMMA,XC,CRTM
    WRITEOUTPUTTAPE2,400,NITR
    WRITEOUTPUTTAPE2,600
    WRITEOUTPUTTAPE2,700,(I,X(I),AS(I),D(I),I=1,M)
    IF(K-10)41,1,1
100 FORMAT(3I3,1P3E12.4)
150 FORMAT(2I3,1P2E12.4)
200 FORMAT(35H1NEUTRON THERMALIZATION (ITERATION))
300 FORMAT(5H N = I3,8H   M1 = I3,8H   M2 = I3,7H   M = I3,8H   H1 = 1
   XPE11.4,8H   H2 = E11.4,8H MASS = E11.4/9H GAMMA = E11.4,8H   XC =
   XE11.4,10H   CRTM = E11.4)
400 FORMAT(22H   NO. OF ITERATION = I4)
500 FORMAT(6(I6,1PE11.4))
600 FORMAT(16H NEUTRON DENSITY/93H        I      X          ASY. SOL.
   X   DENSITY          I      X          ASY. SOL.      DENSITY)
700 FORMAT(2(I9,1PE12.4,2E13.4))
800 FORMAT(25H1ENERGY CHANGE PROBABLITY)
810 FORMAT(22H     MODERATOR MASS = 1PE12.4)
820 FORMAT(14H1INCIDENT X = 1PE11.4)
830 FORMAT(93H     J      X(J)         PROB.         J      X(J)
   XPROB.         J      X(J)         PROB.)
840 FORMAT(3(I6,1PE12.4,E13.4))
850 FORMAT(34H1TOTAL ENERGY TRANSFER PROBABILITY)
860 FORMAT(92H     I      X(I)         V(I)          I      X(I)
   XV(I)          I      X(I)         V(I))
    END(0,1,0,0,1)
```