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A SIMPLIFIED THEORY OF NEUTRON THERMALIZATION

by

LUIS G. DE SOBRINO

Grad. Escuela Naval Militar (Spain) (1951)
Dipl. Escuela de Estudios Superiores (Spain) (1956)
M.S. Massachusetts Institute of Technology (1958)

SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF SCIENCE

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

June, 1960

Signature redacted

Signature of Author.....
Department of Nuclear Engineering, May 14, 1960

Signature redacted

Certified by.....
Thesis Supervisor

Accepted by.....
Chairman, Departmental Committee
on Graduate Students

Abstract

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by

Luis G. de Sobrino

Submitted to the Department of Nuclear Engineering on May 14, 1960 in partial fulfillment of the requirements for the degree of Doctor of Science.

A simplified theory of neutron thermalization based on the heavy gas model is studied.

The influence of the crystalline binding in the thermal neutron spectrum is first considered by the use of an asymptotically valid approximation to the Boltzmann equation in an infinite homogeneous medium. The results are compared with the results of the heavy gas model, and it is seen that the use of this approximation constitutes an improvement over the use of the gaseous model without the assumption of a heavy mass.

The simplified model is then applied to then applied to the spatially dependent problem. To this end, a generalization of the Wilkins equation is studied and its solutions are tabulated.

The results of the application of the theory to bare and heterogeneous systems are compared with the results of experiments available in the literature. The agreement of theoretical and experimental results is found to be good.

Thesis Supervisor: Melville Clark, Jr.,
Associate Professor of
Nuclear Engineering.

Acknowledgments

The author wishes to acknowledge the helpful assistance of his thesis supervisor, Professor M. Clark, Jr., whose suggestions and encouragement have made possible the completion of this thesis.

The author also wishes to thank the M. I. T. Computation Center where part of the numerical work was performed and Mr. L. J. Donadieu for his helpful assistance in the programming of the digital computer.

The writer also wishes to express his thanks for financial assistance to the Junta de Energía Nuclear, Spain.

Finally, the author is indebted to Mrs. Ruth C. Kugelman who skillfully typed the final form.

TABLE OF CONTENTS

INDEX OF TABLES

INDEX OF FIGURES

Page

INTRODUCTION

1. The Problem of Neutron Thermalization

The problem of neutron thermalization deals with the distribution of neutrons of energies near the thermal energies of the medium. In such circumstances the nuclei of the media with which the neutrons interact cannot be assumed at rest. The neutrons will not always loose energy in interacting with the nuclei but can also gain energy. If an equilibrium is reached, neutrons will gain energy on the average with the same probability that they will loose it, and the resulting equilibrium distribution will be a thermal distribution at the temperature of the moderator.

In general, such an equilibrium distribution cannot be achieved. Neutrons will be absorbed by the nuclei of the moderator or they will leak out of it due to the finite size of the body. In such circumstances, a steady-state distribution can be reached only in the presence of a source, and, unless the source and the absorption cross sections have very definite energy and spatial dependence, the steady-state distribution will differ from the thermal equilibrium distributions.

Because of their very nature, substances other than gases, have binding forces among their constituent atoms of magnitude comparable with the energies of thermal agitation. These forces cannot, therefore, be ignored in considering the interaction of the neutron with the substance in question.

The thermal motion of the atoms of the moderator was first studied theoretically by Wigner and Wilkins (9), who neglected the effects of chemical binding and considered that the atoms of the moderator behaved like those in a perfect gas. Since then numerous authors have studied the problem both theoretically and experimentally. Three review articles that discuss the work are available in the literature (47, 48, 49). The main emphasis has been directed to the calculation of the spectrum in an infinite homogeneous medium. Numerical calculations have been performed using different models to take into account the effect of the binding forces. The nature of these forces in solids is fairly well understood, and the infinite medium spectrum can in principle be calculated with a good physical basis. The nature of the binding forces in a liquid is not well understood and detailed

calculations taking into account the effect of the liquid binding forces are not reliable until more advances are made in the theory of liquids. Little work has been done in the space dependent problem, the introduction of a leakage term was proposed by Hurwitz et al. on physical grounds. The work by Honeck (50) constitutes an exception; he developed a code based on the gaseous model to obtain the spatial and energy dependence of the flux in cylindrical cells of an heterogeneous system.

On the experimental side the emphasis has been mostly on homogeneous or quasi-homogeneous water systems. Only recently the measurement of the spectrum in fuel and moderators or uranium-water lattices has been undertaken. Some early measurements were done in heavy water and graphite but they were routine measurements performed as part of the set up of spectrometers. Therefore, no detailed results about the spectra were obtained, with the exception of the graphite measurement by Taylor.

2. Purpose and Outline of the Present Work

The purpose of the present thesis is to develop simple approximate methods that would enable the

calculation of neutron spectra with sufficient simplicity, and reasonable accuracy. To this end it is first necessary to choose a sufficiently simple model with few parameters that gives a reasonable description of the spectrum.

The first part of the thesis-chapters I to IV-is dedicated to the study of the effects of chemical binding in the infinite homogeneous medium. In chapters I and II, a review of the existing literature on the all important calculations of the inelastic scattering cross sections is made. In chapter III an approximate, asymptotically valid, differential equation for the energy distribution of neutrons is obtained. The method uses Placzek's asymptotic expansion for the cross section and is the natural extension of Wilkins' equation for heavy gaseous moderators. The results are only valid asymptotically and for heavy moderators. In chapter IV, the method is applied to beryllium and carbon. The results are compared with the results of a simple Wilkins' calculation and it is found that the error introduced by the heavy mass approximation is in the right direction to account for chemical

binding effects.

In chapter V the problem of spatially dependent spectra is considered. Feynmore's method is used to establish the limits of validity of the introduction of a leakage term into the equation for the infinite medium.

It now becomes necessary to choose a simple model for the process of thermalization. In view of the results obtained in chapter IV and V the Wilkins model is chosen with "1/v" absorption and constant leakage. This selection makes necessary the study of a second order linear differential equation of the second order which is undertaken from a purely mathematical point of view in chapter VI. Numerical results and tables are presented in Appendices A and B.

In chapter VII, the result of previous chapters are applied to specific systems. Since the Wilkins model fulfills the conditions of neutron conservation, detailed balance and correct asymptotic behavior, regardless of the mass of the moderator, it is hoped that its application to experimentally determined water spectra gives reasonable values. The examples worked out for homogeneous systems in chapter VII show that the

hopes were well founded. The application of the method to a water moderated lattice is also made, and the results compare reasonably well with the experiment.

Conclusions and recommendations for future work are stated in chapter VIII.

Chapter I

THE PROBLEM OF NEUTRON THERMALIZATION.

1. The Boltzmann Equation for Neutrons.

The macroscopic behavior of neutrons in a material system is described quite generally by the following integro-differential equation

$$\frac{x^{-\frac{1}{2}}}{v_o}\frac{\partial}{\partial t}\phi(\underline{r},x,\underline{\Omega},t) + \underline{\Omega}\cdot\nabla\phi(\underline{r},x,\underline{\Omega},t) + \Sigma\phi(\underline{r},x,\underline{\Omega},t) =$$

$$= \frac{1}{4\pi}\int d\underline{\Omega}' \int_0^{\infty} \Sigma(x',\underline{\Omega}',\rightarrow x,\underline{\Omega})\ \phi(\underline{r},x',\underline{\Omega}',t)dx +$$

$$+ S(\underline{r},x,\underline{\Omega},t) \qquad (1.1.1)$$

where $\underline{r}$ is the position vector, x is the energy measured in units of kT, v_o is the neutron speed at kT, k is Boltzmann's constant, T is the absolute temperature of the material medium, $\underline{\Omega}$ is a unit vector pointing in the direction of the velocity, $\phi(\underline{r},x,\underline{\Omega},t)$ is the directional flux per unit energy, solid angle and volume, Σ is the total macroscopic neutron cross section of the material system, $\Sigma(x',\underline{\Omega}',\rightarrow x,\underline{\Omega})$ is its macroscopic differential inelastic scattering cross section, and $S(\underline{r},x,\underline{\Omega},t)$ is the number of neutrons introduced in the system per unit time, energy, solid angle and volume.

In writing equation (1.1.1), neutrons are considered to interact with the system as a whole, rather than with

its individual nuclei. It is also assumed that the density of neutrons is so small that neutron-neutron collisions are negligible.

As any other equation describing the macroscopic behavior of an ensemble of particles, equation (1.1.1) implies a subdivision of phase space in elementary cells. A consideration of the size of these cells will clarify the physical situation.

Each cell should contain a sufficiently large number of neutrons in order that statistical considerations be applicable.

The properties of the system should not change appreciably in one cell. The size of the cells must be such that the interactions of a neutron in one cell be independent of the properties of the system in any different cell.

2. The Formulation of the Problem of Neutron Thermalization.

The problem of neutron thermalization is concerned with the solution of equation (1.1.1) in the energy range in which the thermal and binding energies of the atoms of the medium in which the neutrons move are comparable with the energy of the neutrons. This medium will be referred to as the moderator.

The lower limit of the range is taken as that energy below which the nondirectional flux-or simply the flux-

is so small that it does not contribute appreciably to the over-all neutron interaction rate.

The high limit is taken at an energy which is large compared with the thermal and binding energies of the atoms of the moderator, but small compared with the energies of the resonances of the nuclei present, in such a way that the neutron flux obeys the asymptotic low energy behavior predicted by slowing down theory. In general, it is possible to find such a high limit in usual moderators. Moderators which contain appreciable amounts of Pu^{239} constitute an exception; the 0.3 ev. resonance must be included in the thermal range.

In order to tackle the thermalization problem analytically, it is first necessary to obtain expressions for the properties of the moderator that appear in equation (1.1.1), namely, the source, the total cross section and the inelastic scattering cross section.

All neutrons produced by fission or other neutron multiplying reactions are produced at energies extremely high compared with the thermal range that do not depend on the energy of the thermal neutrons. The spatial dependence of the flux in the thermal range is very slightly affected by the distribution in space of very high energy sources, because of the randomizing effect of the collisions. For these reasons, the source will be

taken as an externally applied source, independent of the distribution in energy in the thermal range. The spatial distribution of the fission sources will, in general, be approximated by use of a simple monoenergetic approximation for the thermal flux.

Obtaining analytical expressions for the cross sections is a more difficult problem and will be treated in the next few sections.

3. The Scattering Cross Section of Matter for Slow Neutrons.

The interaction of neutrons with aggregates of atoms, as such, is considered in contrast to the interaction of neutrons with individual nuclei. The subject matter of this section has its place in the quantum theory of matter, rather than in nuclear physics.

The scattering of slow neutrons by matter has been studied theoretically by several authors (1,2,3,4, 5, 6, 7). The formalism that is most convenient for our purposes is the formalism developed by Glauber (4) and Zemach and Glauber (6).

In the following study, the interaction of the neutrons with the nuclei is the only one considered. The interaction of the magnetic moment of the neutrons with any magnetic field present in the moderator (magnetic scattering) is neglected. (Only in magnetic substances is this interaction important.) It is assumed that the interaction of the neutrons with the moderator nuclei is

a point interaction responding to a δ-function potential. This approximation is known as that of the Fermi pseudo-potential (7) and is valid to a high degree of accuracy (5) if the scattering cross section is calculated in the first Born approximation.

In the derivation of the expression for the cross section, we adopt a system of units in which the rationalized Planck's constant $\hbar$ is taken as unity, $\underline{p}$ and $\underline{p}'$ denote the initial and final momenta of the scattered neutron, x and x' the corresponding energies in units of kT.

Let us consider a system that is initially in a state φ_a and that, as a consequence of the interaction with a neutron, changes its state to φ_b.

All the calculations will be performed per unit volume of the system.

In the Fermi pseudopotential approximation, the potential seen by the neutron is

$$V(\underline{r}) = \frac{2\pi}{m} \sum_i a_i \delta(\underline{r} - \underline{r}_i) \qquad (1.3.1)$$

where $\underline{r}_i$ is the position vector of the ith nucleus of the system, a_i is its bound scattering length and m is the neutron mass.

The Born approximation with the potential (1.3.1) gives for the scattering cross section (8)

$$\Sigma_2(\underline{p}\to\underline{p}') = \frac{p'}{p}\left|\langle\varphi_a,p\left|\sum_i a_i\delta(\underline{r}-\underline{r}_i)\right|p',\varphi_b\rangle\right|^2\delta(x_b+x'-x_a-x) \tag{1.3.2}$$

x_a and x_b are the initial and final energies of the system. The second δ-function expresses conservation of energy. The notation for the matrix element is as usual:

$$\langle\varphi_1,p\mid V(\underline{r}_1,\underline{r}_2)\mid p',\varphi_2\rangle \equiv \iint\varphi_a(\underline{r}_1)e^{i\underline{p}\cdot\underline{r}_2}\,V(\underline{r}_1,\underline{r}_2)e^{-i\underline{p}'\cdot\underline{r}_2}\,*$$

$$*\;\varphi_b(\underline{r}_1)\,d\underline{r}_1\,d\underline{r}_2 \tag{1.3.3}$$

By virtue of the properties of the δ-function, (1.3.2) can be immediately written

$$\Sigma_2(\underline{p}\to\underline{p}') = \frac{p'}{p}\left|\langle\varphi_a\left|\sum_i a_i e^{i\underline{P}\cdot\underline{r}_i}\right|\varphi_b\rangle\right|^2\delta(x_b+x'-x_a-x) \tag{1.3.4}$$

where $\underline{P} = \underline{p} - \underline{p}'$.

In order to obtain the total differential cross section for neutron scattering of the system in state φ_a, (1.3.4) must be summed over all possible final states. To this end, we write the δ-function in Fourier integral form and obtain

$$\Sigma_1(x,\underline{\Omega}\to x',\underline{\Omega}') = \frac{p'}{p}\sum_b\left|\langle\varphi_a\left|\sum_i a_i e^{i\underline{P}\cdot\underline{r}_i}\right|\varphi_b\rangle\right|^2\frac{1}{2\pi}\,*$$

$$*\int_{-\infty}^{\infty}dt\;e^{-it(x_b-x_a)}e^{-it(x'-x)} \tag{1.3.5}$$

but, since φ_a and φ_b are eigenfunctions of the system corresponding to the energies x_a and x_b we may write

$$\sum_b e^{-it(x_b - x_a)} \langle \varphi_a | a_i e^{i\underline{P}\cdot\underline{r}_i} | \varphi_b \rangle \langle \varphi_b | a_j^* e^{-i\underline{P}\cdot\underline{r}_j} | \varphi_a \rangle =$$

$$= a_i a_j^* \langle \varphi_a | e^{itH} e^{i\underline{P}\cdot\underline{r}_i} e^{-itH} e^{-i\underline{P}\cdot\underline{r}_j} | \varphi_a \rangle \qquad (1.3.6)$$

where H is the hamiltonian of the system and we have made use of the rule of matrix multiplication.

Substitution of this expression into (1.3.5) yields after averaging over all states φ_i in a thermal distribution

$$\Sigma(x,\underline{\Omega} \to x',\underline{\Omega}') = \frac{1}{2\pi} \frac{p'}{p} \sum_i \sum_j a_i a_j^* \int_{-\infty}^{\infty} dt\, e^{-it(x' - x)} \Big\langle e^{itH} * e^{i\underline{P}\cdot\underline{r}_i} e^{-itH} e^{-i\underline{P}\cdot\underline{r}_j} \Big\rangle_T \qquad (1.3.7)$$

the subscript T denotes the thermal average. Equation (1.3.7) constitutes the general expression for the scattering cross section of a system for neutrons.

Equation (1.3.7) may be written in a simpler form by making use of Heisenberg's equation of motion

$$\Sigma(x,\underline{\Omega} \to x',\underline{\Omega}') = \frac{1}{2\pi} \frac{p'}{p} \sum_i \sum_j a_i a_j^* \int_{-\infty}^{\infty} dt\, * e^{-it(x' - x)} \Big\langle e^{i\underline{P}\cdot\underline{r}_i(t)} e^{-i\underline{P}\cdot\underline{r}_j(o)} \Big\rangle_T \qquad (1.3.8)$$

where $\underline{r}_i(t)$ represents now the position Heisenberg operator.

4. Coherent and Incoherent Cross-Sections, Pair- and Self-Distribution Functions.

Consider a uniform moderator formed by atoms of the same chemical species. Spin and isotopic disorder will introduce fluctuations in the scattering lengths a_i. The products $a_i a_j^*$ have to be averaged over the system. Performing the average, we get

$$\langle a_i a_j^* \rangle = \begin{cases} |\langle a \rangle|^2 & (i \neq j) \\ \langle |a|^2 \rangle & (i = j) \end{cases} \qquad (1.4.1)$$

The incoherent σ_{inc} and coherent σ_{coh} bound atom cross sections are defined by

$$\sigma_{coh} = 4\pi |\langle a \rangle|^2$$
$$\sigma_{inc} = 4\pi \left[\langle |a|^2 \rangle - |\langle a \rangle|^2 \right] \qquad (1.4.2)$$

In the case under consideration, we may write

$$\Sigma(x, \underline{\Omega} \to x', \underline{\Omega}') = \Sigma_{coh}(x, \underline{\Omega} \to x', \underline{\Omega}') + \Sigma_{inc}(x, \underline{\Omega} \to x', \underline{\Omega}') \qquad (1.4.3)$$

where the coherent and incoherent differential cross sections are respectively defined by

$$\Sigma_{coh}(x, \underline{\Omega} \to x', \underline{\Omega}') =$$
$$= \frac{1}{8\pi^2} \frac{p'}{p} \sigma_{coh} \sum_i \sum_j \int_{-\infty}^{\infty} dt \; e^{-it(x'-x)} \left\langle e^{i\underline{P} \cdot \underline{r}_i(t)} e^{-i\underline{P} \cdot \underline{r}_j(o)} \right\rangle_T \qquad (1.4.4)$$

$$\Sigma_{inc}(x, \underline{\Omega} \rightarrow x', \underline{\Omega}') =$$

$$= \frac{1}{8\pi^2} \frac{p'}{p} \sigma_{inc} \sum_i \int_{-\infty}^{\infty} dt \; e^{-it(x'-x)} \left\langle e^{i\underline{P}\cdot\underline{r}_i(t)} e^{-i\underline{P}\cdot\underline{r}_i(o)} \right\rangle_T$$

(1.4.5)

It is convenient to define the pair distribution function, which is the Fourier transform of the sum of the matrix elements appearing in (1.4.4) (3).

$$G_p(\underline{r},t) = \frac{1}{2\pi^3 N} \sum_i \sum_j \int d\underline{k} \; e^{-i\underline{k}\cdot\underline{r}} \left\langle e^{i\underline{k}\cdot\underline{r}_i(t)} e^{-i\underline{k}\cdot\underline{r}_j(o)} \right\rangle_T$$

(1.4.6)

where N is the number of nuclei per unit volume.

Similarly we define the self-distribution function as the Fourier transform of the matrix element in (1.4.5)

$$G_s(\underline{r},t) = \frac{1}{2\pi^3 N} \sum_i \int d\underline{k} \; e^{-i\underline{k}\cdot\underline{r}} \left\langle e^{i\underline{k}\cdot\underline{r}_i(t)} e^{-i\underline{k}\cdot\underline{r}_i(o)} \right\rangle_T$$

(1.4.7)

These distribution functions can be given a simple and convenient classical physical interpretation. To this end, we next transform (1.4.6). We may write

$$G_p(\underline{r},t) = \frac{1}{2\pi^3 N} \sum_i \sum_j \int d\underline{k} \; e^{-i\underline{k}\cdot\underline{r}} \left\langle e^{i\underline{k}\cdot\underline{r}_i(t)} \int d\underline{r}' \; e^{-i\underline{k}\cdot\underline{r}'} \delta\left[\underline{r}' - \underline{r}_j(o)\right] \right\rangle_T$$

(1.4.8)

or, using again the Fourier representation of the δ-function,

$$G_p(\underline{r},t) = \frac{1}{N}\sum_{i}\sum_{i\neq j}\int d\underline{r}' \langle \delta\left[\underline{r} - \underline{r}_j(t) + \underline{r}'\right] \delta\left[\underline{r}' - \underline{r}_j(o)\right]\rangle_T \tag{1.4.9}$$

The seemingly obvious reduction of the δ-functions is not permissible because of the noncommutativity of the position operators.

In the classical approximation the physical interpretation of (1.4.9) is clear. Interpreting the position operators as classical position vectors, (1.4.9) defines $G_p(\underline{r},t)$ as the probability of finding a nucleus at $\underline{r}$ at time t if a <u>different</u> nucleus was at the origin at time 0.

A similar transformation leads to a classical definition of the self-distribution function: The self-distribution function $G_s(\underline{r},t)$ represents the probability that a nucleus initially at the origin at time 0 be found at $\underline{r}$ at time t.

In terms of the distribution functions the macroscopic differential scattering cross sections can be written

$$\Sigma_{coh}(x,\underline{\Omega}\rightarrow x',\underline{\Omega}') = N\,\frac{\sigma_{coh}}{8\pi^2}\,\frac{p'}{p}\int_{-\infty}^{\infty} dt\; e^{-it(x'-x)}\int d\underline{r}\; e^{i\underline{P}\cdot\underline{r}}\, G_p(\underline{r},t) \tag{1.4.10}$$

$$\Sigma_{inc}(x,\underline{\Omega} \rightarrow x',\underline{\Omega}') = N \frac{\sigma_{inc}}{8\pi^2} \frac{p'}{p} \int_{-\infty}^{\infty} dt\, e^{-it(x'-x)} \int d\underline{r}\, e^{i\underline{P}\cdot\underline{r}} G_s(\underline{r},t) \qquad (1.4.11)$$

The formalism here developed will be applied in the following chapters to different moderators of interest.

We have still to determine adequate analytical expressions for the total cross section. The total scattering cross section can be, of course, obtained by integration of the differential scattering cross section. The absorption cross section, if not "1/v", will be assumed as given experimentally.

Chapter II

THE CALCULATION OF THE SCATTERING CROSS SECTIONS FOR DIFFERENT MODERATORS

1. Introduction

The formalism developed in the preceding chapter will be applied to different types of moderators.

Moderators consisting of a single species of atoms have incoherent cross sections that can be expressed by similar analytical expressions, regardless of the nature of the interatomic forces. This fact is a consequence of the physical nature of the self-distribution function. Since the number of atoms of the system is very large, the self-distribution function will be very approximately gaussian, with a width that will, in general, depend on time. In this case, we may write

$$G_s(\underline{r},t) = \frac{1}{[-\pi\mu w(t)]^{3/2}} \exp\left[-\frac{r^2}{-\mu w(t)}\right] \quad (2.1.1)$$

where it has been found convenient to factor out of the width of the gaussian, $-\mu w(t)$, the quantity μ that denotes the ratio of the neutron mass to the mass of the nucleus.

Substituting the expression (2.1.1) into (1.4.11) and performing the $\underline{r}$ integration we find for the incoherent cross section:

$$\sum_{inc}(x,\underline{\Omega}\rightarrow x',\underline{\Omega}') = \frac{N\sigma_{inc}}{8\pi^2}\left(\frac{x'}{x}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty} dt \exp\left[-i(x-x')t + \mu x^2 w(t)\right] \quad (2.1.2)$$

where we have written

$$\underline{\chi} = \frac{\underline{P}}{2M} \qquad (2.1.3)$$

Part of the work in this chapter will be devoted to finding the form of the function w(t).

In certain instances, it is possible to approximate the total inelastic differential scattering-cross section by an expression similar to (2.1.2). This approximation, called the incoherent approximation will also be discussed in this chapter.

We shall discuss mainly the gaseous and solid moderators. Although the gaseous moderator is a highly impractical one, the theory is simple and many of the features of the reactor spectra can be understood with its help. The solid model is useful because it is a realistic model and the theory of solids has reached a state of development such that it is possible to calculate the cross sections with a high degree of accuracy.

Liquid moderators are used extensively in reactors; however, the theory of liquids is not sufficiently well developed to permit the calculation of the scattering cross sections. Some remarks about liquids are also included in this chapter.

2. The Monoatomic Perfect Gas

In the case of a monoatomic perfect gas, the classical

model gives results identical with the quantum-mechanical model; however, for the sake of generality, and as an illustration of the methods that are necessary to treat more complicated moderators, it seems convenient to apply the general formalism developed in Chapter I to the calculation of the scattering cross section.

The only motion to be considered is the translational motion of the atoms that constitute the gas. Since the positions of two different atoms are totally uncorrelated, the average matrix element appearing in (1.4.4) is, obviously, zero. The coherent cross section is, therefore, zero as we would intuitively expect.

The average matrix element appearing in (1.4.5) will be evaluated next:

Heisenberg's equation of motion yields (8)

$$\frac{d\underline{r}_i(t)}{dt} = \frac{1}{i\hbar}\left[r_i(t), H(t)\right] \qquad (2.2.1)$$

where the brackets denote the commutator of two operators:

$$\left[A,B\right] \equiv AB - BA \qquad (2.2.2)$$

To evaluate the commutator in (2.2.1), we note that, since different atoms are not correlated, the part of the hamiltonian due to atoms other than i commutes with i. Now, the hamiltonian of the system is the sum of the hamiltonians of the individual free atoms, and is, of course, independent of time. (It should be remembered that the hamiltonian

refers to the initial state of the system):

$$H = \sum_i \frac{p_{si}^2}{2M} \qquad (2.2.3)$$

where $\underline{p}_{si}$ is the momentum of the ith atom of the system and M is its mass.

Using (2.2.3) in (2.2.1) we obtain

$$\frac{d\underline{r}_i(t)}{dt} = \frac{\underline{p}_{si}}{M} \qquad (2.2.4)$$

and,

$$\underline{r}_i(t) = \frac{\underline{p}_{si}}{M} t + \underline{r}_i(0) \qquad (2.2.5)$$

We have, therefore:

$$\left\langle e^{i\underline{P}\cdot\underline{r}_i(t)} e^{-i\underline{P}\cdot\underline{r}_i(0)} \right\rangle_T = \left\langle e^{i\underline{P}\cdot\left(\frac{\underline{p}_{si}}{M} t + \underline{r}_i(0)\right)} e^{-i\underline{P}\cdot\underline{r}_i(0)} \right\rangle_T \qquad (2.2.6)$$

In order to perform the operator product in the right-hand side of the preceding equation, we recall that for any two operators A and B that commute with their commutator

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]} \qquad (2.2.7)$$

Applying this rule, we obtain

$$e^{i\underline{P}\cdot\left(\frac{\underline{p}_{si}}{M} t + \underline{r}_i(0)\right)} e^{-i\underline{P}\cdot\underline{r}_i(0)} = e^{\frac{it}{2M}(\underline{P}^2 + 2\underline{P}\cdot\underline{p}_{si})} \qquad (2.2.8)$$

Operating with the operator in (2.2.8) on the wave function of the system, which is just the product of all the free particle wave functions of its atoms, we obtain

$$\langle \varphi_a | e^{\frac{it}{2M}(\underline{P}^2 + 2\underline{P}\cdot\underline{p}_{si})} | \varphi \rangle_a = e^{\frac{it}{2M}(\underline{P}^2 + 2\underline{P}\cdot\underline{p}_{si})} \qquad (2.2.9)$$

where we have used the symbol $\underline{p}_{si}$ to denote both the Heisenberg momentum operator and its corresponding eigenvalue. The value (2.2.9) has to be averaged over all the possible initial states defined by the Maxwellian distribution at temperature T. The momentum distribution is:

$$\mathcal{M}(\underline{p}) = \frac{1}{(2\pi M)^{3/2}} e^{\frac{-p^2}{2M}} \qquad (2.2.10)$$

We now peform the integration:

$$\langle e^{i\underline{P}\cdot\underline{r}_i(t)} e^{-i\underline{P}\cdot\underline{r}_i(0)} \rangle_T = \frac{1}{\sqrt{2\pi}\, M^{3/2}} \int_{-1}^{1} d\chi \int_0^{\infty} dp\, p^2 e^{\frac{-p^2}{2M}} e^{\frac{it}{2M}(P^2 + 2Pp\chi)} \qquad (2.2.11)$$

where we have taken the z axis along $\underline{P}$, and where χ is the cosine of the colatitude.

$$\langle e^{i\underline{P}\cdot\underline{r}_i(t)} e^{-i\underline{P}\cdot\underline{r}_i(0)} \rangle_T = \frac{2}{(2\pi M)^{1/2} Pt} e^{\frac{itP^2}{2M}} \int_0^{\infty} dp\, p e^{\frac{-p^2}{2M}} \sin \frac{Pt}{M} p$$

$$= e^{\frac{p^2}{2M}(it - t^2)} \qquad (2.2.13)$$

Substituting the expression for the average matrix element into (1.4.5) and taking (2.1.3) into account, we obtain the differential inelastic scattering cross section

$$\Sigma(x,\underline{\Omega} \rightarrow x';\underline{\Omega}') = \frac{\Sigma_b}{8\pi^2}\frac{p'}{p}\int_{-\infty}^{\infty} dt\; e^{-it(x'-x)}e^{\mu x^2(it-t^2)} \qquad (2.2.14)$$

Comparison with (2.1.2) shows that for a perfect monoatomic gas

$$w_g(t) = it - t^2 \qquad (2.2.15)$$

Equation (2.2.14) can be integrated in a straightforward, but laborious, manner over t, and over all possible changes in direction of the incident neutron. The result is the complicated kernel derived by Wigner and Wilkins (9) from classical principles.

We are not interested, however, in the exact form of the kernel, but, rather, in obtaining simpler approximations that make the Boltzmann equation more tractable.

3. Crystalline Solid

The calculation of the scattering cross section for a crystalline solid requires the use of quantum mechanics.

The calculation is lengthy, and we shall not perform it in detail. The general method has been illustrated in

previous section for the perfect monoatomic gas. Here, we shall outline the procedure used in references ( ) and ( ).

A crystal formed by a single atomic species of equivalent atoms is considered.

The main problem is the calculation of the average matrix elements appearing in (1.4.4) and (1.4.5). In order to solve it, we need to know the position operators $\underline{r}_i(t)$, corresponding to the ith nucleus.

The nuclei of the crystal can be considered to be harmonically bound; with this hypothesis the $\underline{r}_i(t)$ are simply given by a superposition of all possible normal modes, i.e., modes at which all the atoms vibrate with the same frequency. Let $\underline{b}_i$ represent the equilibrium position of the ith atom, then (10).

$$\underline{r}_i(t) = \underline{b}_i + \sum_s \int \xi_f(\underline{f}) \underline{c}_{is}(\underline{f}) e^{i\underline{f}\cdot\underline{b}_i} q_{\underline{f},s}(t)\, d\underline{f} \qquad (2.3.1)$$

where $\underline{f}$ is the propagation vector, $q_{\underline{f},s}(t)$ are the normal coordinates, i.e., the periodic solutions of the simple harmonic oscillator equation

$$\ddot{q}_{f,s} + \omega_s^2(f) q = 0 \qquad (2.3.2)$$

The integration extends over all possible propagation vectors $\underline{f}$, and $\xi_f(f)$ is the density of normal modes per unit volume in $\underline{f}$ space.* The quantities $\underline{C}_{is}(\underline{f})$ are the

---

* Actually, the $\underline{f}$'s constitute a discrete set, but little error is made if the corresponding sum is replaced by an integral, due to the large number of permitted values of f.

amplitudes corresponding to the normal modes. The subscript s refers to the different values of the frequency ω that correspond to each $\underline{f}$.

The normal modes q(t) can be represented by means of the annihilation and creation operators η and η^+ used in the quantization of the harmonic oscillator (11). It is through the use of these operators that the equivalence of a gas of particles obeying the Bose-Einstein statistics and a set of harmonic oscillators, becomes apparent. The set of oscillators forming the solid can be regarded as a gas of particles which are called phonons. A normal oscillator q_{fs} in its nth quantum state is exactly equivalent to n phonons being in a state defined by the propagation vector $\underline{f}$, and the polarization s.

The interaction of the neutron with the vibrating nuclei of the crystal can be looked upon as the interaction of the neutron with the phonon gas. A particular interaction resulting in a jump of an oscillator $q_{f,s}$ from its nth to its (n-m)th state, corresponds to an interaction in which m phonons in the state ($\underline{f}$,s) disappear; such an interaction is called an m-phonon interaction.

The concept of the phonon gas helps to explain the method of calculation of the matrix elements that constitute our target.

The expression (2.3.1) is substituted into the matrix

elements. The product of exponentials can be evaluated using the rule (2.2.7) and the commutation properties of η and η^+.

To evaluate the thermal average of the resulting expressions, use is made of the known equilibrium distribution for a Bose-Einstein gas, which is just Planck's distribution.

Proceeding in this way, one gets after considerable algebra

$$\left\langle e^{i\underline{P}.\underline{r}_i(t)} e^{-i\underline{P}.\underline{r}_j(0)} \right\rangle_T = e^{i\underline{P}.(\underline{b}_i-\underline{b}_j)} \exp\left\{\mu \sum_{\alpha\beta} \kappa_\alpha \kappa_\beta \left[C_{\alpha\beta}(\underline{b}_j,t) + C_{\alpha\beta}(\underline{b}_j,0)\right]\right\} \tag{2.3.3}$$

where

$$C_{\alpha\beta}(\underline{b},t) = \sum_s e_\alpha^s e_\beta^s \int \xi(\underline{f}) \left\{ e^{i(\underline{f}.\underline{b}-\omega_s t)} \frac{1}{e^{\omega_s}-1} + e^{-i(\underline{f}.\underline{b}-\omega_s t)} \left(\frac{1}{e^{\omega_s}-1} + 1\right)\right\} \frac{d\underline{f}}{\omega_s(\underline{f})} \tag{2.3.4}$$

We now substitute into the expressions (1.4.4) and (1.4.5), taking into account our hypothesis of equivalence of all the atoms of the lattice, and get for the cross sections

$$\Sigma_{coh}(x,\underline{\Omega} \to x';\underline{\Omega}') = \frac{N\sigma_{coh}}{8\pi^2}\left(\frac{x'}{x}\right)^{1/2} \sum_j e^{i\underline{P}\cdot\underline{b}_j} \; * \;$$

$$* \int_{-\infty}^{\infty} dt \; \exp\left\{-it(x'-x) + \mu \sum_{\alpha\beta} x_\alpha x_\beta \left[C_{\alpha\beta}(\underline{b}_j,t) - C_{\alpha\beta}(0,0)\right]\right\}$$

(2.3.5)

$$\Sigma_{inc}(x,\underline{\Omega} \to x';\underline{\Omega}') = \frac{N\sigma_{inc}}{8\pi^2}\left(\frac{x'}{x}\right)^{1/2} \; * \;$$

$$* \int_{-\infty}^{\infty} dt \; \exp\left\{-it(x'-x) + \mu \sum_{\alpha\beta} x_\alpha x_\beta \left[C_{\alpha\beta}(0,t) - C_{\alpha\beta}(0,0)\right]\right\}$$

(2.3.6)

with $C_{\alpha\beta}$ given by (2.3.4). Here x_α, x_β represent the components of the vector $\underline{\varkappa}$ defined in (2.1.3).

In the usual case of a polycrystal, these results are to be averaged over all possible orientations of the grains, i.e., over all possible directions of the vectors $\underline{e}^s$.

Several physical considerations can be made, regarding the expressions for the cross section. If $\mu \to 0$, i.e., for extremely heavy nuclei, the integrals reduce to δ-functions, the scattering, of course, is elastic in the laboratory system. The factor $\sum_j e^{i\underline{P}\cdot\underline{b}_j}$ in (2.3.5) gives Bragg's law. The factors $(e^{\omega_s} - 1)^{-1}$ in (2.3.4) arise from the

average number of phonons of energy ω in thermal equilibrium.

Both (2.3.5) and (2.3.6) are very complicated expressions and require simplification before they can be used for our purposes.

The first approximation that we shall make is the so-called incoherent approximation. It was first introduced by Placzek. Its accuracy has been discussed by Kothari and Singwy (5) . In the incoherent approximation the summation appearing in (2.3.5) is replaced by an integral, the integration can be carried out more easily after expansion of the exponential. A result is obtained similar to (2.3.6) but with σ_{coh} instead of σ_{inc}. In replacing the sum by the integral, an error is committed that Kothari and Singwy show to be the smaller, the larger the energy change of the neutron.

Elastic scattering is very badly represented by the incoherent approximation but the error in the total inelastic cross section was found in several examples to be about ten percent. The error in the calculation of reactor spectra is expected to be smaller than that in the cross section because elastic scattering does not contribute to the process of thermalization and because the importance of inelastic scattering increases with the change in energy of the neutron.

The expression that we shall use is, therefore

$$\Sigma(x,\underline{\Omega}\rightarrow x';\underline{\Omega}') = \frac{N\sigma_b}{8\pi^2}\left(\frac{x'}{x}\right)^{1/2}\int_{-\infty}^{\infty} dt\ \exp\Big\{-it(x'-x) + \mu\sum_{\alpha\beta}\chi_\alpha\chi_\beta\left[C_{\alpha\beta}(0,t) - C_{\alpha\beta}(0,0)\right]\Big\} \tag{2.3.7}$$

Here, σ_b is the total bound atom cross section.

It is interesting, partly for the applications, and partly because of the physical insight that will be gained, to particularize (2.3.7) for an isotropic crystal.

In such a case, the averaging over the orientations of the crystal need not be performed.

Let $\xi(\omega)$ be the density of phonons of frequency ω; changing the variable of integration in (2.3.4), we obtain for the cross section (2.3.7)

$$\Sigma(x,\underline{\Omega}\rightarrow x';\underline{\Omega}') = \frac{\Sigma_b}{8\pi^2}\left(\frac{x'}{x}\right)^{1/2}\int_{-\infty}^{\infty} dt\ \exp\Big\{-it(x'-x) + \mu\chi^2 w_s(t)\Big\} \tag{2.3.8}$$

with

$$w_s(t) = \int_0^{\infty}\frac{d\omega}{\omega}\xi(\omega)\left[\frac{e^{-i\omega t}-1}{e^{\omega}-1} + (e^{i\omega t}-1)\left(\frac{1}{e^{\omega}-1}+1\right)\right] \tag{2.3.9}$$

Returning now to the interpretation of w(t) as the width of the (gaussian) self-distribution function, we compare the width corresponding to a solid (2.3.9) with the width (2.2.15) that corresponds to a perfect gas.

First of all, we note that for very small t, both w_g and w_s approach it. A high energy neutron, (small collision time), will "see" in both cases a free nucleus. The term it gives rise to the inelasticity of the cross section produced by the recoil of the free atom. The next term in the expansion of $w_s(t)$ is proportional, though not equal, to t^2. This fact means that for neutrons with energy large compared with the temperature of the solid but slower than the ones considered before, the solid moderator will still appear like a gas, though with a temperature different from the real temperature of the solid and depending on the phonon distribution.

We also note that for large values of t, the width of the gas increases without bound. The fact is physically evident, since the position at time t of an atom initially at the origin becomes more and more unpredictable as t increases, the atoms of the perfect gas being free to move.

On the contrary the width of the solid is always bounded which is the mathematical expression of the

physical fact that, although the nuclei in a crystal can move, their motion is restricted to the neighborhood of their equilibrium position.

4. Remarks on the Scattering Cross Section of Other Kinds of Moderators

Liquid moderators are of great interest in reactor applications; however, the theory of liquids has not yet reached a stage of development that permits the calculation of the neutron scattering cross section. The calculation can be carried out with good accuracy for the individual molecules (6); however, the nature of the intermolecular forces is not well understood.

Qualitatively, one would expect that the width $w_e(t)$ would increase without bound for large values of t, although this increase should be slower than in the case of a perfect gas. A model based on these considerations has been proposed by Vineyard (12).

A model of the liquid cannot be incisively tested by comparing theoretical spectra with experimental measurements because the spectra are insensitive to the model and to small changes in the cross section. A direct measurement of the cross section seems much more reasonable for this purpose. For these reasons, liquid moderators will not be discussed here.

Moderators consisting of hydrogen bound to heavy

metals, like zirconium hydride, are also of interest in reactor applications; they can be approximated by a set of noninteracting harmonically bound hydrogen atoms. The cross section is easily calculated from formula (2.3.9) by using a delta function for the phonon density. However, no satisfactory analytical method of treating this case has been found, due to the highly singular nature of the resulting kernel that transforms the integral equation into an infinite order difference equation.

Chapter III

THE ASYMPTOTIC SOLUTION OF THE BOLTZMANN EQUATION IN AN INFINITE HOMOGENEOUS MEDIUM

1. Introduction

In an infinite homogeneous medium, the steady-state neutron flux depends only on the energy. Boltzmann's equation (1.1.1) reduces to

$$\Sigma(x)\,\phi(x) = \int_0^\infty dx' \Sigma(x' \to x)\,\phi(x') + S(x) \quad (3.1.1)$$

We are interested in an approximate solution of (3.1.1). We shall start with an expression for the cross section of the form (2.1.2). The cross section will be expanded using Placzek's inverse mass expansion (14). No hypothesis will be made about the form of the width w(t). As a result, a fourth order differential equation involving the moments of w(t) will be obtained.

The expression (2.1.2) is not valid for anisotropic moderators of which graphite is an important example. The necessary modifications to include moderators with a certain degree of anisotropy will be carried out.

The approximation to (3.1.1) obtained in the mannner described is only valid, in general, asymptotically. The first few coefficients of an

asymptotic expansion for the flux are given explicitly.

2. The Expansion of the Cross Section

It was pointed out by Placzek (14) that for moderately heavy moderators, it is convenient to expand the exponential appearing in the expression (2.1.2) in powers of the ratio μ of the neutron mass to the scatterer mass. The resulting expansion is expected to converge rather fast, at least in the case of a solid, due to the rapid oscillations of the terms of the type $e^{i\omega t} - 1$, appearing in the expression of the width (2.3.9), for large powers of $w(t)$. Experimental evidence showed that the convergence was very good.

Since we are interested in moderators such that $\mu \sim 0.1$, we shall use Placzek's expansion to order μ^2.

Expansion of (2.1.2) with use of the incoherent approximation yields:

$$\Sigma(x,\underline{\Omega} \rightarrow x',\underline{\Omega}') = \frac{\Sigma_b}{8\pi^2}\left(\frac{x'}{x}\right)^{1/2}\left\{2\pi\delta(x - x') + \right.$$

$$+ \mu x^2 \int_{-\infty}^{\infty} dt\, e^{-i(x'-x)t} w(t) + \frac{1}{2}\mu^2 x^4 \int_{-\infty}^{\infty} dt\, e^{-i(x'-x)t} *$$

$$\left. * w^2(t) + O(\mu^3)\right\} \qquad (3.2.1)$$

We now integrate over all possible changes in direction of the neutron, and noting that

$$x^2 = x + x' - 2(xx')^{1/2}\cos\theta \qquad (3.2.2)$$

where θ is the angle between the initial and final directions of the scattered neutron, we obtain

$$\Sigma(x\rightarrow x') = \frac{\Sigma_b}{2\pi}\left(\frac{x'}{x}\right)^{1/2}\left\{\mu(x + x')\int_{-\infty}^{\infty} dt\, e^{-i(x'-x)t}\, w(t) + \right.$$

$$\left. + \frac{1}{2}\mu^2\left[(x+x')^2 + \frac{4}{3}xx'\right]\int_{-\infty}^{\infty} dt\, e^{-i(x'-x)t}\, w^2(t) + O(\mu^3)\right\} \qquad (3.2.3)$$

where we have omitted elastic terms that do not contribute to (3.2.1).

We further approximate (3.2.3) by expanding $w(t)$ in powers of it.

$$w(t) = \sum_{n=1}^{\infty} w_n (it)^n \qquad (3.2.4)$$

This expansion was also suggested by Placzek (14); it has been used by Zemach and Glauber (6) in the calculation of the scattering cross section of methane giving good agreement with experimental results.

It use in reactor spectra calculations was suggested by Hurwitz et al. (15), and has been used by Kazarnovsky and coworkers (16) and by Corngold (17) in his calculations for gaseous moderators.

Kazarnovsky restricted his calculations to first

order in μ. Corngold did not make any restrictions on the mass of the moderator, but he assumed a gaseous model.

It is convenient to note that, since at high energies (small collision time t), the width w(t) of any scattering system approaches the width (2.2.15) of a perfect gas, we have quite generally

$$w_1 = 1 \tag{3.2.5}$$

The expression (3.2.4) is now substituted into (3.2.3); we make use of the identity

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i(x'-x)t}\,(it)^n\,dt = \delta^{(n)}(x - x') \tag{3.2.6}$$

where $\delta^{(n)}(x - x')$ is the nth derivative of the δ-function, and obtain to order μ^2 for the inelastic cross section

$$\Sigma(x\to x') = \Sigma_b\left(\frac{x'}{x}\right)^{1/2}\left\{\mu(x+x')\sum_{n=1}^{\infty} w_n\delta^{(n)}(x - x') + \right.$$

$$\left. + \frac{1}{2}\mu^2\left[(x+x')^2 + \frac{4}{3}xx'\right]\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} w_n w_m \delta^{(n+m)}(x - x')\right\} \tag{3.2.7}$$

Inspection of the preceding expression shows that with the approximations used, the integral equation (3.1.1)

will be transformed into an infinite order differential equation. The approximation is an asymptotic one as can be expected from the fact that the expansion of w(t) has been an expansion about the origin, that is, valid for small collision times or high neutron energies. It should be possible to find a solution for the differential equation in terms of an asymptotic series without truncating the equation. However, the domain of validity of the asymptotic series would not be greatly extended and the mathematical complications that arise would tend to obscure the result. We have, therefore, decided to cut the differential equation, arbitrarily, after the fourth derivative. It is, then, consistent to consider only the first three moments of the width w(t). With this new approximation, the total inelastic scattering cross section becomes

$$\int_0^\infty \Sigma(x\rightarrow x')\,dx' = \Sigma_b\left[\mu(-2 + \frac{w_2}{2x}) + \mu^2(3 - \frac{w_2}{x})\right] \qquad (3.2.8)$$

In deriving (3.2.7) we have used the fact that

$$\int_a^b f(x)\delta^{(n)}(x)\,dx = (-1)^n f^{(n)}(0) \qquad (3.2.9)$$

if the interval of integration includes the origin.

The fact that the expansion of the cross section is of an asymptotic nature, is apparent in (3.2.8). If we add to (3.2.8) the elastic term and make $x \to \infty$, the total scattering cross section becomes

$$\Sigma_s \to \Sigma_b(1 - 2\mu + 3\mu^2) \approx \frac{\Sigma_b}{(1+\mu)^2} \qquad (3.2.10)$$

so that to the order of our approximation, Σ_s becomes the free atom cross section. This fact is to be expected since the only errors inherent to the incoherent approximation are produced by the ordering of the atoms resulting from the interatomic binding forces and these can be disregarded for sufficiently high neutron energies.

3. The Approximation to the Integral Equation

As already has been mentioned, the expression (3.2.7) constitutes the basis for the transformation of the integral equation into a differential equation.

We substitute (3.2.7) into the kernel of the integral equation. By making use of (3.2.9), truncating after the fourth derivative, and considering only the first three moments of the width, we obtain a lengthy expression for the integral term involving ϕ and its first four derivatives. This expression is

now combined with (3.2.8) and the absorption cross section in accordance with (3.1.1). A fourth order differential equation results. The procedure is entirely straightforward and for this reason the details are not given.

We furthermore assume that the absorption cross section is of the form

$$\Sigma_a = \frac{\Sigma_o}{x^{1/2}} \qquad (3.3.1)$$

where Σ_o is the cross section at kT.

In order to remove the half integral power, the change of independent variable

$$y = x^{1/2} \qquad (3.3.2)$$

is made and the following fourth order differential equation is obtained.

$$+\mu\frac{w}{3}y\,\frac{d^4\phi}{dy^4} + \left[\frac{w_3}{2} + \mu\left(\frac{4w_2}{3}y^2 - \frac{2\bar{w}}{3}\right)\right]\frac{d^3\phi}{dy^3} + \left[w_2 y - \frac{3w_3}{2}y^{-1} + \right.$$

$$\left. + \mu\left(\frac{4}{3}y^3 + 2\bar{w}\,y^{-1}\right)\right]\frac{d^2\phi}{dy^2} + \left[2y^2 - w_2 + 3w_3 y^{-2} + \right.$$

$$\left. + \mu\left(\frac{4}{3}y^2 + 2w_2 - 4\bar{w}\,y^{-2}\right)\right]\frac{d\phi}{dy} + \left[4y - 3w_3 y^{-3} + \right.$$

$$\left. + \mu\left(-\frac{16}{3}y + 4w\,y^{-3}\right) - \Delta\right]\phi = 0 \qquad (3.3.3)$$

In writing (3.2.13) we have put

$$\Delta = \frac{2\Sigma_o}{\mu\Sigma_b} \qquad (3.3.4)$$

$$\bar{w} = w_2^2 + 2w_3 \qquad (3.3.5)$$

and we have also assumed that the energies of source neutrons are very high compared with the thermal energy so that we may write (3.1.1) as a homogeneous equation and select the solution that behaves properly at infinity.

The moments w_n appearing in (3.3.3) will be determined next: For a gas, we obtain immediately from (2.2.15)

$$w_2 = 1 \qquad (3.3.6)$$

$$w_n = 0 \quad n > 2$$

and for an isotropic solid (2.3.9) yields

$$w_n = \frac{1}{n!}\int_0^\infty \omega^{n-1}\,\xi(\omega)\,d\omega, \quad (n \text{ odd})$$

$$w_n = \frac{1}{n!}\int_0^\infty \omega^{n-1}\,\frac{e^\omega + 1}{e^\omega - 1}\,\xi(\omega)\,d\omega, \quad (n \text{ even}) \qquad (3.3.7)$$

Several features of equation (3.3.3) are of interest. We note firstly that for a heavy gas, $\mu \ll 1$; the equation to first order in μ, becomes a second order differential equation. This simple and useful equation was first proposed by Wilkins (18) and is known as the Wilkins equation.

Secondly we note that although, in general, equation (3.3.3) has only asymptotic validity, this is not the case for a gas, since then the expansion (3.2.4) of the width is exact because of the simple form (2.2.15). In this case, however, the expansion in μ is not valid because of the fact that the width $w(t)$ increases as t^2 for large t. The expansion is therefore valid only for $\mu t^2 \lesssim 1$, or, since the square of the collision time is inversely proportional to the energy, for $\mu/x \lesssim 1$.

4. The Modification of the Equation for Anisotropic Solids

The preceding theory is based on the expression (2.1.2) valid only for isotropic moderators. The case of anisotropic moderators is of interest in reactor calculation because graphite has a strongly anisotropic lattice.

Krumhansl and Brooks (19) have developed a model for graphite in which the phonon spectrum is considered to be different for displacements parallel and perpendicular to the layer planes. It is also assumed that both components of the atomic displacements do not interact. Keenson and Pearlman (20) have determined the pertinent constants from measurements of the low temperature specific heat of graphite, and Kothari and Singwi (22) have calculated with the use of these constants, the inelastic

scattering cross section for cold neutrons, obtaining good agreement with experimental results.

We are going to consider now the modifications of the theory developed in the preceding section for crystals having asymmetry similar to the model of graphite just discussed, i.e., an asymmetry characterized by an ellipsoid of revolution.

We start with equation (2.3.7) and again change the variable f to ω. Let $\xi^{(p)}(\omega)$ represent the distributions of phonons of polarization $\underline{e}^{p}$, we then have

$$C_{\alpha\beta}(0,t) - C_{\alpha\beta}(0,0) = \sum_{p} e^{s}_{\alpha} e^{s}_{\beta} \int \xi^{(s)}(\omega) \left[\frac{e^{-i\omega t}-1}{e^{\omega}-1} + \right.$$

$$\left. + (e^{i\omega t}-1)\left(\frac{1}{e^{\omega}-1} + 1\right) \right] \frac{d\omega}{\omega} \qquad (3.4.1)$$

In specializing for the type of anisotropy under consideration, let $\xi^{(1)}(\omega)$ and $\xi^{(2)}(\omega)$ represent the distribution of phonons corresponding to the displacements normal to the layer planes and in the layer planes respectively. We have to integrate over all possible orientations of the grains. To this end, we take a coordinate system with axes along the three principal axes of the polarization ellipsoid. Let the z-axis be along the polarization vector $\underline{e}^{1}$ and the x and y axis

be directed in such a way that the vector $\underline{\varkappa}$, representing the change in momentum of the neutron lie in the z-y plane (Fig. 3.1) and form an angle ζ with the z-axis.

To simplify the notation, let us write

$$g_i(t) = \int \xi^{(i)}(\omega)\left[\frac{e^{-i\omega t}-1}{e^{\omega}-1} + (e^{i\omega t}-1)\left(\frac{1}{e^{\omega}-1}+1\right)\right]\frac{d\omega}{\omega} \qquad (3.4.2)$$

We then have, omitting the argument of $g_i(t)$

$$\sum_{\alpha,\beta,s} \varkappa_\alpha \varkappa_\beta e^s_\alpha e^s_\beta g_s = \varkappa^2(g_1\cos^2 + g_2\sin^2\zeta) \qquad (3.4.3)$$

Or putting $\nu = \cos\zeta$, we obtain for the cross section averaged over all orientations of the grains

$$\Sigma(x,\underline{\Omega}\to x',\underline{\Omega}') = \frac{\Sigma_b}{8\pi^2}\left(\frac{x'}{x}\right)^{1/2}\int_{-\infty}^{\infty} dt\, e^{-i(x'-x)t} * \int_0^1 d\nu\, e^{\mu\varkappa^2[g_1\nu^2 + g_2(1-\nu^2)]} \qquad (3.4.4)$$

We now want to evaluate the integral I, over ν. Use of the definition of the error function

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}\,dt \qquad (3.4.5)$$

yields

$$I = \frac{\sqrt{\pi}}{2}\frac{e^{\mu\varkappa^2 g_2}}{\sqrt{\mu\varkappa^2(g_2-g_1)}}\operatorname{erf}\left[\sqrt{\mu\varkappa^2(g_2-g_1)}\right] \qquad (3.4.6)$$

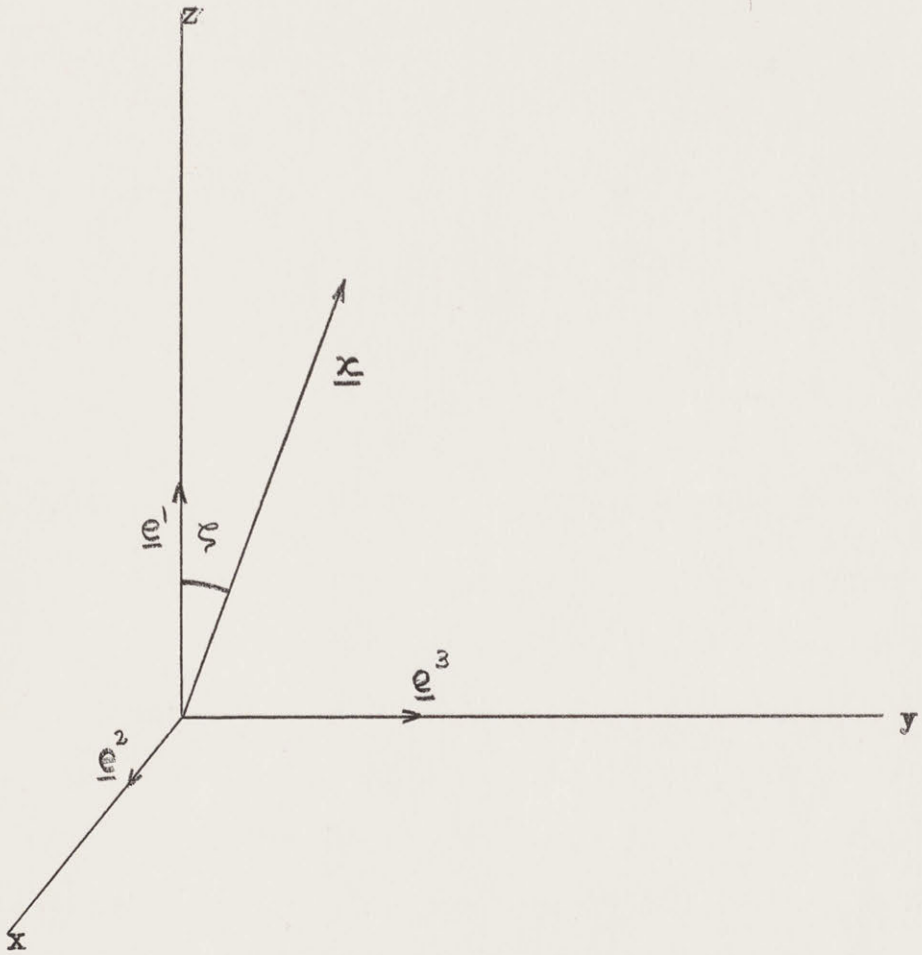

Fig. 3.1. System of coordinates used in the averaging of the cross section over all orientations of the grains.

Using the Taylor expansion of the error function (21), we obtain to order μ^2

$$I = 1 + \mu x^2 \frac{g_1(t) + 2g_2(t)}{3} +$$

$$+ \frac{1}{2}\mu^2 x^4 \left\{ \left[\frac{g_1(t) + 2g_2(t)}{3} \right]^2 + \frac{4}{45}\left[g_1(t) - g_2(t) \right]^2 \right\} \qquad (3.4.7)$$

Let us define

$$w(t) = \frac{g_1(t) + 2g_2(t)}{3} \qquad (3.4.8)$$

$$u(t) = g_1(t) - g_2(t) \qquad (3.4.9)$$

Comparison of (3.4.7) with the expression (3.2.1) shows that the theory can be extended to anisotropic scattering if $w^2(t)$ is replaced by $w^2(t) + u^2(t)$ in the terms of second order in μ.

We note that to first order in μ, the cross section is independent of the degree of anisotropy, since (3.4.8) is nothing else but the average of the phonon distributions of different polarizations. We also note that the new definition of w(t) (3.4.8) is consistent with our previous definition.

A derivation entirely similar to the one that led to equation (3.3.3) shows that for the anisotropic moderator under consideration, the corresponding fourth order differential equation is

$$\mu\frac{w}{3}y\,\frac{d^4\phi}{dy^4} + \left[\frac{w_3}{2} + \mu\left(\frac{4\bar{w}_2}{3}y^2 - \frac{2\bar{w}}{3}\right)\right]\frac{d^3\phi}{dy^3} +$$

$$+\left[w_2 y - \frac{3w_3}{2}y^{-1} + \mu\left(\frac{4\bar{w}_1}{3}y^3 + 2\bar{w}\,y^{-1}\right)\right]\frac{d^2\phi}{dy^2} +$$

$$+\left[2y^2 - w_2 + 3w_3 y^{-2} + \mu\left(\frac{4\bar{w}_1}{3}y^2 + 2\bar{w}_2 - 4\bar{w}\,y^{-2}\right)\right]\frac{d\phi}{dy} +$$

$$+\left[4y - 3w_3 y^{-3} + \mu\left(-\frac{16\bar{w}_1}{3} + 4\bar{w}\,y^{-3}\right) - \Delta\right]\phi = 0 \qquad (3.4.10)$$

where we have used the following notation, consistent with the notation previously introduced

$$\bar{w}_1 = 1 + \frac{4}{45}u_1^2$$

$$\bar{w}_2 = w_2 + \frac{4}{45}u_1 u_2 \qquad (3.4.11)$$

$$\bar{w} = w_2^2 + 2w_3 + \frac{4}{45}(u_2^2 + 2u_1 u_3)$$

and u_n are the moments of $u(t)$ defined by

$$u(t) = \sum_{n=1}^{\infty} u_n (it)^n \qquad (3.4.12)$$

Equation (3.4.10) is a more general form of (3.3.3) and reduces to it in the case of isotropy, $u(t) = 0$.

5. Some Remarks on the Wilkins Equation

As it was pointed out in section 3, equation (3.3.3) or the more general (3.4.10) becomes the Wilkins equation when the perfect gas model is considered and all powers of the mass ratio μ, except the first, are neglected.

The Wilkins equation is

$$y \frac{d^2\phi}{dy^2} + (2y^2 - 1) \frac{d\phi}{dy} + (4y - \Delta) \phi = 0 \quad (3.5.1)$$

or, in terms of the energy variable $x = y^2$

$$x \frac{d^2\phi}{dx^2} + x \frac{d\phi}{dx} + (1 - \frac{\Delta}{4x^{1/2}}) \phi = 0 \quad (3.5.2)$$

Here, the absorption cross section has been assumed 1/v. This restriction is not necessary and without it the Wilkins equation may be written

$$x \frac{d^2\phi}{dx^2} + x \frac{d\phi}{dx} + (1 - \frac{\Sigma_a(x)}{2\mu \Sigma_b}) \phi = 0 \quad (3.5.3)$$

The preceding equations are extremely attractive because of their simplicity. They have been derived as a particular case of the more general equation (3.4.10); their usefulness, however, extends beyond the validity of the hypotheses that led to their derivation, because they satisfy two fundamental conditions that every equation describing the spectrum of neutrons over the full energy range, must satisfy. These conditions are

a) The condition of detailed balance, which requires that the steady-state distribution of neutrons in an infinite homogeneous moderator without sources or sinks be a Maxwellian distribution.*

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* Quantum effects in the distribution are entirely negligible in all practical cases because of the low density of the neutron gas.

b) The condition that the asymptotic behavior of the flux, in an infinite homogeneous medium in the presence of absorption and high energy sources, must have the 1/x dependence predicted by slowing down theory.

That these conditions are satisfied by (3.5.3) can be readily verified.

The fourth order differential equation that results from (3.4.10) applied to the perfect gas, also satisfies these conditions.

Therefore, both the Wilkins equation and the fourth order differential equation for the perfect gas can be expected to represent reasonably well the overall behavior of the spectrum when the absorption is small.

In the case of a solid (3.4.10) will give with good accuracy the asymptotic form of the spectrum but it does not satisfy the condition of detailed balance, and therefore it cannot represent at all the overall behavior of the spectrum even for very small absorption.

The properties mentioned are a result of the fact, already noted in section 3, that the expansion of the width in powers of it and subsequent truncation after the first four terms, yields an exact result for the width of a gas but not for the width of a solid.

6. The Asymptotic Expansion for the Flux

It is easy to find an asymptotic series for the flux in (3.4.10) that behaves at infinity as required by slowing down theory. We substitute in (3.4.10) the series

$$\phi = \frac{1}{y^2} \sum_{n=0}^{\infty} a_n y^{-n}$$

and identify coefficients.

The first few coefficients are given next, explicitly, for convenience

$$a_0 = 1$$

$$a_1 = -\frac{\Delta}{2} - \mu \frac{5}{3} \Delta \bar{w}_1$$

$$a_2 = \frac{\Delta^2}{8} + 2w_2 + \mu\left(\frac{11}{12} \Delta^2 \bar{w}_1 + 8 w_2 \bar{w}_1 - 9 \bar{w}_2\right)$$

$$a_3 = -\frac{\Delta^3}{48} - \frac{19}{12} \Delta w_2 - \mu \left[\frac{\Delta^3}{4} \bar{w}_1 + \Delta\left(\frac{116}{9} \bar{w}_1 w_2 - \frac{26}{3} \bar{w}_2\right)\right]$$

$$a_4 = \frac{\Delta^4}{384} + \frac{55}{96} \Delta^2 w_2 + 6 w_2^2 - \frac{15}{4} w_3 + \mu \left[\frac{13}{288} \Delta^4 \bar{w}_1 + \Delta^2 \left(\frac{267}{36} \bar{w}_1 w_2 - \frac{89}{24} \bar{w}_2\right) + \right.$$

$$\left. + 56 w_2^2 \bar{w}_1 - 69 w_2 \bar{w}_2 - 20 w_3 \bar{w}_1 + 10 \bar{w} \right]$$

These coefficients when particularized for a gaseous moderator coincide with the values given by Corngold (17)* to order μ.

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* Note that the Δ used in reference (17) is the Δ in this work multiplied by the ratio of the bound to the free atom cross section.

Chapter IV

APPLICATION TO SEVERAL MODERATORS

1. Introduction

In the preceding chapter, an approximate asymptotic solution to the Boltzmann equation was given. In this chapter, the explicit solution for beryllium and graphite at different temperatures and in systems with different absorption will be given. The results are compared with the results given by the simple Wilkins' equation, and it will be found that the difference between the Wilkins solution and the more accurate gaseous model is in the direction of the correction due to crystalline binding, and that, at least in the energy range covered by the asymptotic solution, the use of the Wilkins' equation instead of the more accurate equation for the gaseous model, actually constitutes an improvement in the calculation of the neutron spectra.

2. Beryllium

Beryllium is considered to have a Debye phonon spectrum with a Debye temperature of 1000°K. This model has been used by Bandhari (23) to calculate the total scattering cross section for beryllium in the thermal range. The results are in excellent agreement with the experimental measurements. Nelkin (24)

used this model in conjunction with the incoherent approximation and the lowest term in the inverse mass expansion of the cross section to calculate the spectrum of thermal neutrons in beryllium by numerical integration of the integral equation.

Let θ represent the Debye temperature in units of kT. For a Debye model of the phonon spectrum we have

$$\xi(\omega) = \frac{3\omega^2}{\theta^3} \qquad (4.2.1)$$

and therefore the pertinent moments are

$$w_2 = \overline{w}_2 = \frac{3}{2\theta^3} \int_0^\theta \omega^3 \, \frac{e^\omega + 1}{e^\omega - 1} \, d\omega \qquad (4.2.2)$$

$$w_3 = \frac{1}{2\theta^3} \int_0^\theta \omega^4 \, d\omega$$

$$= \frac{\theta^2}{10} \qquad (4.2.3)$$

if $\theta \lesssim 4$, that is, if the Debye temperature is less than about four times the temperature of the moderator the series expansion for w_2 in powers of θ converges very rapidly, and we have

$$w_2 = 1 + \frac{\theta^2}{20} + \ldots \qquad (4.2.4)$$

Equations (4.2.3) and (4.2.4) show that the effect of crystalline binding increases as the square of the

ratio of the Debye temperature to the temperature of the moderator. This effect is measured by the width of the Gaussian self-distribution function of the solid compared with the corresponding quantity for a gas.

Figure 4.1 shows the effect of the crystalline binding in the asymptotic part of the spectrum for beryllium at 600°K and 300°K. Two values of Δ are shown, the value $\Delta = 0.4$ can be considered as typical for a thermal reactor. The value $\Delta = 0.8$ corresponds to a slightly under-moderated reactor. The small circles have been obtained with the Wilkins' equation. It can be seen that the use of this simple equation constitutes an improvement over the use of the more complicated gas model, at least in the energy range under consideration.

Table 4.1 lists the values of the pertinent moments used in calculating the solution.

Table 4.1

Moments Used in the Calculation of Beryllium Spectra

	Temperature of Beryllium	
	300°K	600°K
w_2	1.499	1.134
w_3	1.111	0.278
w	4.469	1.843

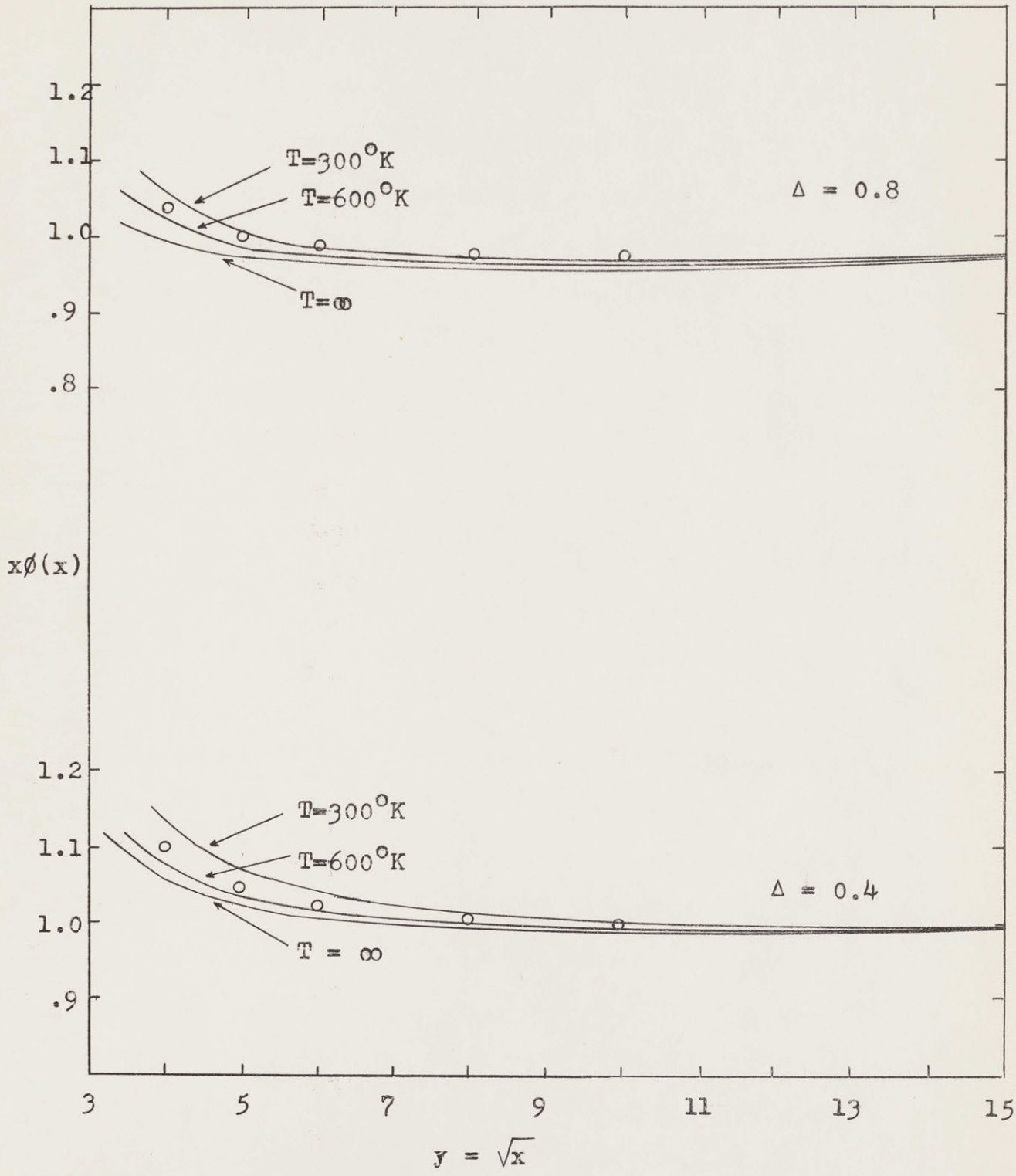

Fig. 4.1. The asymptotic part of the spectrum in beryllium. The circles are the result of the heavy gas model.

3. Graphite

As we briefly mentioned in the preceding chapter, Krumhansl and Brooks (19) developed a model for graphite in which the phonon spectrum is considered to be different for displacements perpendicular and parallel to the layer planes and both components of the displacement are assumed independent from each other. By theoretical considerations they found that both spectra can be approximated by a parabolic dependence on ω near the origin and by a linear dependence over the rest of the interval.

By measurements of the specific heat of graphite at low temperatures Keenson and Pearlman (20) determined the necessary constants. More recently Baldock (25) has computed with great detail the phonon spectrum for displacements perpendicular to the layer planes. Schofield and Hassit (26) have computed the neutron distribution in graphite in the presence of plutonium at 300°K by numerical solution of the integral equation. They used Baldock's model for the distribution of the transverse modes and Krumhansl's model for the vibrations along the planes; however, they found small differences between the constants using Baldock's spectrum and those computed using the corresponding Krumhansl spectrum. We shall use Krumhansl's model.

From the constants given by Keenson, it follows that the parabolic part of the distributions is en-

tirely negligible in our application; for our purposes both spectra can be considered to be linear with Debye temperatures of 1000°K for the transverse modes and 2500°K for the planar modes. With this model we may write

$$\xi^{(i)}(\omega) = \frac{2\omega}{\theta_i^2} \qquad (4.2.4)$$

Because of the independence of the modes, the total number of phonons corresponding to each of three principal displacements is the same, insuring that

$$\begin{aligned} \bar{w}_1 &= 1 \\ \bar{w}_2 &= w_2 \end{aligned} \qquad (4.2.5)$$

As in the case of beryllium the effect of chemical binding on the moments is seen to be quadratic in θ_1 and θ_2 for values of these ratios not much larger than unity.

Figure 4.2 shows the asymptotic solution for the neutron flux for the same values of the temperature and the thermalization parameter Δ used in the previous section. The Wilkins solution showed by the circles still constitutes an improvement over the solution for the gaseous model; also the difference between both of them is smaller than in the case of beryllium because of the higher value of the graphite mass.

Table 4.2 shows the values of the moments used

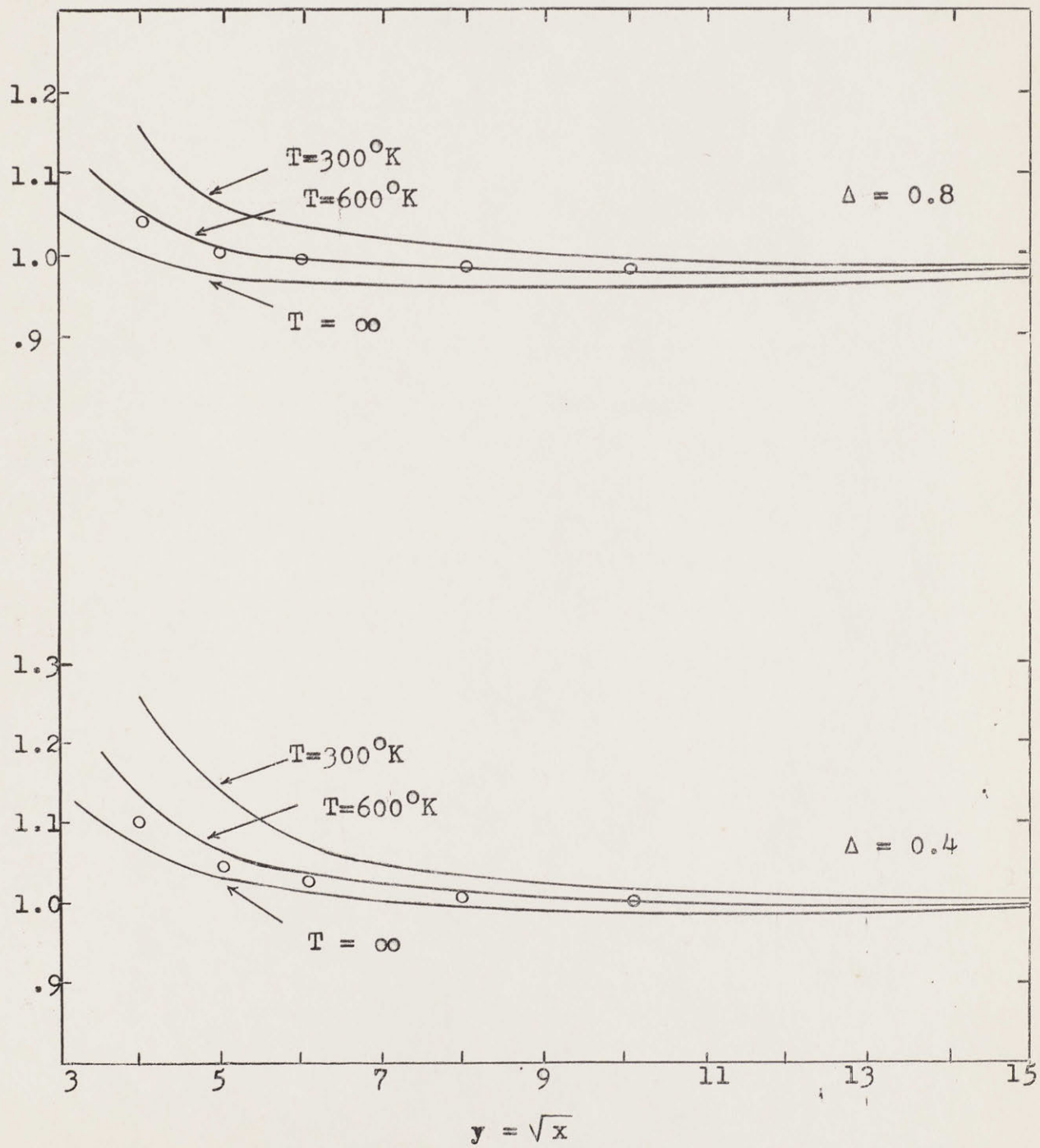

Fig. 4.2. The asymptotic part of the spectrum in graphite. The circles are the result of the heavy gas model.

in the calculation.

Table 4.2

Moments Used in the Calculation of Graphite Spectra

	Temperature of Graphite	
	300°K	600°K
w_2	2.376	1.449
w_3	5.864	1.046
w	17.55	4.325

The large values of the moments caused by the high Debye temperature of the planar modes are to be noted.

Chapter V

THE SPACE DEPENDENT PROBLEM

1. Introduction

In the present chapter, we shall present the theory of the space dependent Boltzmann equation when the energy dependence of the neutron flux is taken into account.

The complication of the problem is very great and simplifications have to be made in order to be able to treat analytically even the simplest problem. We shall start with the general equation and proceed with the simplifications finding the conditions under which they are valid. The approach taken by Feynman (27,28) in his method is admirably suited for the discussion of the simplifications and it will be followed.

A note about the time dependent problem is also included at the end of the chapter.

The treatment presented is purely formal and serves as an introduction to the work of later chapters.

2. The Approximation to the Boltzmann Equation

We are interested in the steady-state version of Boltzmann's equation (1.1.1). The first approximation that we shall make is that the inelastic scattering cross section is isotropic. This

approximation is certainly good for heavy gaseous moderators. In fact, the approximation is better at thermal energies than at epithermal energies. A simple calculation based on the expression (3.2.1) for the cross section yields for the average cosine of the scattering angle in a gaseous moderator

$$\langle \cos \theta \rangle = \frac{2}{3} \mu \left(1 - \frac{\mu}{2x}\right) \qquad (5.2.1)$$

which shows the dependence of the anisotropy on energy. Expression (5.2.1) is valid, of course, only asymptotically. The reduction of the anisotropy is a consequence of the highly disordered motion of the moderator atoms.

In liquid moderators, the reduction of the anisotropy at thermal energies is even greater because of the increase in apparent mass of the molecules of the moderator caused by the increase in the effect of intermolecular binding with decreasing energy. Drozdov et al. (29) report calculations done with a phenomenological model of scattering by water that show that the average cosine of the scattering angle has a value of only 0.4 at an energy of $4kT$.

Crystalline binding in solids should greatly increase the apparent mass of the scattering nuclei and therefore reduce the scattering anisotropy.

Coherent effects must be also taken into account. Bragg scattering, however, is very selective in energy, and, although it may strongly affect the isotropy at certain energies, its overall effect is expected to be small. Calculations of the transport cross section of beryllium carried out by Bandhari (23) confirm this point.

With the assumption of isotropy, an integral equation for the flux can be obtained from (1.1.1) (27)

$$\phi(\underline{r},x) = \frac{1}{4\pi}\int_V d\underline{r}'\left\{\int_0^\infty \frac{e^{-\Sigma(x)|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|^2}\Sigma(x'\to x)\phi(\underline{r}',x')\,dx' + 4\pi S(\underline{r},x)\right\} \qquad (5.2.3)$$

where the source is assumed to be isotropic.

We make use of the basic idea underlying the method of Feynman (27,28) that consists in expanding the solution of (5.2.3) in a series of spatial eigenfunctions in which the energy plays the role of a parameter. To this end it is convenient to introduce the emission density $H(\underline{r},x)$ defined by (27)

$$H(\underline{r},x) = \frac{1}{4\pi}\int_0^\infty dx'\,\Sigma(x'\to x)\phi(\underline{r},x') + S(\underline{r},x) \qquad (5.2.4)$$

that represents the total number of neutrons appearing with energy x at the point $\underline{r}$ per unit volume and energy. The inversion of (5.2.4) can be easily performed. Physical

intuition dictates

$$\phi(\underline{r},x) = \int_V d\underline{r}' \; \frac{e^{-\Sigma(x)|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|^2} H(\underline{r}',x) \quad (5.2.5)$$

which can be readily verified by elimination of $H(\underline{r},x)$ between this equation and (5.2.4). Substituting (5.2.5) into (5.2.4) we obtain an integral equation for the emission density,

$$H(\underline{r},x) = \frac{1}{4\pi} \int_V d\underline{r}' \int_0^\infty \frac{e^{-\Sigma(x')|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|^2} \Sigma(x' \rightarrow x) * H(\underline{r}',x') \, dx' + S(\underline{r},x) \quad (5.2.6)$$

Feynman used this equation instead of (5.2.3) because for the work to follow if is convenient to have in the exponential the cross section at energy x'.

As can be seen from the form in which the integral equations have been written, we are restricting the problem to the case in which the cross sections are independent of position. More complicated systems will be considered later.

We now expand the solution of (5.2.6) in a series of space eigenfunctions, having the energy as a parameter

$$H(\underline{r},x) = \sum_{\ell=0}^{\infty} f_\ell(x) \, Z_\ell(\underline{r},x) \quad (5.2.7)$$

The normalized eigenfunctions $Z_\ell(\underline{r},x)$ are defined by the eigenvalue problem

$$Z_\ell(\underline{r},x) = \frac{\Sigma(x) + 2\mu\Sigma_b\lambda_\ell(x)}{4\pi} \int_V \frac{e^{-\Sigma(x)|\underline{r}-\underline{r}'|}}{|\underline{r}-\underline{r}'|^2} Z_\ell(\underline{r}',x)\, d\underline{r}' \tag{5.2.8}$$

and constitute an orthogonal set. The form of the eigenvalue $\lambda_\ell(x)$ has been chosen for later convenience.

The source is also expanded in a series of the space eigenfunctions

$$S(\underline{r},x) = \sum_{\ell=0}^{\infty} S_\ell(x)\, Z_\ell(\underline{r},x) \tag{5.2.9}$$

The series (5.2.7) and (5.2.9) are now substituted into the integral equation (5.2.6); the result is multiplied by $Z_p(\underline{r},x)$ and integrated over the volume of the system. Use is made of the orthonormality of the set $Z_\ell(\underline{r},v)$ and of the integral equation (5.2.8). The result is

$$f_p(x) = \sum_\ell \int_0^\infty \frac{\Sigma(x'\to x) f_\ell(x')}{\Sigma(x') + 2\mu\Sigma_b\lambda_\ell(x')} A_{\ell p}(x'|x)\, dx' + S_\ell(x) \tag{5.2.10}$$

where

$$A_{\ell p}(x'|x) = \int_V Z_\ell(\underline{r},x') Z_p(\underline{r},x)\, d\underline{r} \tag{5.2.11}$$

Let us now change the dependent variable

$$\varphi_p(x) = \frac{f_p(x)}{\Sigma(x) + 2\mu\Sigma_b\lambda_p(x)} \qquad (5.2.12)$$

We obtain

$$\left[\Sigma(x) + 2\mu\Sigma_b\lambda_p(x)\right]\varphi_p(x) = \sum_\ell \int_0^\infty \Sigma(x' \to x)\,\varphi_\ell(x')A_{\ell p}(x'|x)\,dx' + S_\ell(x)$$

(5.2.13)

The system (5.2.13) is still exact except for the assumption of isotropy of the scattering kernel.

If the dimensions of the system are large compared with the mean free path, it is permissible to use the diffusion approximation in (5.2.8). The buckling $B_p(x)$ is then related to the eigenvalue $\lambda_p(x)$ by the equation

$$\frac{1}{1 + \frac{2\mu\Sigma_b\lambda_p(x)}{\Sigma(x)}} = \frac{\Sigma(x)}{B_p(x)} \tan^{-1} \frac{B_p(x)}{\Sigma(x)}$$

(5.2.14)

But, since the system is large $\left[B(x)/\Sigma(x)\right]^2 \ll 1$ and we may write

$$\lambda_p(x) = \frac{B_p(x)^2}{6\mu\Sigma_b\Sigma(x)} \qquad (5.2.15)$$

However, with the assumption of large system, the change of extrapolation length with energy is negligible and

the spatial eigenfunctions are the same for all energies; this fact means that

$$A_{\ell p}(x' | x) = \delta_{\ell p}$$

and (5.2.13) becomes

$$\left[\Sigma(x) + 2\mu\Sigma_b\lambda_p(x)\right]\varphi_p(x) = \int_0^\infty \Sigma(x' \to x)\varphi_p(x)\, dx' + S_\ell(x) \qquad (5.2.17)$$

with $\lambda p(x)$ given by

$$\lambda_p(x) = \frac{B_p^2}{6\mu\Sigma_b\Sigma(x)} \qquad (5.2.18)$$

The function $\varphi_p(x)$ is, then, given by the solution of an equation analogous to the equation for the infinite medium with an extra term $2\mu\Sigma_b\lambda_p(x)$. To neglect this term in the left-hand side of (5.2.17) on the grounds that B/Σ is small, is not permissible because the (large) contribution of the elastic scattering cross section to Σ cancels from both sides of (5.2.17).

The equation (5.2.17) is, of course, valid whatever the dimensions of the system if the total cross section is independent of energy.

In the cases in which (5.2.17) is valid consideration of (5.2.5), (5.2.7), (5.2.8), and (5.2.12) yields

$$\phi(\underline{r},x) = 4\pi \sum_{\ell=0}^{\infty} \varphi_\ell(x) Z_\ell(\underline{r}) \qquad (5.2.19)$$

If the conditions stated for the validity of (5.2.17) are not fulfilled, it is necessary to solve (5.2.13) . In general, it will be sufficient to use a perturbation approach because the spatial eigenfunctions at different energies would not differ much from each other. This idea is basic to Feynman's method.

In the following chapter we shall study the solutions of equation (5.2.17) with the heavy gas model.

Feynman's method is also very useful in treating the case of several media only one of which scatters inelastically. This medium will be called the moderator. The usefulness of this problem for cell calculations is obvious. The fuel, because of its heavy mass, can be considered to scatter neutrons without changing its energy.

We shall outline the basis of the method; a detailed description can be found in several references (27,28). We shall assume that sources are present only in the moderator. This assumption does not constitute any restriction in the usual case of high energy sources because neutrons can only attain thermal energies by moderation in the moderator.

The first collision distribution in the moderator of neutrons produced in the other media should be included in the source.

The emission density is expanded in a series of spatial eigenfunctions, orthogonal in the volume of the moderator,

$$H(\underline{r},x) = \sum_{\ell=0}^{\infty} f_\ell(x) Z_\ell(\underline{r},x) \qquad (5.2.20)$$

The functions $Z_\ell(\underline{r},x)$ are defined by

$$Z_\ell(\underline{r},x) = \left[\Sigma(x) + 2\mu\Sigma_b\lambda_\ell(x)\right] \int_{\text{mod}} K(\underline{r},\underline{r}'|x) Z_\ell(\underline{r}',x)\, dr' \qquad (5.2.21)$$

The cross sections are the cross sections of the moderator. The definition of the kernel $K(\underline{r},\underline{r}'|x)$ is given next: Consider a fictitious system in which all parameters are independent of energy and have the values that the parameters of the real system have at energy x; $K(\underline{r},\underline{r}'|x)$ is the probability that a neutron originating at $\underline{r}'$ in the moderator of the fictitious system, suffers its first collision in the moderator at $\underline{r}$. Obviously $K(\underline{r},\underline{r}'|x)$ is symmetric in $\underline{r}$ and $\underline{r}'$. The orthogonality of the set $Z_\ell(\underline{r},x)$ follows from this property.

By inserting the series into the integral equation

for the flux, using the orthogonality relation and the equation (5.2.21), a system of integral equations like (5.2.13) is obtained. The parameters in the system of equations refer to the moderator, and the series (5.2.20) gives the emission density in the moderator only. Once the emission density is known, the flux can be obtained by the equation analogous to (5.2.5) which in this case reads

$$\phi(\underline{r},x) = \int_{\text{mod}} d\underline{r}'\ K(\underline{r},\underline{r}'|x)\ H(\underline{r}',x) \qquad (5.2.22)$$

The flux in the other media can be obtained by solving monoenergetic problems at each energy, since no change of energy of the neutrons occur.

The simplifications that were made in the case of a single medium, when the dimensions were large compared with the mean free path, cannot be carried to the present problem without great care. Even when the dimensions of the moderator are large compared with the mean free path, a rapid change with energy of the cross sections of the other media can affect sensibly the spatial eigenfunctions of the moderator at different energies.

3. Note on the Time Dependent Problem

Inspection of the general equation (1.1.1) shows

that it can be reduced to a time independent equation by performing a Laplace transformation with respect to time. The resulting equation has the same structure than the time independent equation but with an added absorption cross section of magnitude s/v (30), where s is the parameter of the Laplace transformation. The general methods outlined in the preceding sections can be applied to the Laplace transformed equation, but considerable care must be taken in using approximations similar to those described before, even when the system is large compared with the mean free path. The fact that a term in s/v constitutes a part of the mean free path of the Laplace transformed problem should be kept in mind. Generally, in solving a time dependent problem, one is interested in obtaining a relaxation constant that is given by the value of s, when the problem is considered as an eigenvalue problem where s is the eigenvalue. If the relaxation constant is large, it is no longer possible to neglect the change in the spatial eigenfunctions with energy, caused by the variation of s/v with energy even if the dimensions of the system are large compared with the mean free path.

Chapter VI

THE GENERALIZED WILKINS EQUATION

1. Introduction

In the preceding chapter, we have seen that in several simple systems, the zeroth order solution of the space and energy dependent Boltzmann equation can be expressed as a sum of eigenfunctions of the spatially dependent problem with coefficients that are functions of energy defined as the solutions of integral equations of the form

$$\left[\Sigma(x) + 2\mu\Sigma_b\lambda(x)\right]\varphi(x) = \int \Sigma(x' \rightarrow x)\,\varphi(x')\,dx' + S(x) \qquad (6.1.1)$$

In order to be able to treat the problem analytically, it is necessary to study the solutions of (6.1.1). A considerably simplified model has to be chosen to calculate the cross sections in order to make the problem tractable. The heavy gas or Wilkins model is the simplest one, and as it was shown in chapter IV, it is a reasonable one to use. If this model is used, (6.1.1) becomes

$$2\mu\Sigma_b\left\{x\frac{d^2}{dx^2} + x\frac{d}{dx} + 1 - \frac{\Sigma_a(x)}{2\mu_b} - \lambda(x)\right\}\varphi(x) = -S(x) \qquad (6.1.2)$$

Simple analytical expressions for $\Sigma_a(x)$ and $\lambda(x)$ are needed; it is natural to take a 1/v dependence for $\Sigma_a(x)$ and a constant value for $\lambda(x)$. Since both $\lambda(x)$ and $\Sigma_a(x)$ enter additively in (6.1.2), the foregoing hypotheses on the form of $\Sigma_a(x)$ and λ allows us to treat exactly dependences of $\lambda(x)$ and $\Sigma(x)$ as the energy of the form $A + B/x^{1/2}$.

As regards the source, two cases are at present of interest: a) A high energy source. For all practical purposes, fission sources and other commonly used sources can be considered to be of infinite energy compared with thermal energies. b) No sources present. This case is of interest in pulsed neutron experiments.

These two cases require that we consider the solutions of the equation

$$x \frac{d^2\varphi}{dx^2} + x \frac{d\varphi}{dx} + \left(1 - \frac{\Delta}{4x^{1/2}} - \lambda\right)\varphi = 0 \qquad (6.1.3)$$

that are regular at the origin.

Equation (6.1.3) will be studied in the present chapter from a purely mathematical point of view.

For a reference to the methods used in this chapter, see, e.g., ref. (31).

2. The Behavior of the Solutions around the Singular Points.

In order to study equation (6.1.3) it is convenient to change both the dependent and independent variables. We make the changes

$$= xe^{-x} \qquad (6.2.1)$$

$$x^{1/2} = y \qquad (6.2.2)$$

and obtain

$$y \frac{d^2\psi}{dy^2} + (3 - 2y^2) \frac{d\psi}{dy} - (\Delta + 4y\lambda)\psi = 0 \qquad (6.2.3)$$

We note first that for $\Delta = 0$ a solution of (6.2.3) regular at the origin is the confluent hypergeometric function $\Phi(\lambda, 2; y^2)$ as defined in ref. (32). Upon returning now to our original equation (6.2.3), inspection shows that the origin is a regular singular point and that there is no other singular point for finite values of y. The indicial equation at the origin is

$$s(s - 1) = 0 \qquad (6.2.4)$$

suggesting the existence of a solution regular at the origin and a solution with a logarithmic singularity at the origin.

In order to obtain the solution regular at the origin, ψ_1 , we substitute the series

$$\psi_1(\lambda,\Delta;y) = \sum_{n=0}^{\infty} a_n y^n \qquad (6.2.5)$$

and obtain the following values for the coefficients

$$\begin{aligned} a_0 &= 1 \\ a_1 &= \frac{\Delta}{3} \qquad (6.2.6) \\ a_n &= \frac{\Delta}{n(n+2)} a_{n-1} + \frac{2(n-2+2\lambda)}{n(n+2)} a_{n-2} \end{aligned}$$

The normalization has been chosen in such a way that

$$\psi_1(\lambda,0;y) = \Phi(\lambda,2;y^2) \qquad (6.2.7)$$

The solution independent of ψ_1 has a logarithmic branch point at the origin and can be obtained by the formula

$$\psi_2(y) = C\,\psi_1(y) \int e^{-\int^y dy'\left(\frac{3}{y'} - 2y'\right)} \frac{dy}{[\psi_1(y)]^2} \qquad (6.2.8)$$

where the explicit dependence on the parameters has been omitted for brevity. Performing operations, we obtain

$$\psi_2(y) = C\,\psi_1(y)\int \frac{e^{y^2}}{y^3[\psi_1(y)]^2}\,dy \qquad (6.2.9)$$

Considering (6.2.5), formula (6.2.9) gives an expression of the form

$$\psi_2(\lambda,\Delta;y) = A\,\psi_1(y)\log y + \frac{1}{y^2} + \frac{b_{-1}}{y} + \sum_{n=1}^{\infty} b_n y^{-n} \qquad (6.2.10)$$

For $\Delta = 0$, we have the relation

$$\psi_2(\lambda,0;y) = \Gamma(\lambda)\Psi(\lambda,2;y^2) - (\lambda-1)\left[\frac{\Gamma'(\lambda)}{\Gamma(\lambda)} + 1 - 2\gamma\right]\Phi(\lambda,2;y^2) \qquad (6.2.11)$$

Here, $\Psi(a,c;x)$ is the second solution of the confluent hypergeometric equation as defined in ref. (32), and γ is Euler's constant.

Direct substitution of (6.2.10) into the differential equation (6.2.3), yields the values of the coefficients:

$$A = \frac{-\Delta^2+4(\lambda-1)}{2}; \quad b_{-1} = -\Delta; \quad b_1 = \frac{5\Delta^3+(32-44\lambda)\Delta}{3};$$

$$b_2 = \frac{7\Delta^4-(20+28\lambda)\Delta^2+48\lambda-192}{48}; \qquad (6.2.12)$$

$$b_n = \frac{\Delta}{n(n+2)}\,b_{n-1} + \frac{2(n-2+2\lambda)}{n(n+2)}\,b_{n-2} + 2A\left[(2n+3)a_n - 2a_{n-2}\right]$$

Since no singularities of the solution exist for finite y aside from the origin, the radii of convergence of (6.2.5) and the power series in (6.2.10) are infinite, and, therefore, both series converge absolutely and uniformly for all finite values of y.

We now proceed to investigate the point of infinity. To this end, we make the substitution $y = 1/z$ in the original equation and obtain

$$z^3 \frac{d^2\psi}{dz^2} + (2 - z^2) \frac{d\psi}{dz} - (\Delta + \frac{4}{z}\lambda)\psi = 0 \qquad (6.2.13)$$

The point $z = 0$ is an irregular singular point, the nature of the singularity, however, is such that one solution with a branch point exists. The indicial equation is

$$2s - 4\lambda = 0 \qquad (6.2.14)$$

We therefore substitute a series of the form

$$\psi_3(z) = z^{2\lambda} \sum_{n=0}^{\infty} c_n z^n \qquad (6.2.15)$$

into (6.2.13) and obtain the coefficients:

$$c_o = 1; \qquad c_1 = \frac{\Delta}{2}$$

$$c_n = \frac{\Delta}{2n} c_{n-1} - \frac{(2\lambda+n-2)(2\lambda+n)}{2n} c_{n-2} \qquad (6.2.16)$$

The radius of convergence of the series (6.2.15) is zero. This fact can be readily seen by considering the behavior of the recurrence relation (6.2.16) for large values of n. The divergence of the series is a result of the fact that the point z=0 is an irregular singular point.

Returning to the variable y, we obtain

$$\psi_3(\lambda,\Delta;y) \sim y^{-2\lambda} \sum_{n=0}^{\infty} c_n y^{-n} \qquad (6.2.17)$$

where we have used the symbol $\sim$ to denote that there is a solution $\psi_3(y)$ represented asymptotically by (6.2.17).

We now want to investigate whether a solution with a different asymptotic representation exists. To this end, we return again to equation (6.2.13) and note that a solution independent of (6.2.15) exists given by

$$\psi_4(z) = \psi_3(z) \; e^{-\int^z (\frac{2}{z'^3} - \frac{1}{z'}) \, dz'} \frac{dz}{[\psi_3(z)]^2}$$

$$= \psi_3(z) \int \frac{z \exp(z^{-2})}{[\psi_3(z)]^2} \, dz \qquad (6.2.18)$$

This expression suggests a solution containing an essential singularity of the form $\exp(z^{-2})$. In consequence, we

make in (6.2.13) the substitution

$$\psi(z) = e^{z^{-2}} \chi(z) \qquad (6.2.19)$$

The result is

$$z^3 \frac{d^2\chi}{dz^2} - (2+z^2) \frac{d\chi}{dz} - (\Delta + \frac{4\lambda-8}{z})\chi = 0 \qquad (6.2.20)$$

which has a solution with a branch point at z=0, with index $s = -(2\lambda-4)$. Substitution of the corresponding series into the equation yields the coefficients. It is again found that the radius of convergence of the series is zero. Returning to the previous variables, we find a solution, independent of $\psi_3(y)$ given asymptotically by

$$\psi_4(\lambda,\Delta;y) \sim y^{2\lambda-4} e^{y^2} \sum_{n=0}^{\infty} d_n y^{-n} \qquad (6.2.21)$$

where

$$d_0=1; \qquad d_1 = -\frac{\Delta}{2} \qquad (6.2.22)$$

$$d_n = -\frac{\Delta d_{n-1}}{2n} + \frac{(n+2-2\lambda)(n-2\lambda)}{2n} d_{n-2}$$

In short, we have found two solutions expressed about the origin by (6.2.5) and (6.2.10) and two

solutions expressed asymptotically by (6.2.17) and (6.2.21). Our task is now to relate the solutions about the origin to the solutions about the point of infinity.

3. The Joining of the Solutions

Since the generalized Wilkins equation is of the second order, ψ_1 must be a linear combination of ψ_3 and ψ_4. The coefficients will, of course, depend on the parameters λ and Δ of the equation. We, therefore, write

$$\psi_1(\lambda,\Delta;y) = P(\lambda,\Delta)\psi_3(\lambda,\Delta;y) + Q(\lambda,\Delta)\psi_4(\lambda,\Delta;y) \tag{6.3.1}$$

Extreme care must be exercised in studying the asymptotic behavior of ψ_1 (and ψ_2), because, the point of infinity being an irregular point, both functions should exhibit a Stoke's phenomenon.

In order to study the asymptotic behavior of ψ_1, the form of the coefficients a_n for large values of n is needed. To this end, let

$$\alpha_n = \frac{a_n}{a_{n+1}} \tag{6.3.2}$$

$$A_n = \frac{(n+1)(n+3)}{2(n-1+2\lambda)} \tag{6.3.3}$$

$$B_n = \frac{\Delta}{2(n-1+2\lambda)} \qquad (6.3.4)$$

The recurrence relation (6.2.6) gives the following terminating continuous fraction expression for α_n

$$\alpha_n = \frac{A_n}{B_n+} \frac{A_{n-1}}{B_{n-1}+} \cdots\cdots\cdots \frac{A_2}{B_2+} \frac{A_1}{B_1+A_o} \qquad (6.3.5)$$

that can also be written

$$\alpha_n = \frac{A_n}{B_n + \alpha_{n-1}} \qquad (6.3.6)$$

We have already proved that the series for $_1$ is absolutely convergent in the finite y-plane; therefore, for sufficiently large m, $\alpha_m \geqslant 1$, and there will exist an M such that for $m > M$

$$B_m < \epsilon \alpha_m \qquad (6.3.7)$$

ϵ being an arbitrarily small number. Since the sequence B_n decreases monotonically, we may write

$$\alpha_n = \frac{A_n A_{n-2} \cdots A_{m+2}}{A_{n-1} A_{n-3} \cdots A_{m+1}} \alpha_m \left[1 + o(\epsilon)\right] \qquad (6.3.8)$$

where we have assumed that both n and m are even.

From (6.3.6), (6.3.7), and (6.3.8) we may also write

$$a_n = \frac{a_m}{A_{n-1}A_{n-3}\cdots A_{m+1}}\left[1 + O(\epsilon)\right] \quad (6.3.9)$$

for n and m even.

A similar reasoning yields for n even and m odd

$$a_n = \frac{a_{m+1}}{A_{n-1}A_{n-3}\cdots A_{m+2}}\left[1 + O(\epsilon)\right] \quad (6.3.10)$$

By (6.3.3) and (6.3.9), (6.3.10) can be written

$$a_n = \frac{\Gamma(\frac{n}{2} + \lambda)}{\Gamma(\frac{n+4}{2})\Gamma(\frac{n+2}{2})} \frac{\Gamma(\frac{m+4}{2})\Gamma(\frac{m+2}{2})}{\Gamma(\frac{m}{2} + \lambda)} a_m \left[1 + O(\epsilon)\right]$$

n,m even (6.3.11)

$$a_n = \frac{\Gamma(\frac{n}{2} + \lambda)}{\Gamma(\frac{n+4}{2})\Gamma(\frac{n+2}{2})} \frac{\Gamma(\frac{m+5}{2})\Gamma(\frac{m+3}{2})}{\Gamma(\frac{m+3}{2} + \lambda)} a_{m+1}\left[1 + O(\epsilon)\right]$$

n even, m odd (6.3.12)

Consider first the case m even and let n = 2p. We have,

$$a_{2p} = \frac{\Gamma(\frac{m+4}{2})\Gamma(\frac{m+2}{2})}{\Gamma(\frac{m}{2} + \lambda)} a_m \left[1 + O(\epsilon)\right] \frac{\Gamma(p + \lambda)}{\Gamma(p+2)\Gamma(p+1)}$$

(6.3.13)

Similarly, for n odd, we put n = 2p+1 and obtain

$$a_{2p+1} = \frac{\Gamma(\frac{m+5}{2})\,\Gamma(\frac{m+3}{2})}{\Gamma(\frac{m+1}{2}+\lambda)}\, a_{m+1}\left[1 + O(\epsilon)\right]\frac{\Gamma(p+\lambda+\frac{1}{2})}{\Gamma(p+\frac{5}{2})\,\Gamma(p+\frac{3}{2})}$$

(6.3.14)

The asymptotic behavior of the -function yields

$$\Gamma(z) \to \sqrt{2\pi}\; z^{z-\frac{1}{2}}\, e^{-z} \qquad (6.3.15)$$

We may write for large p

$$\frac{\Gamma(p+\lambda+\frac{1}{2})}{\Gamma(p+\frac{5}{2})\Gamma(p+\frac{3}{2})} \to \frac{\Gamma(p+\lambda-\frac{1}{2})}{\Gamma(p+2)\Gamma(p+1)}$$

(6.3.16)

We are now going to determine separately the asymptotic behavior of the functions represented by the series $\sum_p a_{2p} y^{2p}$ and $\sum_p a_{2p+1} y^{2p+1}$. To this end, it is convenient to write the series expansion of the confluent hypergeometric function (32)

$$\Phi(a,c;z) = \frac{\Gamma(c)}{\Gamma(a)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(c+n)} \frac{z^n}{n!} \qquad (6.3.17)$$

The following theorem (33) is now used: "Let

$$f(z) = \sum_{n=0}^{\infty} a_n z^n \; ; \quad g(z) = \sum_{n=0}^{\infty} b_n z^n$$

where a_n and b_n maintain a constant sign for $n \geq N$, with N arbitrary but finite. If the series converges for $0 < z < \alpha$, where α is real and positive, and diverges for $z = \alpha$; and if, as $n \to \infty$

$$a_n \to C\, b_n$$

then as $z \to a$

$$f(z) \to C\, g(z) \text{ "}$$

Comparison of (6.3.13) and (6.3.17) shows that

$$\sum_{p=0}^{\infty} a_{2p} y^{2p} \to \frac{\Gamma(\frac{m+4}{2})\Gamma(\frac{m+2}{2})}{\Gamma(\frac{m}{2}+\lambda)} a_m \left[1 + O(\epsilon)\right] \frac{\Gamma(\lambda)}{\Gamma(2)} \Phi(\lambda, 2; y^2) \tag{6.3.18}$$

In a similar way, we obtain

$$\sum_{p=0}^{\infty} a_{2p+1} y^{2p+1} \to y \frac{\Gamma(\frac{m+5}{2})\Gamma(\frac{m+3}{2})}{\Gamma(\frac{m+1}{2}+\lambda)} a_{m+1} \left[1 + O(\epsilon)\right] *$$

$$* \frac{\Gamma(\lambda - \frac{1}{2})}{\Gamma(2)} \Phi(\lambda - \tfrac{1}{2}, 2; y^2) \tag{6.3.19}$$

We now make use of the asymptotic behavior of the confluent hypergeometric function (32) for real and positive values of the argument and obtain

$$\frac{\Gamma(\lambda)}{\Gamma(2)}\,\Phi(\lambda,2,y^2)\to y^{2\lambda-4}\,e^{y^2} \qquad (6.3.20)$$

and

$$\frac{\Gamma(\lambda-\frac{1}{2})}{\Gamma(2)}\Phi(\lambda-\tfrac{1}{2},2;y^2)\to y^{2\lambda-3}e^{y^2} \qquad (6.3.21)$$

Remembering that the series (6.2.5) defining ψ_1 is absolutely convergent, we may write

$$\psi_1(\lambda,\Delta;y)=\sum_{p=0}^{\infty} a_{2p}y^{2p}+\sum_{p=0}^{\infty} a_{2p+1}y^{2p+1} \qquad (6.3.22)$$

The asymptotic behavior of ψ_1, for y real, follows from (6.3.13), (6.3.14) and (6.3.19) through (6.3.21).

$$\psi_1(\lambda,\Delta;y)\to\lim_{m\to\infty}\left[\frac{\Gamma(\frac{m+4}{2})\Gamma(\frac{m+2}{2})}{\Gamma(\frac{m}{2}+\lambda)}a_m+\frac{\Gamma(\frac{m+5}{2})\Gamma(\frac{m+3}{2})}{\Gamma(\frac{m+1}{2}+\lambda)}a_{m+1}\right]y^{2\lambda-4}e^{y^2} \qquad (6.3.23)$$

where we have used the fact that as $m\to\infty$, ϵ can be taken as small as desired. As already stated, the asymptotic form (6.3.23) is only valid for y real, because of the restriction imposed by the theorem.

Comparing (6.3.23) with (6.3.1) and the asymptotic series for ψ_4, (6.2.21), we may write

$$Q(\lambda,\Delta) = \lim_{m\to\infty}\left[\frac{\Gamma(\frac{m+4}{2})\Gamma(\frac{m+2}{2})}{\Gamma(\frac{m}{2}+\lambda)}\,a_m + \frac{\Gamma(\frac{m+5}{2})\Gamma(\frac{m+3}{2})}{\Gamma(\frac{m+1}{2}+\lambda)}\,a_{m+1}\right]$$

(6.3.24)

In order to have the complete relationship between ψ_1 and the solutions around the point of infinity ψ_3 and ψ_4, it is necessary now to derive an expression for $P(\lambda,\Delta)$. Fortunately, the laborious process leading to (6.3.24) can be avoided.

Consider again the original equation (6.2.3) and let us change both the dependent and the independent variables

$$\psi = e^{y^2}\chi\ ; \qquad y = -it \tag{6.3.25}$$

Performing operations, we obtain

$$t\frac{d^2\chi}{dt^2} + (3 - 2t^2)\frac{d\chi}{dt} - \left[i\Delta + 4(2-\lambda)t\right]\chi = 0$$

(6.3.26)

Upon comparison of (6.3.26) with (6.2.3), we learn that

$$e^{y^2}\psi_1(2-\lambda;i\Delta;iy) \tag{6.3.27}$$

is another solution of (6.2.3). The absence of singularities at the origin shows that (6.3.27) is

proportional to ψ_1 and its value at this point shows that

$$\psi_1(\lambda,\Delta;y) = e^{y^2}\psi_1(2-\lambda,i\Delta;iy) \quad (6.3.28)$$

For y pure imaginary, iy is real and the theorem quoted above can be used. Its application shows that, for y pure imaginary

$$\psi_1(\lambda,\Delta;y) \to Q(2-\lambda,i\Delta)\ e^{-i\pi\lambda}y^{-2\lambda} \quad (6.3.29)$$

and comparing with (6.3.1) and the asymptotic series for ψ_3, (6.2.17) we obtain

$$P(\lambda,\Delta) = e^{-i\pi\lambda}Q(2-\lambda,i\Delta) \quad (6.3.30)$$

which completes our investigation of the relationship among ψ_1, ψ_3, and ψ_4.

The expression (6.3.24) obtained for $Q(\lambda,\Delta)$ is, however, not very convenient for numerical calculation. In the next section, a power expansion in Δ for $Q(\lambda,\Delta)$ is obtained.

4. The Expansion of $Q(\lambda,\Delta)$ in Powers of Δ

As was mentioned at the end of the last section, the expression (6.3.24) for the joining factor $Q(\lambda,\Delta)$ does not lend itself easily to numerical calculation.

In this section, we shall obtain an expression of the coefficients a_m as polynomials in Δ, and, as a consequence, a series expansion of $Q(\lambda,\Delta)$ in powers of Δ. The approach is based on the solution of the difference equation (6.2.6).

The expression (6.3.24) suggests that we make the change of variable

$$a_n = \frac{\Gamma(\frac{n}{2} + \lambda)}{\Gamma(\frac{n+4}{2})\Gamma(\frac{n+2}{2})} f(n) \quad (6.4.1)$$

With this change of variables, the recurrence relation (6.2.6) becomes

$$f(n) - \Delta g(n)\, f(n-1) - f(n-2) = 0 \quad (6.4.2)$$

where

$$g(n) = \frac{1}{4} \frac{\Gamma(\frac{n-1}{2} + \lambda)\Gamma(\frac{n+2}{2})\Gamma(\frac{n}{2})}{\Gamma(\frac{n}{2} + \lambda)\Gamma(\frac{n+3}{2})\Gamma(\frac{n+1}{2})} \quad (6.4.3)$$

Two initial conditions are needed to determine the solutions of the difference equation (6.4.2); these conditions are provided by the values of a_o and a_1 in (6.2.6). Using these values in conjunction with (6.4.1), we obtain

$$f(0) = \alpha = \frac{1}{\Gamma(\lambda)} \qquad (6.4.4)$$

$$f(1) = \beta = \frac{\pi\Delta}{8\Gamma(\lambda+\frac{1}{2})} \qquad (6.4.5)$$

We now substitute in (6.4.2) a series of the form

$$f(n) = \sum_{j=0}^{\infty} A_j \Delta^j \qquad (6.4.6)$$

Direct substitution of this series into the difference equation yields a system of recurrent difference equations for the coefficients A_j

$$\begin{aligned} A_0(n) - A_0(n-2) &= 0 \\ A_1(n) - A_1(n-2) &= g(n)\, A_0(n-1) \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ A_j(n) - A_j(n-2) &= g(n)\, A_{j-1}(n-1) \end{aligned} \qquad (6.4.7)$$

The system (6.4.7) can now be solved by successive steps. Because of the nature of the initial conditions, the values of the coefficients A_j are different for n even and n odd. We shall denote this difference by using the subscripts e and o for n even and odd respectively.

The first equation of the system (6.4.7), gives evidently

$$A_o(n_e) = \alpha \; ; \qquad A_o(n_o) = 0 \qquad (6.4.8)$$

The second equation yields (34)

$$A_1(n_o) = \frac{\beta}{\Delta} + \alpha \sum_{p=1}^{\infty} g(2p+1) - \alpha \sum_{p=1}^{\infty} g(n+2p) \qquad (6.4.9)$$

or, taken into account (6.4.3), (6.4.4), and (6.4.5),

$$A_1(n_o) = \alpha \sum_{p=1}^{\frac{n+1}{2}} g(2p-1) \qquad (6.4.10)$$

$$A_1(n_e) = 0$$

By proceeding in this way, the general form, which can be proved by induction, is obtained. For n even we have

$$A_n(n_e) = \alpha \sum_{p_1=1}^{n/2} \sum_{p_2=1}^{p_1-1} \sum_{p_3=1}^{p_2} \cdots \sum_{p_n=1}^{p_{n-1}} g(2p_1)g(2p_2+1) \, * \, * \, g(2p_3+1) \cdots g(2p_n-1) \qquad (6.4.11)$$

$$A_n(n_o) = 0$$

Similarly for n odd we get

$$A_n(n_o) = \alpha \sum_{p_1=1}^{\frac{n-1}{2}} \sum_{p_2=1}^{p_1} \sum_{p_3=1}^{p_2-1} \cdots \sum_{p_{n=1}}^{p_n-1} g(2p_1+1)g(2p_2) *$$

$$* \quad g(2p_3+1) \ldots g(2p_n-1)$$

(6.4.12)

$$A_n(n_e) = 0$$

These formulas, however, are not particularly advantageous for the calculation of the coefficients a_n of the power series for ψ_1; the recursion relation being a more expedient method for the computation. The usefulness of (6.4.12) is for the computation of $Q(\lambda,\Delta)$. By (6.3.24) and (6.4.1) we have:

$$Q(\lambda,\Delta) = \lim_{n\to\infty} \left[f(n) + f(n+1)\right] \quad (n, \text{ even})$$

(6.4.13)

By (6.4.4), (6.4.6), (6.4.11), and (6.4.12), we obtain

$$Q(\lambda,\Delta) = \frac{1}{\Gamma(\lambda)}\left\{1 + \Delta \sum_{p=1}^{\infty} g(2p-1) + \Delta^2 \sum_{p=1}^{\infty}\sum_{q=1}^{p} g(2p)g(2g-1) + \right.$$

$$\left. + \Delta^3 \sum_{p=1}^{\infty}\sum_{q=1}^{p}\sum_{r=1}^{q} g(2p+1)g(2q)g(2r-1) + \ldots \right\}$$

(6.4.14)

This formula has been used to calculate $Q(\lambda,\Delta)$. The numerical calculations and results are discussed in Appendix A.

Tables of the function $y^2e^{-y^2}\psi_1(\lambda,\Delta;y)$ together with the discussion of the numerical calculation are given in Appendix B.

5. The Eigenvalue Problem

When low energy sources of neutrons are present, or in studying the decay of neutrons in the absence of sources in small systems, it is convenient to examine the eigenvalue problem defined by the eigenvalue equation

$$y\frac{d^2W_n}{dy^2} + (3-2y^2)\frac{dW_n}{dy} - (\Delta + 4y\gamma_n)W_n = 0 \qquad (6.5.1)$$

and the boundary conditions that W_n be regular at the origin and have a nonexponential behavior at infinity.

Equation (6.5.1) can be written in Sturm-Liouville form

$$\frac{d}{dy}\left[y^3e^{-y^2}\frac{dW_n}{dy}\right] - (\Delta y^2e^{-y^2} + 4y^3e^{-y^2}\gamma_n)W_n = 0 \qquad (6.5.2)$$

The coefficients are seen to fulfill all the requirements that insure the orthogonality and

completeness of the set W_n in the range $(0,\infty)$ (35). The orthogonality relation can be immediately written

$$\int_0^\infty W_n(y)W_m(y)\, y^3 e^{-y^2}\, dy = N_n \delta_{nm} \tag{6.5.3}$$

where the N_n are the normalization constants.

Instead of considering γ as the eigenvalue parameter, it is possible to so consider Δ. We denote by $\bar{W}_n$ the corresponding eigenfunctions for fixed γ, the orthogonality relation reads instead of (6.5.3)

$$\int_0^\infty \bar{W}_n(y)\, \bar{W}_m(y)\, y^2 e^{-y^2}\, dy = \bar{N}_n \delta_{nm} \tag{6.5.4}$$

In a physical problem, the eigenvalues γ_n for fixed Δ are related to the negative leakage (or inward flow of neutrons) necessary to maintain the nth energy distribution mode for a given absorption. The eigenvalues Δ_n for fixed γ are related to the (negative) absorption cross section necessary to maintain the nth energy mode for a fixed leakage. In time dependent problems with no sources present, the Δ_n are closely related to the decay constants of the different energy modes.

The equation determining the eigenvalues can be obtained from (6.3.1). Since $\psi_4(\gamma,\Delta;y)$ increases exponentially at infinity, and since $\psi_1(\gamma,\Delta;y)$ is regular at the origin, it is evident that the eigenvalues are the solutions of

$$Q(\gamma,\Delta) = 0 \qquad (6.5.5)$$

This equation can, of course, be used to determine either the λ_n or the Δ_n.

Equation (6.5.5) in conjunction with formula (6.4.14) has been used to calculate the first few eigenvalues. The numerical calculation is discussed and a table of eigenvalues is given in Appendix A. Tables of eignefunctions are given in Appendix B.

The normalization of the eigenfunctions has been chosen in such a way that

$$W_n(y) = \psi_1(\gamma_n,\Delta;y)$$
$$\bar{W}_n(y) = \psi_1(\gamma,\Delta_n;y) \qquad (6.5.6)$$

A useful relation that gives pairs of values of λ and Δ that satisfy (6.5.5) is easily obtained from a consideration of the recurrence relationship (6.2.6), which, for convenience, is repeated here:

$$a_n = \frac{\Delta}{n(n+2)}\, a_{n-1} + \frac{2(n-2+2\gamma)}{n(n+2)}\, a_{n-2} \qquad (6.5.7)$$

Let $\gamma = -m/2$ where m is zero or a positive integer; if Δ is a root of $a_{m+1} = 0$, equation (6.5.5) is satisfied.

The proof is immediate; for $\gamma = -m/2$, we have from (6.5.7)

$$a_{m+2} = \frac{\Delta}{(m+2)m}\, a_{m+1} \qquad (6.5.8)$$

and if $a_{m+1} = 0$, then $a_{m+2} = 0$ and in general $a_n = 0$ for $n > m$. The power series expansion of ψ_1 terminates; ψ_1 behaves at infinity as y^m and therefore, (6.5.5) is satisfied. This property has been used in Appendix A to extrapolate the formulas obtained for the eigenvalues from (6.4.14).

Chapter VII

APPLICATIONS TO SPECIFIC SYSTEMS

1. Introduction

In this chapter, we treat some of the applications of the theory developed in the preceding chapters. We consider first the problem of the calculation of neutron spectra in bare homogeneous systems. Unfortunately, the detailed measurements of spectra have been limited up to now to water systems. Furthermore, the measurements have been designed to simulate the spectrum in infinite media and have not been directed to the influence of leakage. The applicability of the Wilkins approximation to water systems (not discussed theoretically) is tested by comparison with experiments. The approximation is seen to be applicable in the range of absorption studied.

The problem of the neutron spectrum in lattices is considered next. A very simplified model equivalent to the first order approximate solution of the system of integral equations (5.2.13), is considered. The result of the calculations is seen to be in agreement with the experimentally measured moderator spectra.

2. Bare Homogeneous Systems With High Energy Sources

It was shown in Chapter V that in a bare homogeneous

system with dimensions large compared with the mean free path, the neutron flux can be represented by

$$\phi(\underline{r},x) = 4\pi \sum_{n=0}^{\infty} \varphi_n(x) Z_n(\underline{r}) \qquad (7.2.1)$$

where the $Z_n(\underline{r})$ are the spatial eigenfunctions and $\varphi_n(x)$ are the solutions of the equation

$$[\Sigma(x) + 2\mu\Sigma_b\lambda_n(x)]\varphi_n(x) = \int_0^{\infty} \Sigma(x' \rightarrow x)\, \varphi_n(x')\, dx' + S_n(x) \qquad (7.2.2)$$

$\lambda_n(x)$ are the spatial eigenvalues as defined by (5.2.8) and $S_n(x)$ is the contribution of the source to neutrons in the nth spatial mode as defined by (5.2.9).

If the source neutrons are emitted at energies very large compared with thermal energies, then we can assume with a high degree of accuracy that the source neutrons are monoenergetic. The accuracy is a consequence of the fact that they have already reached the asymptotic behavior predicted by slowing down theory when they attain thermal energies. We can, therefore, write

$$S_n(x) = S_n\delta(x - x_o) \qquad (7.2.3)$$

where x_o is the energy of the source neutrons.

In order to solve (7.2.2) we use the Wilkins approximation and assume 1/v absorption and constant total cross section in the thermal region. With these assumptions, we obtain instead of (7.2.2)

$$x\frac{d^2\varphi_n}{dx^2} + x\frac{d\varphi_n}{dx} + \left(1 - \frac{\Delta}{4x^{1/2}} - \lambda_n\right)\varphi_n = -\frac{S_n}{2\mu\Sigma_b}\delta(x - x_o) \qquad (7.2.4)$$

We want to reduce (7.2.4) to the equation studied in Chapter VI. To this end, we put $\varphi_n = xe^{-x}g_n$ and $x = y^2$. Changing the variables in (7.2.4), we obtain:

$$y\frac{d^2g_n}{dy^2} + (3 - 2y^2)\frac{dg_n}{dy} - (\Delta + 4y\lambda_n)g_n = -\frac{y_o^{-2}e^{y_o^2}S_n}{\mu\Sigma_b}\delta(y - y_o) \qquad (7.2.5)$$

The solution of (7.2.5) can easily be written by application of the methods for obtaining the Green's function of a second order linear differential operator (*5*), in terms of the functions studied in the previous chapter

$$g_n(y) = \frac{S_n}{2\mu\Sigma_b Q(\lambda_n,\Delta)}\begin{cases}\psi_1(\lambda_n,\Delta;y)\,\psi_3(\lambda_n,\Delta;y_o) & y < y_o \\ \psi_3(\lambda_n,\Delta;y)\,\psi_1(\lambda_n,\Delta;y_o) & y > y_o\end{cases} \qquad (7.2.6)$$

We are interested only in the region $y < y_o$. Moreover,

since we have assumed $y_o \gg 1$, we can use the asymptotic form for ψ_3 and write

$$g_n(y) = \frac{S_n y_o^{-2\lambda_n}}{2\mu\Sigma_b Q(\lambda_n,\Delta)} \psi_1(\lambda_n,\Delta;y) \qquad (7.2.7)$$

Or returning to our old variables φ_n and x, and taking into account (7.2.1) we may write

$$\phi(\underline{r},x) = \frac{1}{2\mu\Sigma_b} \sum_{n=0}^{\infty} \frac{S_n x_o^{-\lambda_n}}{Q(\lambda_n,\Delta)} Z_n(\underline{r}) x e^{-x} \psi_1(\lambda_n,\Delta;x^{1/2}) \qquad (7.2.8)$$

This relation is the final solution of our problem.

Before proceeding further it is interesting to consider the solution (7.2.8) for energies much higher than thermal. Use of the asymptotic expression (6.3.23) for ψ_1 yields

$$\phi(\underline{r},x) = \frac{1}{2\mu\Sigma_b} \sum_{n=0}^{\infty} S_n Z_n(\underline{r}) \left(\frac{x_o}{x}\right)^{-\lambda_n} \frac{1}{x} \qquad (7.2.9)$$

We now introduce the notation customarily used in age theory. With the assumptions made about the cross sections, we have

$$\tau = \frac{1}{3\xi\Sigma\Sigma_s} \log \frac{x_o}{x} \qquad (7.2.10)$$

$$q(\underline{r},\tau) = \xi \Sigma_s \times \phi(\underline{r},x) \qquad (7.2.11)$$

where τ is the Fermi age, ξ is the average logarithmic energy decrement per collision and q is the slowing down density. We also showed in Chapter V that

$$\lambda_n = \frac{B_n^2}{6\mu\Sigma\Sigma_b} \qquad (7.2.12)$$

In general, we have (37)

$$\Sigma_s = \frac{\Sigma_b}{(1+\mu)^2} \quad ; \qquad \xi = 1 + \frac{(1-\mu)^2}{2\mu} \log \frac{1-\mu}{1+\mu}$$

(7.2.13); (7.2.14)

and for small μ

$$\xi \Sigma_s \approx 2\mu \Sigma_b \qquad (7.2.15)$$

By (7.2.10) through (7.2.15), (7.2.8) becomes:

$$g(\underline{r},\tau) = \sum_{n=0}^{\infty} S_n Z_n(\underline{r}) e^{-B_n^2 \tau} \qquad (7.2.16)$$

which is exactly the result of age theory.

We notice that if, as a result of the discussion in Chapter IV, the Wilkins approximation is used for light moderators, it is then convenient to replace $\mu \Sigma_b$ by $\xi\Sigma_s/2$ in order to have the correct asymptotic behavior. Then we should use

$$\Delta = \frac{4\,\Sigma_o}{\xi\,\Sigma_s} \quad ; \qquad \lambda_n = \frac{DB_n^2}{\xi\,\Sigma_s} \tag{7.2.17}$$

Since the assumptions about the cross sections are certainly not valid at energies large compared with thermal, we shall obtain a more accurate expression for the flux if $x_o^{-\lambda_n}$ is replaced by $e^{-B_n^2\tau_o}$, where τ_o is now the age of source neutrons to the energy kT, calculated with the assumption that the spectrum is 1/E in the range from epithermal down to kT.

Taking into account these considerations, we write instead of (7.2.8)

$$\phi(\underline{r},x) = \frac{1}{\xi\,\Sigma_s} \sum_{n=0}^{\infty} \frac{S_n e^{-B_n^2\tau_o}}{Q(\lambda_n,\Delta)}\, Z_n(\underline{r})\, x e^{-x}\, \psi_1(\lambda_n,\Delta;x^{1/2}) \tag{7.2.18}$$

where λ_n and Δ are given by (7.2.17).

Several considerations regarding (7.2.18) are of interest: We note firstly that if the source neutrons are distributed according to the lowest spatial mode $Z_o(\underline{r})$, then the spectrum is given simply by $xe^{-x}\psi_1(\lambda_o,\Delta;x^{1/2})$.

Secondly we note that even if the above statement is not true, the spectrum will still be represented with good accuracy by $xe^{-x}\psi_1(\lambda_o,\Delta;x^{1/2})$ if the dimensions of the system are sufficiently small compared with the

square root of the age. Mathematically, if

$$S_1 e^{-B_1^2 \tau_o} << S_o e^{-B_o^2 \tau_o} \qquad (7.2.19)$$

then the lowest mode represents the flux well.

In the case of a slab of width 2a with a plane source at the center, the criterion (7.2.19) becomes:

$$e^{-\frac{9\pi^2}{4}\frac{\tau_o}{a^2}} << e^{-\frac{\pi^2}{4}\frac{\tau_o}{a^2}} \qquad (7.2.20)$$

Table 7.1 gives the value of 2a for different moderators such that the contribution of the second harmonic to (7.2.18) is only 10% of the fundamental. The source is assumed to be a fission source. It should be noted that a plane source is much richer in harmonics

Table 7.1

Dimensions of a slab for 10% contribution of the second harmonic to the spectrum, in usual moderators.

Moderator	Width of the Slab
Water	34 cm
Heavy Water	64 cm
Beryllium	58 cm
Graphite	110 cm

than an extended source with reasonable spatial dependence.

It should also be noted that the value of 10% given for the contribution of the second harmonic is an upper limit valid for energies a few times greater than the thermal energies. The actual contribution to lower energies is somewhat less because of the preferential leakage of neutrons in the higher spatial modes. This fact is illustrated in Fig. 7.1 where the spectrum for the fundamental and second harmonic, for a case approximately that of beryllium given in Table 7.1, has been plotted.

3. The Infinite Medium with a Plane Source

When the size of the assembly becomes large compared with the slowing down length, the separation between the spatial eigenvalues becomes very small. When the medium becomes infinite in extent, the spectrum of eigenvalues becomes continuous and equation (7.2.18) is no longer valid. We can, however, transform (7.2.18) into an integral performing the limiting process customary in such cases. We are going to perform such a limiting process in the special case of an infinite medium with a plane source. As it is well known (38), the solution for a point source- and therefore for any source- can be derived from the plane source solution.

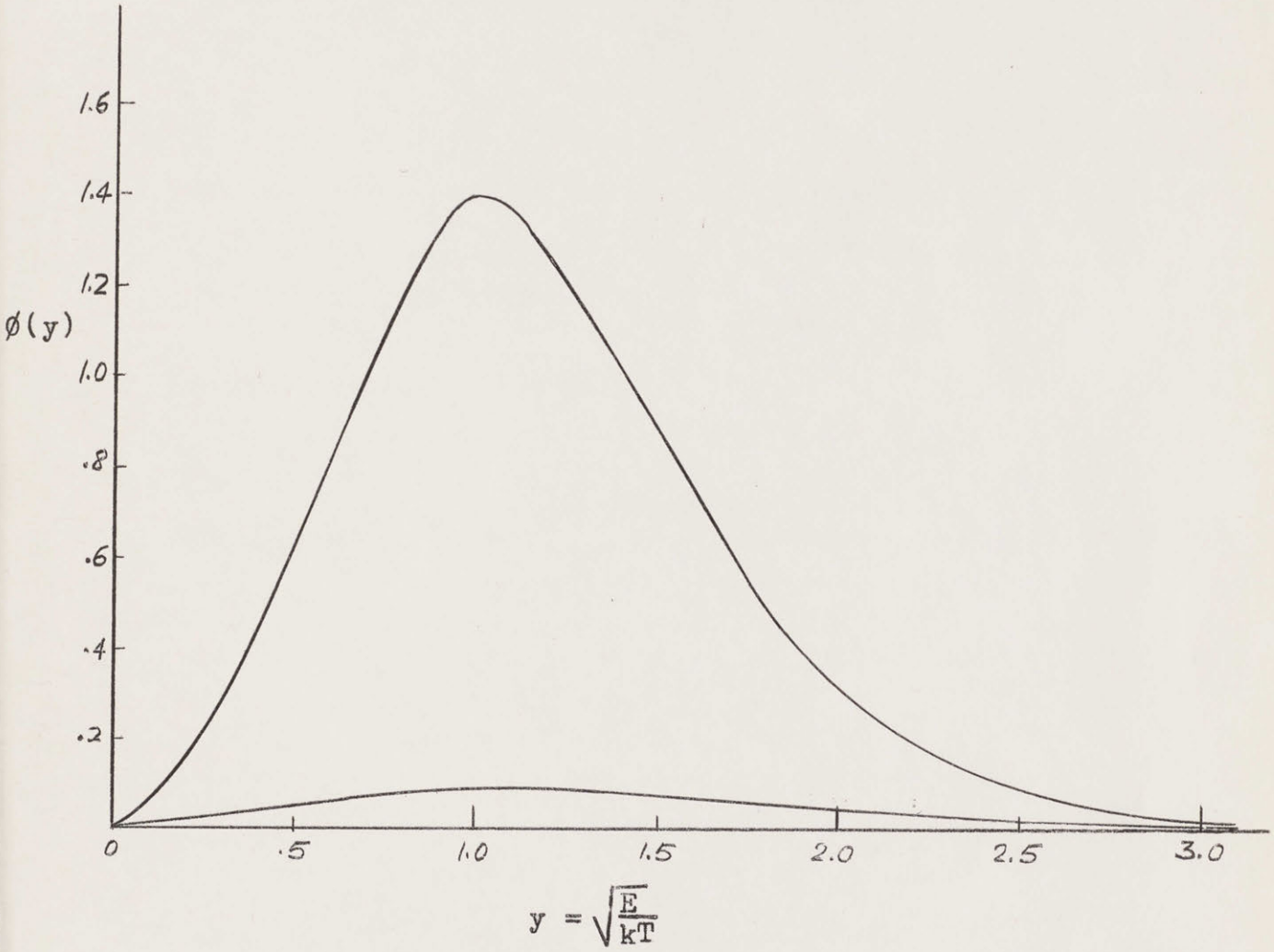

Figure 7.1

Comparison of the spectra of the fundamental and second harmonic in a slab of beryllium, for $\Delta = 0.1$ and 68 cm. thick.

Let us consider a plane slab of width 2a with a plane source of unit strength at the center. Let the z axis be directed normal to the plane of symmetry. The buckling B_n^2 is given by

$$B_n^2 = \left(\frac{2n+1}{2}\,\frac{\pi}{a}\right)^2 \qquad (7.3.1)$$

and the corresponding normalized eigenfunctions by

$$Z_n(z) = \frac{1}{\sqrt{a}} \cos\left[\frac{(2n+1)\pi}{2}\,\frac{z}{a}\right] \qquad (7.3.2)$$

Equation (7.2.18) becomes

$$\phi(z,x) = \frac{1}{\xi\Sigma_s}\,\frac{xe^{-x}}{a} \sum_{n=0}^{\infty} \frac{\exp -\left[\left(\frac{2n+1}{2}\,\frac{\pi}{a}\right)^2 \tau_o\right]}{Q\left[\frac{D}{\xi\Sigma_s}\left(\frac{2n+1}{2}\,\frac{\pi}{a}\right)^2, \Delta\right]} \cos\left[\frac{(2n+1)\pi}{2}\,\frac{z}{a}\right] *$$

$$* \psi_1\left[\frac{D}{\xi\Sigma_s}\left(\frac{2n+1}{2}\,\frac{\pi}{a}\right)^2, \Delta;\ x^{1/2}\right] \qquad (7.3.3)$$

Let

$$\frac{D}{\xi\Sigma_s} = \beta^2 \quad ; \qquad \frac{2n+1}{2}\,\frac{\pi}{a} = k \qquad (7.3.4)$$

We now make $a \to \infty$, the slab becomes an infinite medium. With the definitions (7.3.4), (7.3.3) becomes

$$\phi(z,x) = \frac{1}{\xi\Sigma_s\pi} \int_0^{\infty} dk \cos kz\, \frac{e^{-k^2\tau_o}}{Q(\beta^2k^2, \Delta)}\, xe^{-x} \psi_1(\beta^2k^2, \Delta; x^{1/2}) \qquad (7.3.5)$$

which is the answer to our problem.

The evaluation of the integral in (7.3.5), in closed form seems hopeless. Some approximations, however, can be made. We note first that for energies a few times greater than kT the function $\psi_1(\beta^2k^2,\Delta;x^{1/2})/Q(\beta^2k^2,\Delta)$ varies slowly compared with $e^{-k^2\tau_o}$. This fact follows immediately from the consideration of the asymptotic behavior, (6.3.23), of ψ_1. For low values of x, it may be seen from (A.1) that $Q(\beta^2k^2,\Delta)$ changes to first order linearly in β^2k^2 while the function ψ_1 is rather insensitive to changes in β^2k^2, as can be seen from the tabulations in Appendix B and the series (6.2.5).

Disregarding changes in ψ_1/Q for small values of k which are the values that contribute mostly to the integral (7.3.5), we may write

$$\phi(z,x) \quad \frac{1}{2\pi\xi_1\Sigma_s}\sqrt{\frac{\pi}{\tau_o}}\; e^{-\frac{z^2}{4\tau_o}}\; xe^{-x}\; \frac{\psi_1(o,\Delta;x^{1/2})}{Q(o,\Delta)} \tag{7.3.6}$$

so that to first approximation the spectrum is the same as the spectrum in an infinite homogeneous medium.

In order to find the limits of validity of (7.3.6) we compare first the asymptotic form of (7.3.6) with the result of age theory, namely

$$\phi(z,x) = \frac{1}{2\pi\xi\Sigma_s}\,\frac{1}{x}\sqrt{\frac{\pi}{\tau}}\; e^{-\frac{z^2}{4\tau}} \qquad (7.3.7)$$

From (6.3.23) it is seen that both results are identical if the energy is such that the difference between the age τ corresponding to it and the age τ_o corresponding to the energy kT can be neglected. This difference for ordinary moderators is less than 10% for energies less than 5 kT. If τ_o is replaced by τ in (7.3.6) the correctness of the asymptotic behavior is insured at the cost, however, of introducing large errors for energies less than kT.

We are now interested in finding the limit of validity of (7.3.7) for energies smaller than kT. As was remarked above, ψ_1 is quite insensitive to changes in β^2k^2 for small βk. To find the first order correction to (7.3.6) we take into account the first order change in $Q(\beta^2k^2,\Delta)$ for changes in β^2k^2. We may write for small λ and Δ (A.1)

$$Q(\lambda,\Delta) \approx \lambda + \frac{\sqrt{\pi}}{8}\Delta \qquad (7.3.8)$$

With these assumptions, we may write instead of (7.3.5)

$$\phi(z,x) = \frac{4}{\xi\Sigma_s}\, xe^{-x}\psi_1(o,\Delta;x^{1/2})\,\frac{8}{\sqrt{\pi}\,\Delta}\int_0^\infty dk\,\cos kz\; e^{-k^2\tau_o} * \left[1 - \frac{8\beta^2}{\sqrt{\pi}\,\Delta}\,k^2\right] \qquad (7.3.9)$$

where we have assumed $\beta^2 k^2 \ll \frac{\pi}{8}\Delta$. If the term cos kz is also expanded in a power series in kz, (7.3.9) can easily be integrated to give the expression

$$\phi(z,x) = \frac{4}{\xi\Sigma_s} x e^{-x} \frac{\psi_1(o,\Delta;x^{1/2})}{Q(o,\Delta)} \sqrt{\frac{\pi}{\tau_o}}\, e^{-\frac{z^2}{4\tau_o}} \left(1 - \frac{4\beta^2}{\sqrt{\pi}\,\Delta}\,\frac{1}{\tau_o}\right) \tag{7.3.10}$$

valid for small Δ and small $z^2/4\tau_o$. Comparing (7.3.10) with (7.3.6), we see that, at least for small absorption parameter Δ and distances from the source small compared with the slowing down length τ_o, (7.3.6) is valid if $4\beta^2/\sqrt{\pi}\,\Delta\tau_o \ll 1$. Taking into account the definitions of Δ (7.2.17) and β^2 (7.3.4), we conclude that under the conditions stated the approximation (7.3.6) is valid, for energies less than kT, only if

$$\frac{D}{\Sigma_o} \ll \tau_o \tag{7.3.11}$$

This condition is not always satisfied by ordinary moderators even for $\Delta \sim 0.3$, a value that can be considered typical of a thermal reactor, and care must be exercised in designing an experiment not to distort the lower part of the spectrum.

The physical interpretation of (7.3.12) is immediate. D/Σ_o is a measure of the distance the

neutrons diffuse before being absorbed, while τ_o is a measure of the distance the neutrons travel before reaching thermal energies. Equation (7.3.12) is an expression of the fact that neutrons produced by a plane source should not travel too far from the source before being moderated if their energy spectrum is to be well represented by the spectrum corresponding to a source infinite in extent.

Another limitation of (7.3.6) is that $z \ll \Sigma_\tau$. This limitation is the limitation of age theory, which (7.3.6) approaches asymptotically.

4. Comparison with Experimental Results

Extensive measurements have been made in water systems to determine the energy distribution of neutrons. Spectral measurements in other systems have been directed towards other goals. Unfortunately no measurements have been made to investigate the influence of leakage in the spectrum. The experiments have been designed with the specific purpose of obtaining the spectra for infinite homogeneous media.

The application of our theory, based in the Wilkins approximation, to water systems is justified by the fact that this approximation satisfies the detailed balance and conservation conditions as discussed in Chapter III. That the Wilkins equation may be applied

to water was first suggested by Greeber (41), who compared the results of a Wilkins calculation with a spectrum obtained by Poole (40) in borated water.

In order to test the applicability more thoroughly, we have compared several spectral parameters with experimental results and also with the calculations done by Amster (52) using a Wigner and Wilkins model. The experimental results are due to Poole (40).

The results of the comparison are shown in Table 7.2. The temperature of the moderator is given by kT in ev. The experimental spectra were fit by least squares in the slow energy range by a maxwellian with a most probable energy of E_o, and in the high energy range by a 1/E distribution. The maxwellian was normalized so that the total area under it was unity. With this normalization, the spectrum behaves asymptotically like C/E.

We have calculated the temperature E_o in the same way, and the constant C by the relation

$$C = \frac{Q}{x_o} \frac{e}{\phi(x_o)} \qquad (7.4.1)$$

where Q is the joining factor discussed before, $x_o = E_o/kT$ and $\phi(x)$ the calculated flux. The value of Δ used was obtained from the free atom value of the quantity $\xi\Sigma_s$. In all cases we took $\lambda = 0$.

σ_a barns per H atom	Δ	kT e.v.	E_o meas. ev ±10%	E_o calc. Wilkins	E_o calc. Amster	C meas. ± 10%	C. calc. Wilkins	C calc. Amster
1.5	0.291	0.0251	0.026	0.0271	0.0261	0.067	0.0671	0.072
2.9	0.563	0.0251	0.027	0.0292	0.0276	0.130	0.133	0.139
3.73	0.725	0.0251	0.029	0.0304		0.13	0.175	0.18
4.55	0.884	0.0251	0.032	0.0317	0.0294	0.214	0.216	0.215
3.03	0.588	0.0318	0.037	0.0372	0.0360	0.121	0.141	0.125
4.54	0.881	0.0318	0.037	0.0401	0.0390	0.136	0.207	
7.6	1.477	0.0319	0.0432	0.046	0.0390	0.328	0.38	0.34

Table 7.2

Comparison of Experimental and Theoretical Determinations of Spectra Parameters in Homogeneous Water Systems.

From the table it is seen that both theoretical models represent the experimental results well.

In performing the computations, the calculated value of E_o was seen to obey the relation

$$E_o = kT(1 + 0.30\Delta) \qquad (7.4.2)$$

This result should not be compared with the equation obtained by Coveyou et al (53) using the Wigner and Wilkins model

$$E_o = kT(1 + 0.49\Delta) \qquad (7.4.3)$$

The reason is that they fitted points up to energies of 7.2 kT while we have excluded the "non maxwellian region" by taking an upper limit of 2kT in our calculations.

Recently, Stone and Slovacek (39) have measured the neutron spectrum in water and closely packed uranium-water lattices. The measurements were performed with a slow chopper. Two spectra were measured in pure water at 298°K and 586°K. The values of Δ were obtained from the measured absorption cross section as 0.0636 and 0.0426 respectively. The experimental results are compared with the theoretical ones in Figs. 7.2 and 7.3. Experiments and theory were made to coincide at 1 ev. A strong disagreement

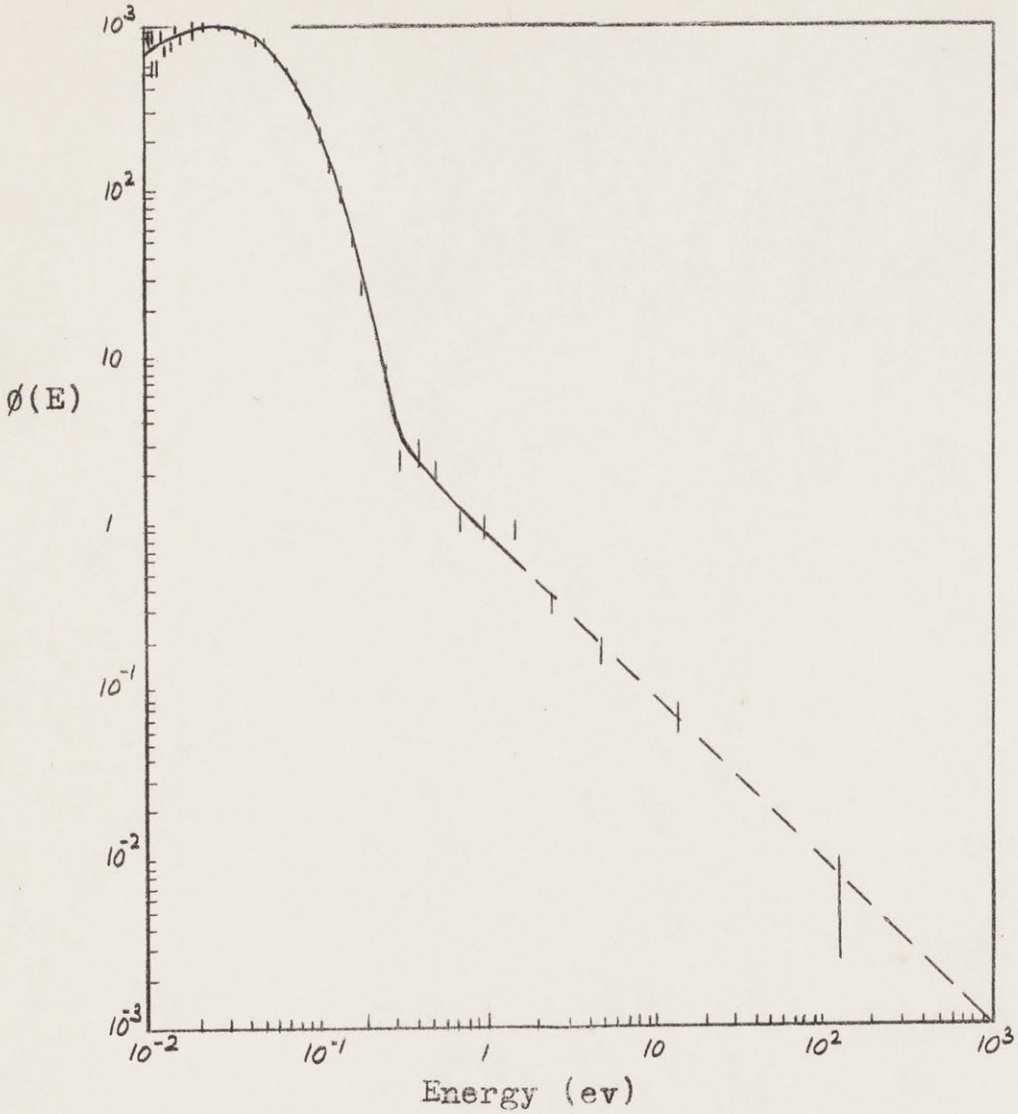

Figure 7.2

Comparison of theoretical and experimental spectra for water at 298°K. The vertical lines are a measure of the statistical experimental error.

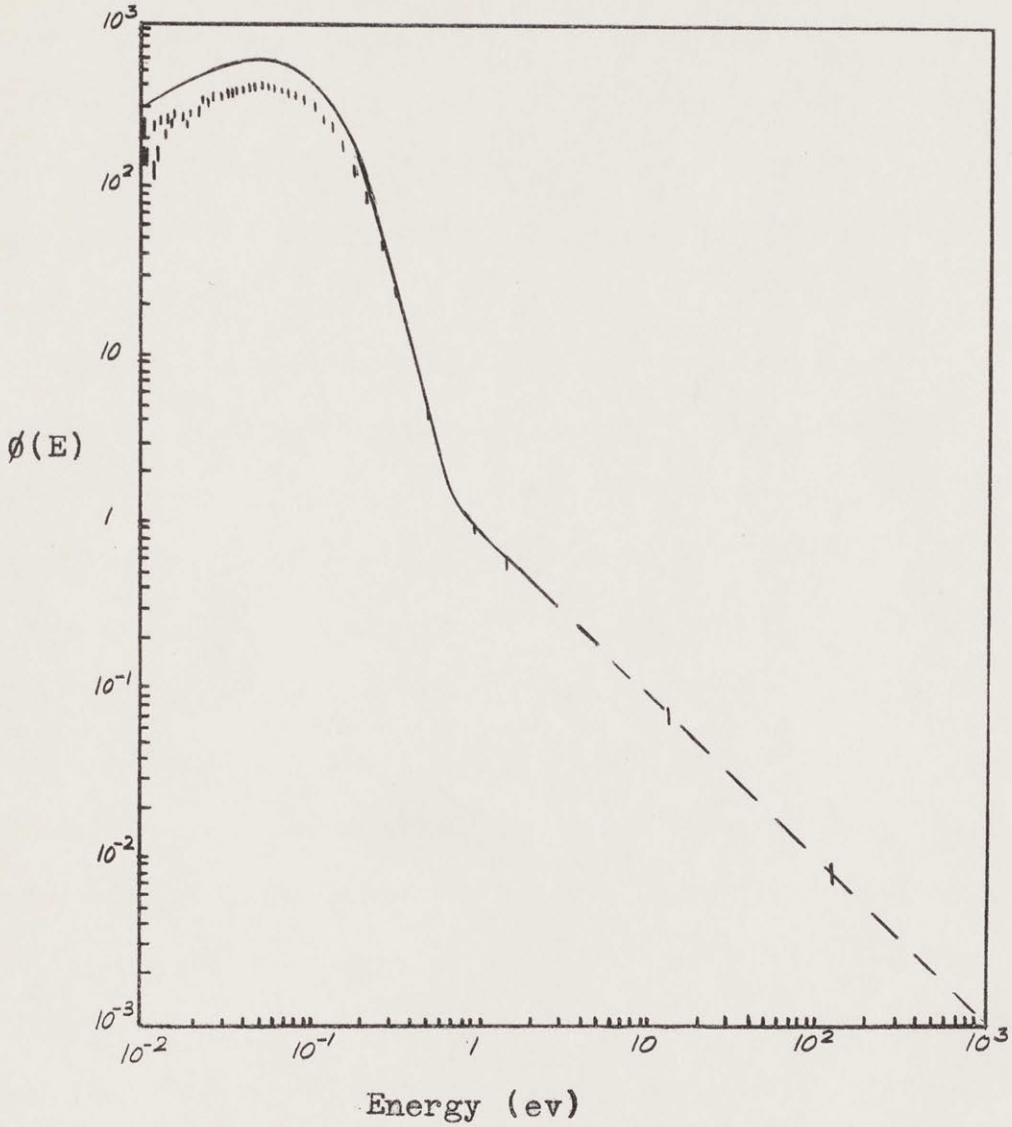

Figure 7.3

Comparison of theoretical and experimental spectra for water at 586°K. The vertical lines are a measure of the experimental statistical error.

is seen at 586°K. However, because of the smallness of the high energy component of the spectrum, a small error in the measurement of the absorption cross section will cause a large relative error in the magnitude of the tail. A similar disagreement was obtained by the authors when they compared the results with a Wigner and Wilkins calculation.

Two spectra were measured also by the same authors in a closely packed uranium water lattice. The uranium was 0.0013 in. thick and clad in zircalloy. Measurements were performed at 298° and 586°K. Because of the thinness of the fuel, the assembly can be assumed to be homogeneous. From the measured values of the cross sections at the most probable energy, Δ has been calculated as 1.14 at 298°K and 1.12 at 586°K. The buckling was also measured by the experimenters, and from these measurements λ was obtained as 0.0014 and 0.011 respectively. No self shielding correction was applied. The comparison of the experimental spectrum with the theoretical results is shown in Figs. 7.4 and 7.5. The agreement is good in spite of the fact that that the absorption cross section is not "1/v" as assumed in our theory.

Finally, in Fig. 7.6 we have compared the result of a Wigner and Wilkins calculation by Amster -reported in Ref. (48) -with the result of a Wilkins calculation

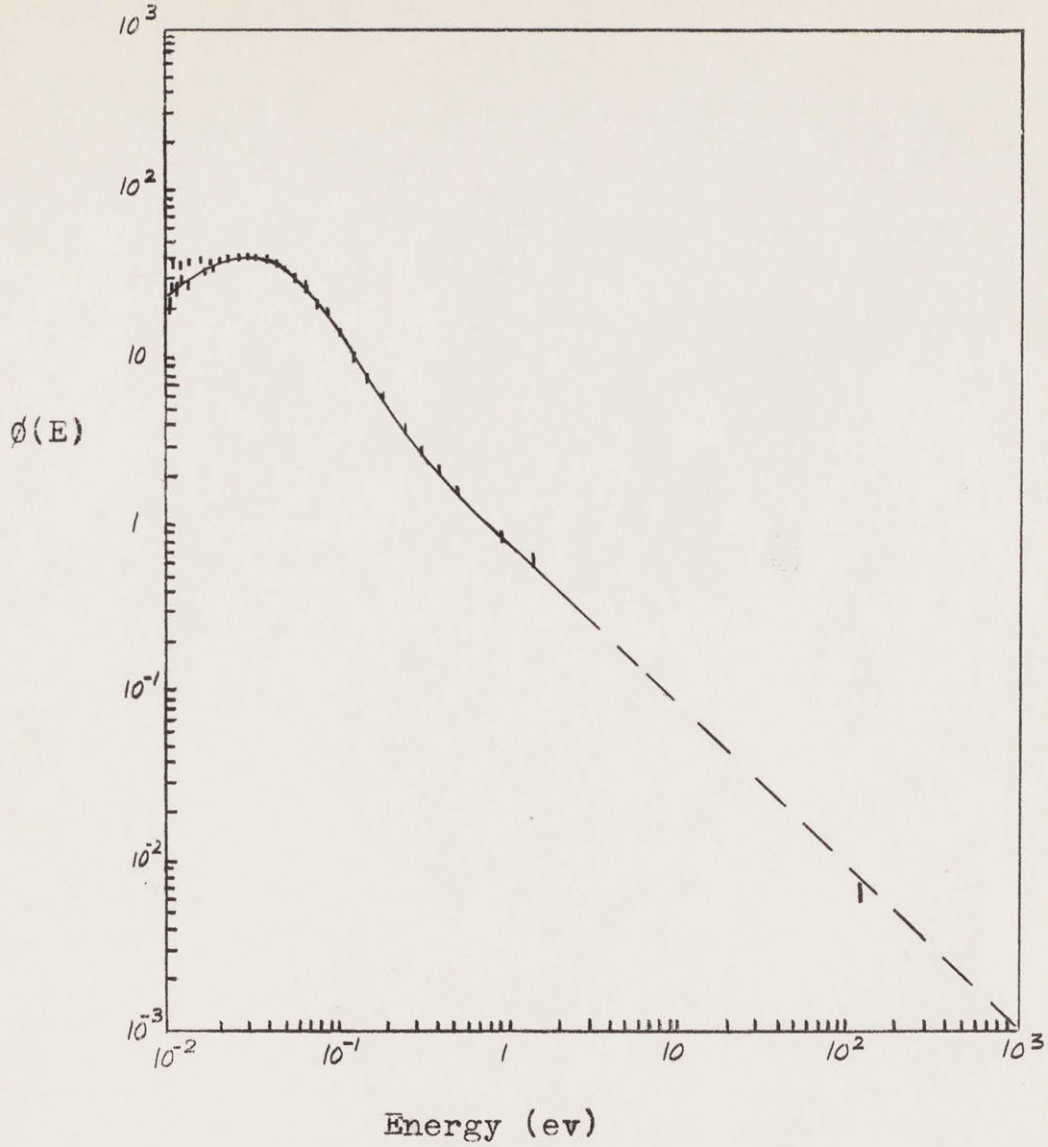

Figure 7.4

Comparison of the theoretical and experimental spectra for a close packed uranium-water lattice at 298°K. The vertical lines are a measure of the statistical experimental error.

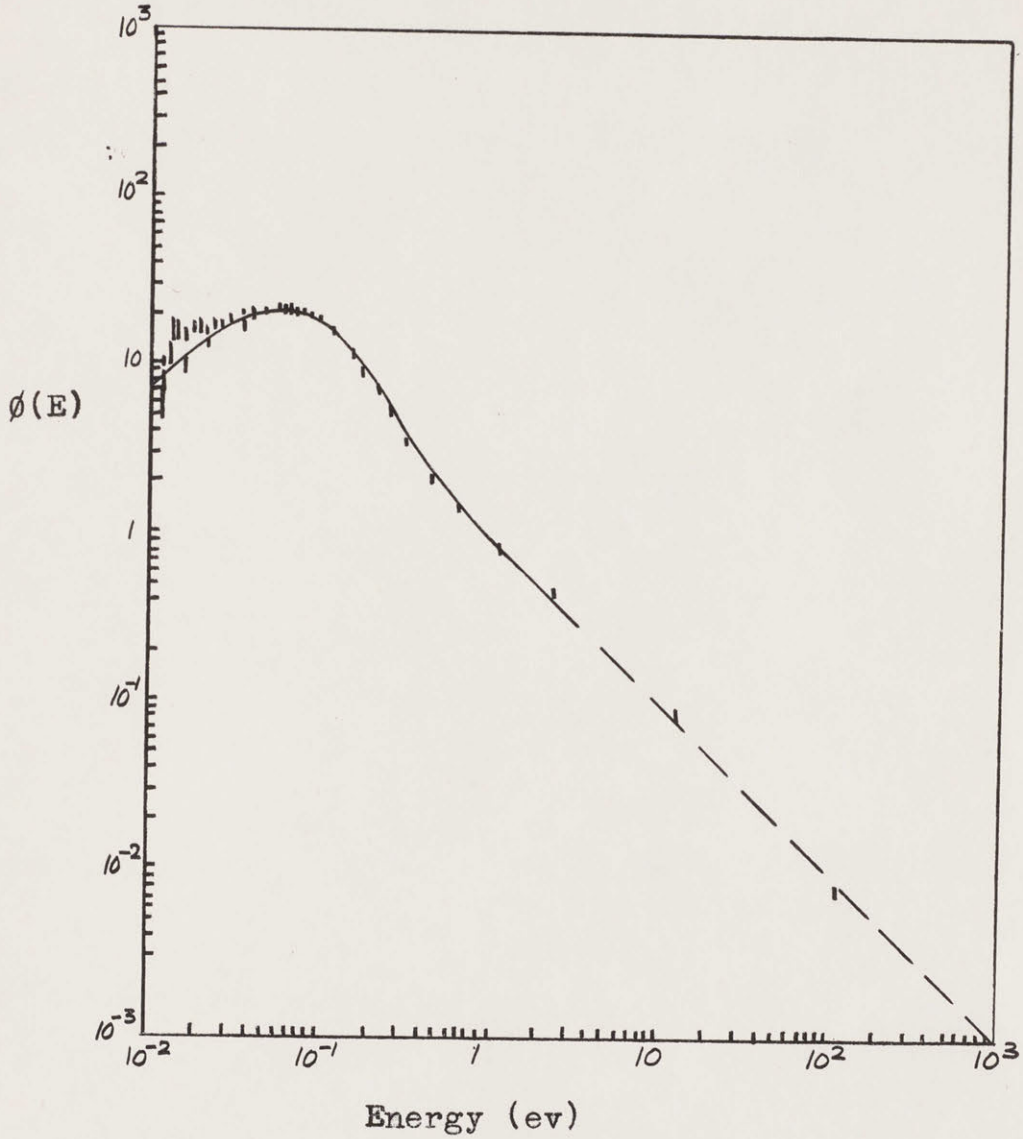

Figure 7.5

Comparison of the theoretical and experimental spectra for a close packed uranium-water lattice at 586°K. The vertical lines are a measure of the statistical experimental error.

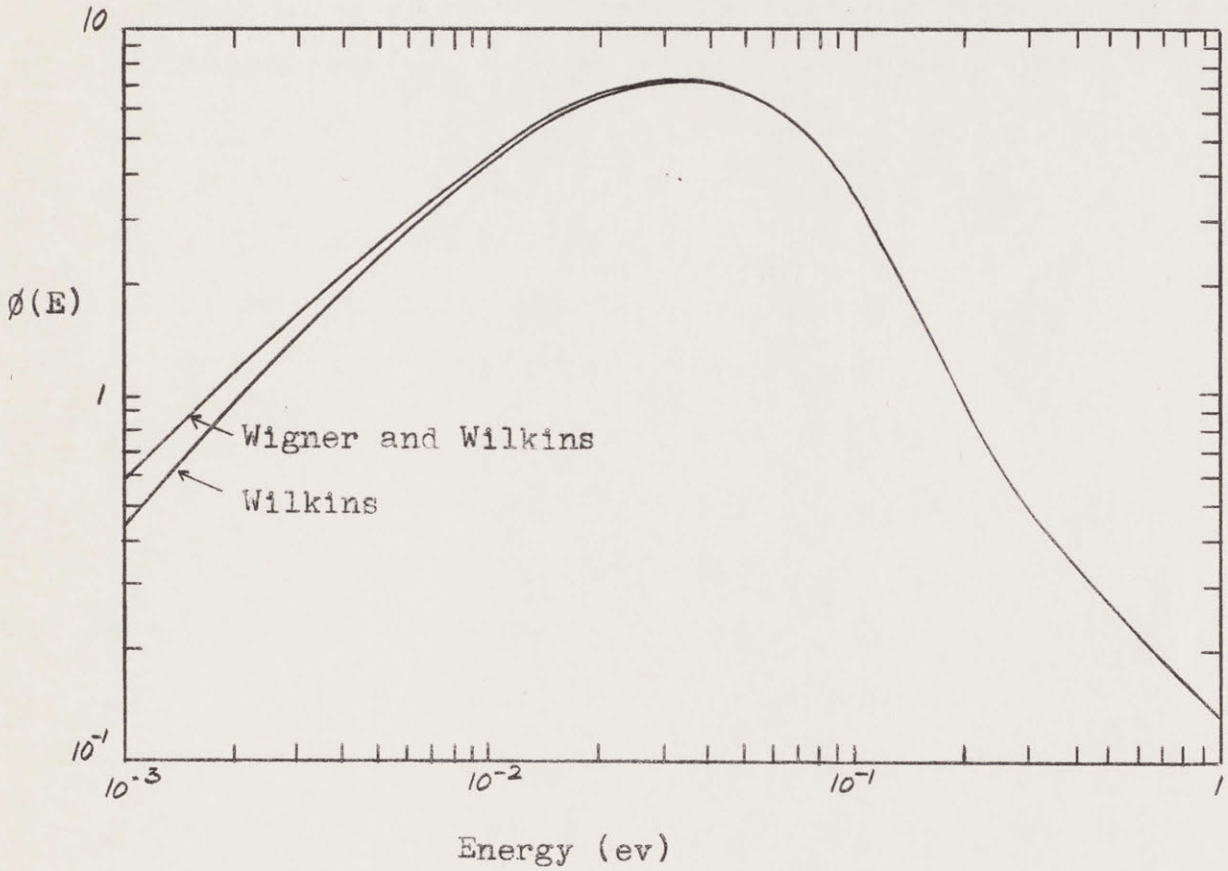

Fig. 7.6

Comparison of a Wigner and Wilkins calculation with a Wilkins calculation for hydrogen at 293°K. $\Delta = 0.8$.

for hydrogen and $\Delta = 0.8$. Both calculations are seen to disagree only in the low energy part of the spectrum. The Wilkins calculation is seen to give a harder spectrum than the gas model. As was explained in Chapter IV for solid moderators, this deviation is in the right direction to account for the effect of chemical binding.

5. Heterogeneous Systems

The cell of a heterogeneous assembly can be considered as a system composed of several media only one of which, the moderator, scatters inelastically. To a very good approximation the fuel, cladding, air channels etc. can be considered not to change the energy of the neutrons. (Systems in which the coolant is water or heavy water and the moderator is a different material cannot be represented by this model.)

In order to treat such a system, the method discussed in Section 5.2 is used. It was shown there that the flux in the moderator can be represented by

$$\phi(\underline{r},x) = 4\pi \sum_{n=0}^{\infty} \varphi_n(x)\, Z_n(\underline{r}) \qquad (7.5.1)$$

where the $Z_n(\underline{r})$ are the spatial eigenfunctions in the moderator and the $\varphi_n(x)$ are the solutions of the equation

$$[\Sigma(x) + \xi\Sigma_s\lambda_n(x)]\,\varphi_n(x) = \int_0^\infty \Sigma(x' \to x)\,\varphi_n(x')\,dx'$$

(7.5.2)

where the source has been assumed to be at very high energies and we have replaced $2\mu\Sigma_b$ by $\xi\Sigma_s$ in accordance with the discussion of Section 7.2. It was also shown there that this approximation is valid as long as the spatial eigenfunctions of the moderator are not very different for different energies. This condition is not satisfied, in general, in a cell of a heterogeneous assembly, because of the change with energy of the nuclear properties of the fuel. We expect, however, to obtain a reasonably accurate spectrum in the thermal region by considering suitably averaged properties of the fuel.

In order to compute the spatial eigenvalues corresponding to the moderator eigenfunctions, we shall use diffusion theory in the moderator with an extrapolation distance at the boundary of the fuel computed by transport theory. We shall restrict our spatial calculations to cylindrical geometry. The modifications for other simple geometries are obvious.

Let the outer radius of the cell be r_1 and the outer radius of the rod r_0. With the usual boundary condition that the gradient of the flux vanishes at the outer boundary of the cell, the spatial eigenfunctions

are given by

$$Z_n(r) = -N_1(B_n r_1)J_o(B_n r) + J_1(B_n r_1)N_o(B_n r) \tag{7.5.3}$$

The notation for the Bessel functions is as in ref. (42). Using the boundary condition at the surface of the cell, we obtain

$$dB_n = - \frac{N_1(B_n r_1)J_o(B_n r_o) - J_1(B_n r_1)N_o(B_n r_o)}{N_1(B_n r_1)J_1(B_n r_o) - J_1(B_n r_1)N_1(B_n r_o)} \tag{7.5.4}$$

which determines B_n. Here d is the linear extrapolation distance. If $B_n r_o$ and $B_n r_1 \lesssim 1$, (7.5.4) can be simplified using the expansions for the Bessel functions, the result is

$$B_n^2 = \frac{2}{\frac{d}{r_o}(r_1^2 - r_o^2) + r_1^2\left[\frac{r_1^2}{r_1^2 - r_o^2}\log\left(\frac{r_1}{r_o}\right) - \frac{3}{4} + \left(\frac{r_o}{2r_1}\right)\right]^2} \tag{7.5.5}$$

For the linear extrapolation distance d we use the results obtained by Kushneriuk and McKay (43) from a variational method in conjunction with the integral Boltzmann equation.

It is interesting to compute the limiting value of

B_n^2 when the rods are very thin compared with their mean free path. In this case we have (43)

$$d = \frac{2}{3r_o\Sigma_{ao}\Sigma_1}(1 + r_o\Sigma_{ao}) + \frac{r_o}{4}(\log 2r_o\Sigma_1 + 0.077) \qquad (7.5.6)$$

here Σ_{ao} is the absorption cross section of the fuel and Σ_1 the transport cross section of the moderator. If $r_o\Sigma_{ao}$ is sufficiently small, we may write instead of (7.5.5)

$$B_n^2 = \frac{2}{\frac{2}{3\Sigma_{ao}\Sigma_1}\frac{r_1^2 - r_o^2}{r_o^2} + r_1^2\left[\frac{r_1^2}{r_1^2 - r_o^2}\log\left(\frac{r_1}{r_o}\right) - \frac{3}{4} + \left(\frac{r_o}{2r_1}\right)\right]^2} \qquad (7.5.7)$$

and in case the second term in the denominator be negligible we get

$$B_n^2 = \frac{3\Sigma_{ao}\Sigma_1 r_o^2}{r_1^2 - r_o^2} \qquad (7.5.8)$$

so that

$$\lambda_n(x) = \frac{DB_n^2}{\xi\Sigma_s} = \frac{1}{\xi\Sigma_s}\frac{\Sigma_{ao}r_o^2}{r_1^2 - r_o^2} \qquad (7.5.9)$$

the quantity in brackets in (7.5.2) becomes then

$$\Sigma_{s1} + \frac{\Sigma_{a1}(r_1^2 - r_o^2) + \Sigma_{ao} r_o^2}{r_1^2 - r_o^2} \qquad (7.5.10)$$

which shows that (7.5.2) amounts to the problem of an infinite homogeneous medium with an absorption cross section very approximately equal to the volume averaged absorption cross sections of fuel and moderator.

In general, if the Wilkins approximation is used and the diffusion approximation to $\lambda_n(x)$ is taken into account, equation (7.5.2) becomes an equation similar to (7.2.4).

$$x \frac{d^2\varphi_n}{dx^2} + x \frac{d\varphi_n}{dx} + (1 - \frac{\Delta}{4x^{1/2}} - \frac{DB_n^2}{\xi \Sigma_s})\varphi_n = - \frac{4\pi s_n}{\xi \Sigma_s} \delta(x-x_o)$$

(7.5.5)

If we are to use the solutions of the equation described in the preceding chapter in order to solve (7.5.5), the energy dependent term $\frac{DB_n^2}{\xi \Sigma_s}$ must be approximated by a function of the form $A + C/x^{1/2}$. Even at energies as large as 10 kT, the absorption cross section is small in natural or slightly enriched uranium. Since the buckling is small at such an energy and decreasing, the term $DB_n^2/\xi\Sigma_s$ must be represented by a function of the type $C/x^{1/2}$. Otherwise, the spectrum will be distorted at such energies. The lower region

of the spectrum will not be much distorted by such a function, since an examination of the tables in Appendix B shows that the form of the functions ψ_1 for $y \lesssim 1$ is fairly insensitive to changes in the parameters.

It is important in performing the approximation mentioned not to destroy neutron conservation so that C must be constrained by the condition

$$C \int_0^\infty x^{-1/2}\, \phi(x)\, dx = \frac{1}{\xi \Sigma_s} \int_0^\infty DB_n^2\, \phi(x)\, dx \qquad (7.5.6)$$

Since the flux is not known we replace it by a maxwellian at the moderator temperature and obtain

$$C = \frac{2}{\sqrt{\pi}} \frac{1}{\xi \Sigma_s} \int_0^\infty DB_n^2\, x e^{-x}\, dx \qquad (7.5.7)$$

With this approximation, the solution of (7.5.5) for high energy sources becomes proportional to

$$x e^{-x} \psi_1(o, \Delta+4C; x^{1/2}) \qquad (7.5.8)$$

(cf. (6.1.3) and (7.2.5) and see (6.2.1)) and can be calculated with the help of the tables given in Appendix B.

Once the spectrum in the moderator is known,

the spatially averaged spectrum in the fuel can be computed by calculating at each energy, the average depression of the flux in the fuel by an of the methods developed for the calculation of the disadvantage factors. In the computations to follow, we have used the integral transport method (45,46) for the calculation of the disadvantage factors.

6. Comparison with Experiments

The only detailed measurements in the fuel and moderator of heterogeneous lattices are, again, in uranium-water lattices.

Two experiments have been selected to compare theory and experiment: a natural uranium-water lattice measured by Mostovoy et al (55) and an enriched uranium-water lattice measured by Poole (40). The parameters of the lattices are described in Table 7.3.

Table 7.3

Parameters of uranium-water lattices

Fuel	r_o cm	r_1 cm	Moderator Temperature	Measurement Method
Natural U.	1.75	2.27	315°K	Slow chopper
1.6% enriched U.	1.52	2.65	293°K	Pulsed source

The transport cross section of water was taken equal to the scattering cross section. The bucklings were obtained as a function of energy by using (7.5.4) in conjunction with the extrapolation distance obtained from the report of Kushneriuk and McKay (43). The cross sections were obtained from the compilation BNL 325. The high values obtained for the lowest buckling in both cases insure that the contribution of all the spatial modes but the lowest is negligible. Calculations were performed in both cases by taking a constant value and a "1/v" for the leakage term DB^2. The resulting parameters, obtained by averaging the energy dependence of DB^2 between 0.01 and 0.3 ev in both cases are shown in Table 7.4.

Table 7.4

Values of λ and Δ used in the computation of the moderator spectrum.

Fuel	Constant Leakage		"1/v" Leakage	
	λ	Δ	λ	Δ
Natural U.	0.20	0.055	0	0.80
Enriched U.	0.098	0.057	0	0.42

In every case the value of $\xi\Sigma_s$ taken was the one corresponding to the free atoms.

Figures 7.7 and 7.8 show the results of the calculations together with the experimental results. The agreement with the moderator spectrum is seen to be very good when the "1/v" leakage is used. The constant leakage overestimates, of course, the high energy tail, since fewer neutrons are allowed to thermalize.

With the moderator spectra calculated from the "1/v" leakage, the spectrum in the fuel was obtained by first calculating, as a function of energy, the depression of the moderator flux near the fuel with respect to the flux in the center of the moderator by means of the formula

$$\frac{\phi(r_o)}{\phi(r_1)} = \frac{N_1(Br_1)J_o(Br_o) - J_1(Br_1)N_o(Br_o)}{N_1(Br_1)J_o(Br_1) - J_1(Br_1)N_o(Br_1)} \qquad (7.6.1)$$

By virtue of the properties of the Bessel functions, (7.6.1) can be reduced to

$$\frac{\phi(r_o)}{\phi(r_1)} = \frac{\pi Br_1}{2}\left[J_1(Br_1)N_o(Br_o) - N_1(Br_1)J_o(Br_o)\right] \qquad (7.6.2)$$

The expression for the fuel disadvantage factor $\phi(r_o)/\phi_o$ is given by the integral transport method (45,46) and may be used to calculate the average spectrum in the fuel.

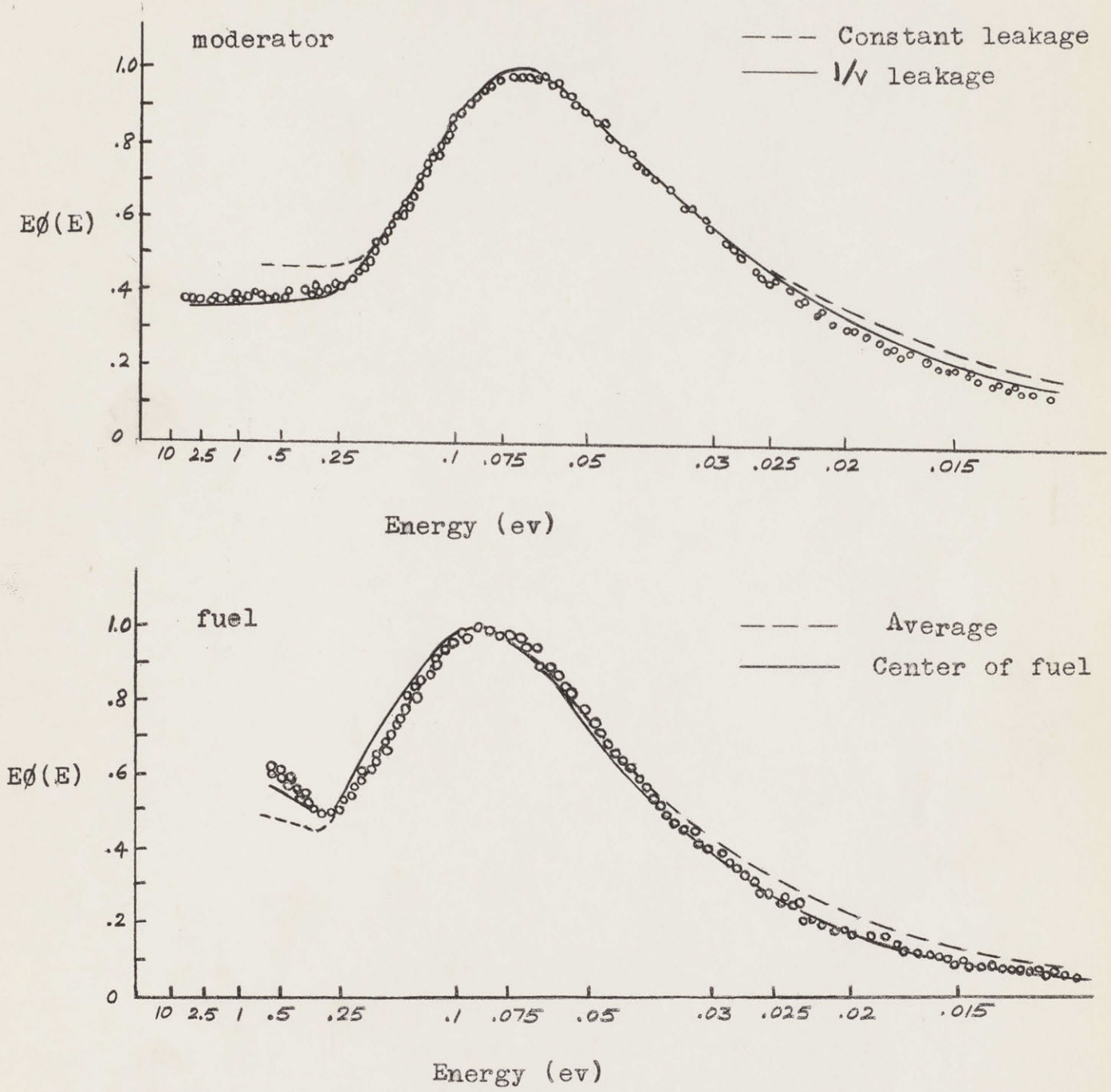

Figure 7.7. Comparison of theoretical and experimental spectra in the moderator and fuel of a natural uranium-water lattice.

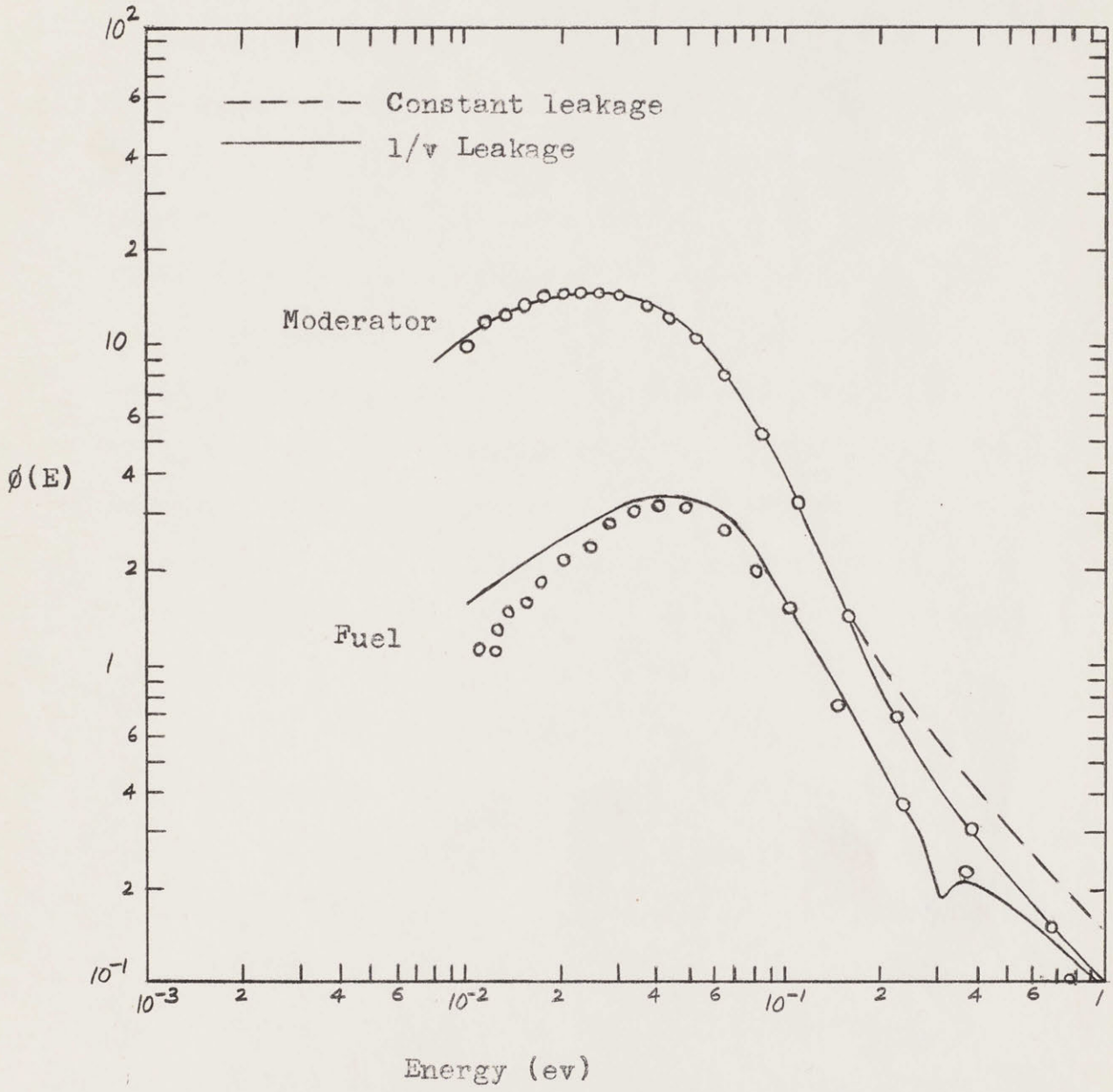

Fig. 7.8. Comparison of theoretical and experimental spectra in moderator and fuel of a slightly enriched uranium-water lattice.

The result is shown in broken lines in the lower part of Fig. 7.7 for the natural uranium lattice. In this experiment a very thin collimator was used and, therefore, the measured spectrum in the fuel is probably a good representation of the spectrum in the center of the fuel. To estimate it, we have assumed that the spatial dependence in the fuel is given by $J_o(\varkappa r)$ and we have adjusted $\varkappa$ at each energy to yield the correct disadvantage factor. The result of the calculation is shown in solid lines in the lower part of Fig. 7.7. The agreement with the experimental results is seen to be good. However, not much significance is attributed to this fact because, as found by Poole, the measured spectrum in the fuel depends on the direction along which the neutron beam is taken.

The calculated average spectrum in the fuel of the enriched uranium lattice is shown in Figure 7.8. The spectrum in the center of the fuel calculated by the method used before gives a spectrum considerably more depressed in the low energy region. We, however, feel that the representation of the spatial dependence of the flux by a function of the form $I_o(\varkappa r)$ is inadequate in the lower energy region where the ratio of the scattering to the total cross section is of the order of 10%. The lack of information about the disposition and size of the collimator used in the experiment also makes difficult the interpretation of the measured spectrum in the fuel.

Chapter VIII

CONCLUSIONS AND RECOMMENDATIONS

1. Conclusions

The influence of the chemical binding in the asymptotic part of the thermal neutron spectra has been studied for isotropic and anisotropic, infinite, homogeneous, solid moderators. Calculations have been performed for beryllium and graphite at 300°K and 600°K. The effect of chemical binding at these temperatures is particularly marked in graphite because of the high Debye temperature of the vibrations in the lattice planes. The theoretical results have been compared with the Wilkins approximation, and it was found that this approximation in the range of energies considered constitutes an improvement over the gaseous model.

The problem of determining the spatial and energy dependence of the neutron flux in finite moderators has been considered, and the Wilkins approximation for the scattering kernel has been used. The solutions of the pertinent differential equation have been studied, calculated numerically, and tabulated. Applications to homogeneous and heterogeneous systems have been studied and the results compared with experiments, when possible. From the comparisons, it is concluded that the theory can be applied to water systems in the range of absorption

practically used in reactor applications. The theory also predicts accurately the neutron spectra in the moderator of natural or slightly enriched uranium lattices. Within the range of validity of the methods used for the calculation of disadvantage factors, the theory can also be used to calculate the average spectrum within the fuel.

The main advantage of the theory is the simplicity of its application. With the tables given, spectrum calculations can be performed with reasonable accuracy without having to resort to expensive machine calculations.

2. Recommendations for Future Study

Further experimental work is necessary to check the validity of the theory in systems with moderators different from water.

On the theoretical side the Feynman-Welton method can be used to obtain accurate machine calculations of spectra in lattices. The assumption of a fuel that does not scatter neutrons inelastically is very probably a very good one. These hypotheses yield a solution in separated form: each term in an infinite sum involves two factors, one of which depends only on the energy, and the other of which depends on the neutron position and contains the energy as a parameter.

The use of the eigenfunctions W_n in the diffusion cooling problem, instead of Laguerre polynomials, should also be investigated in order to improve the theoretical calculations of the diffusion cooling constant.

Finally the representation of the energy dependence of the spectrum in terms of a series of the eigenfunctions W_n is also of interest. The series is very poor for representing the spectrum at energies a few times greater than kT, but for lower energies a good agreement may be obtained with only a few terms.

We conclude by noting the direct applicability of the equation studied in Chapter VI to the study of the time behavior of a Lorentz gas with constant cross section.

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Appendix A

THE CALCULATION OF THE JOINING FACTOR

The direct calculation of the joining factor $Q(\lambda,\Delta)$ can be performed by means of the expression (6.4.14). In the explicit calculation we have neglected terms of order higher than λ^2, Δ^2, or $\lambda\Delta$. The resulting formula is adequate for most practical purposes.

For λ small the Γ-functions appearing in (6.4.14) that depend on λ can be expanded, in general, in a Laurent series around the point $\lambda = 0$. If only the dominant terms are taken into account, the result is

$$Q(\lambda,\Delta) = \lambda + \gamma\lambda^2 + \Delta\frac{\sqrt{\pi}}{8}\left[1 + \lambda(\gamma + 2\log 2 + g)\right] + h\Delta^2 + \ldots \tag{A.1}$$

where the constants g and h are given by

$$g = \frac{2}{\sqrt{\pi}} \sum_{p=1}^{\infty} \frac{\Gamma(p + \frac{3}{2})\Gamma(p)}{\Gamma(p + 2)\Gamma(p+1)} \tag{A.2}$$

and

$$h = \frac{\sqrt{\pi}}{32} \sum_{p=1}^{\infty} \frac{\Gamma(p+1)\Gamma(p - \frac{1}{2})}{\Gamma(p + \frac{3}{2})\Gamma(p + \frac{1}{2})} \tag{A.3}$$

Here, $\gamma = 0.57722\ldots$ is Euler's constant. The series (A.2) can be summed by noting its relationship with the hypergeometric function (32). We have

$$g = \lim_{\epsilon \to 0} \frac{2}{\sqrt{\pi}} \frac{\Gamma(\frac{3}{2})\Gamma(\epsilon)}{\Gamma(2)} \left[F(\tfrac{3}{2}, \epsilon ; 2; 1) - 1 \right]$$

$$= \lim_{\epsilon \to 0} \Gamma(\epsilon) \left[\frac{\Gamma(2)\Gamma(\frac{1}{2} - \epsilon)}{\Gamma(\frac{1}{2})\Gamma(2 - \epsilon)} - 1 \right]$$

$$= \frac{\Gamma'(2)}{\Gamma(2)} - \frac{\Gamma'(\frac{1}{2})}{\Gamma(\frac{1}{2})} = 1 + 2 \log 2 \qquad (A.4)$$

The series (A.3) is related to a higher order confluent hypergeometric function and its sum is not known. Numerical evaluation yields

$$h = 0.1770... \qquad (A.5)$$

(A.1) may be written more explicitly

$$Q(\lambda, \Delta) = \lambda(1 + \gamma\lambda) + \Delta\frac{\sqrt{\pi}}{8} \left[1 + \lambda(1 + \gamma + 4\log 2) \right] + h\Delta^2 + ... \qquad (A.6)$$

As a result of the method used for the numerical determination of the solutions $\psi_1(\lambda, \Delta, y)$ of the differential equation (6.2.3), discussed in Appendix B, the corresponding values of $Q(\lambda, \Delta)$ were obtained. These agree with the results of formula (A.1) within 2% for values of Δ up to about 0.3 and values of λ up to about 0.05.

Tables A.1 and A.2 give values of $Q(\lambda, \Delta)$ calculated numerically from the solution of the differential equation.

Table A.1

VALUES OF THE JOINING FACTOR $Q(\lambda, \Delta)$

$\Delta \backslash \lambda$	0.0	0.01	0.02	0.03	0.04	0.05
0.1	0.0240	0.0351	0.0462	0.0575	0.0689	0.0804
0.2	0519	0641	0763	0887	1011	1137
0.3	0842	0975	1109	1244	1380	1517
0.4	1214	1359	1506	1653	1801	1951
0.5	1639	1798	1958	2118	2280	2442
0.6	2124	2297	2470	2645	2821	2997
0.7	2674	2862	3051	3241	3431	3623
0.8	3296	3500	3705	3911	4118	4325
0.9	4786	4219	4441	4664	4888	5112

Table A.2

VALUES OF THE JOINING FACTOR $Q(\lambda, \Delta)$

$\Delta \backslash \lambda$	0.0	0.2	0.4	0.6
0.4	0.121	0.427	0.738	1.021
0.8	0.330	0.748	1.156	1.514
1.6	1.187	1.931	2.604	3.148

It is also possible to solve the equation $Q(\lambda,\Delta) = 0$ that determines the eigenvalues. To this end, we note that as $\Delta \to 0$ the corresponding values of λ that satisfy the eigenvalue equation are 0, -1, -2, ..., since the equation, for $\Delta = 0$, becomes the Laguerre equation. For small Δ we may, therefore, write

$$\gamma_n = -n + a_n\Delta + b_n\Delta^2 + \ldots \qquad (A.6)$$

where γ_n is the nth eigenvalue for fixed Δ.

Substituting expression (A.6) into the eigenvalue equation, expanding the Γ-functions around $\Delta = 0$ and identifying coefficients of the power series in Δ one obtains after considerable, though straightforward, algebra.

$$a_n = -\frac{1}{4\pi}\sum_{p=1}^{n+1}\frac{\Gamma(p+\frac{1}{2})\Gamma(p-\frac{1}{2})\Gamma(n-p+\frac{3}{2})}{\Gamma(p+1)\Gamma(p)\Gamma(n-p+2)} \qquad (A.7)$$

$$b_n = -a_n\left\{\frac{1}{4\pi}\sum_{p=1}^{n+1}\frac{\Gamma(p+\frac{1}{2})\Gamma(p-\frac{1}{2})\Gamma(n-p+\frac{3}{2})}{\Gamma(p+1)\Gamma(p)\Gamma(n-p+2)}\left[\frac{\Gamma'(n-p+2)}{\Gamma(n-p+2)} + \right.\right.$$

$$\left. - \frac{\Gamma'(p-n-\frac{1}{2})}{\Gamma(p-n-\frac{1}{2})}\right] - \sum_{p=n+1}^{\infty}\left[\frac{1}{4}\frac{\Gamma(p+1)\Gamma(p)\Gamma(p-n-\frac{1}{2})}{\Gamma(p+\frac{3}{2})\Gamma(p+\frac{1}{2})\Gamma(p-n)} + \right.$$

$$\left.\left. - \frac{1}{4}\frac{\Gamma(p+\frac{3}{2})\Gamma(p+\frac{1}{2})\Gamma(p-n)}{\Gamma(p+2)\Gamma(p+1)\Gamma(p-n+\frac{1}{2})}\right]\right\} \qquad (A.8)$$

It is not difficult to sum numerically the series in (A.8) because a simple recurrence relation exists between two consecutive coefficients. Table A.3 gives the values of the coefficients a_n and b_n for the first 10 eigenvalues.

With the property derived at the end of Section 6.5, it is possible to extrapolate the values obtained from (A.6). Table A.4 gives the eigenvalues obtained by this method for several values of Δ.

Table A.3

COFFICIENTS FOR THE DETERMINATION OF THE EIGENVALUES Υ_n

	a_n	b_n
0	-0.22156	0.00819
1	19386	00409
2	17655	00252
3	16422	00175
4	15476	00130
5	14717	00101
6	14088	00081
7	13552	00067
8	13087	00056
9	12681	00048
10	12320	00041

Table A.4

EIGENVALUES Υ_n AS A FUNCTION OF Δ

Δ	Υ_0	Υ_1	Υ_2	Υ_3	Υ_4
0.1	-0.02207	-1.01934	-2.01763	-3.01640	-4.01546
0.2	04399	03861	03521	03277	03085
0.4	08734	07689	07021	06541	06169
0.8	17225	15251	13962	13025	12296
1.6	33539	30001	27601	25822	24420

Appendix B

NUMERICAL INTEGRATION OF THE GENERALIZED WILKINS EQUATION

The generalized Wilkins equation (6.2.3) was numerically integrated using the IBM 704 computer available at the M.I.T.Computation Center. Rather than integrate equation (6.2.3) it was felt convenient to integrate the equation for $\phi(y) = y^2 e^{-y^2} \psi_1(y)$ because it gives directly an expression for the neutron density and, more important, because $\phi(y)$ decreases as $y \to \infty$ while $\psi_1(y)$ increases without limit.

A power series about the origin for $\phi(y)$ can be easily obtained from (6.2.5); the result is

$$\phi(y) = y^2 \sum_{n=0}^{\infty} a'_n y^n \qquad (B.1)$$

$$a'_o = 1; \quad a'_1 = \frac{\Delta}{3}; \quad a'_n = \frac{\Delta}{n(n+2)} a'_{n-1} - \frac{2(n+2-2\lambda)}{n(n+2)} a'_{n-2}$$

An asymptotic series is immediately obtained from (6.2.21)

$$\phi(y) \sim y^{2(\lambda-1)} \sum_{n=0}^{\infty} b_n y^{-n} \qquad (B.2)$$

$$b_o = 1; \quad b_1 = -\frac{\Delta}{2}; \quad b_n = -\frac{\Delta}{2n} b_{n-1} + \frac{(n+2-2\lambda)(n-2\lambda)}{2n} b_{n-2}$$

To perform the numerical integration, the series (B.1) was used for $0 < y \leq 2$. At $y = 2$, the derivative $\phi'(2)$ was calculated using the power series immediately

obtainable from (B.1). The values $\phi(2)$ and $\phi'(2)$ were used as initial conditions to perform a numerical integration for $2 < y \leq 6$ using the four point integration formula provided in the M.I.T. Computation Center FORTRAN loader. For $5 \leq y \leq 10$ the asymptotic series (B.2) was used. The results of the sum of the asymptotic series in the interval $5 \leq y \leq 6$ were compared with the results of the numerical integration. This comparison served two purposes: first, the joining factor $Q(\lambda,\Delta)$ was obtained; second, the constancy of $Q(\lambda,\Delta)$ in the interval provided an estimation of the truncation error caused by the numerical integration. After two trials, the step of integration for $2 < y \leq 6$ was selected as 0.02. The resulting error was estimated not to affect the fifth decimal place.

Tables B.1 and B.2 give values of the functions $\phi(y)$ for different values of λ and Δ useful for practical applications. The results can be extended to values of y greater than 4.0 by use of the asymptotic series in conjunction with the joining factors given in Tables A.1 and A.2.

With the eigenvalues calculated in Appendix A.1, eigenfunctions have been calculated by the procedure explained above. Because of the reduced practical interest, only the first five eigenfunctions for three values of Δ have been tabulated in Table B.3. These eigenfunctions correspond to eigenvalues given in Table A.4.

$\Delta = 0.1$

y \ λ	0.	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	00993	00993	00993	00994	00994	00994
0.2	03869	03870	03871	03871	03872	03873
0.3	08309	08313	08317	08320	08324	08328
0.4	13821	13832	13844	13855	13866	13878
0.5	19808	19834	19859	19885	19911	19937
0.6	25648	25697	25746	25795	25844	25893
0.7	30776	30857	30939	31021	31103	31185
0.8	34743	34867	34990	35114	35239	35363
0.9	37265	37437	37611	37785	37959	38134
1.0	38230	38457	38685	38913	39143	39373
1.1	37697	37979	38262	38546	38832	39119
1.2	35857	36190	36526	36864	37203	37544
1.3	32992	33372	33754	34139	34526	34916
1.4	29432	29848	30268	30691	31117	31546
1.5	25504	25946	26393	26843	27298	27758
1.6	21503	21960	22422	22888	23359	23835
1.7	17668	18128	18593	19064	19540	20022
1.8	14169	14621	15080	15545	16016	16494
1.9	11107	11544	11988	12439	12896	13361
2.0	08528	08943	09365	09795	10232	10677
2.1	06427	06815	07212	07616	08029	08449
2.2	04767	05127	05495	05872	06256	06650
2.3	03493	03824	04163	04510	04866	05231
2.4	02540	02842	03152	03471	03799	04135
2.5	01844	02119	02402	02694	02994	03302
2.6	01346	01595	01853	02119	02394	02678
2.7	00996	01223	01457	01700	01952	02212
2.8	00753	00959	01173	01396	01626	01865
2.9	00586	00774	00970	01174	01385	01605
3.0	00472	00644	00823	01010	01205	01408
3.1	00392	00550	00715	00888	01068	01256
3.2	00337	00482	00635	00794	00961	01136
3.3	00296	00431	00572	00721	00876	01038
3.4	00266	00392	00523	00661	00806	00957
3.5	00243	00359	00482	00611	00746	00889
3.6	00224	00333	00447	00568	00696	00830
3.7	00208	00310	00418	00531	00651	00777
3.8	00194	00290	00391	00499	00612	00731
3.9	00182	00272	00368	00469	00576	00689
4.0	00171	00257	00347	00443	00544	00651

Table B.1

THE FUNCTION $y^2 e^{-y^2} \psi_1(\lambda, \Delta; y)$

Table B.1 (Cont'd)

$\Delta = 0.2$

y \ λ	0.	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	00997	00997	00997	00997	00997	00997
0.2	03895	03896	03897	03897	03898	03899
0.3	08393	08397	08401	08405	08408	08412
0.4	14010	14021	14033	14044	14055	14067
0.5	20150	20176	20202	20228	20255	20281
0.6	26189	26238	26288	26338	26388	26437
0.7	31547	31630	31713	31796	31880	31964
0.8	35761	35887	36013	36140	36267	36394
0.9	38525	38702	38880	39057	39236	39415
1.0	39712	39945	40178	40413	40648	40884
1.1	39362	39652	39943	40236	40730	40825
1.2	37655	37999	38346	38695	39045	39397
1.3	34868	35262	35658	36056	36457	36861
1.4	31330	31763	32200	32639	33082	33528
1.5	27374	27836	28301	28771	29245	29723
1.6	23302	23780	24263	24751	25244	25742
1.7	19363	19846	20334	20829	21329	21836
1.8	15736	16213	16697	17187	17684	18188
1.9	12536	12998	13468	13946	14430	14922
2.0	09814	10255	10704	11161	11626	12099
2.1	07573	07989	08412	08844	09284	09733
2.2	05783	06170	06565	06969	07381	07802
2.3	04390	04747	05513	05487	05870	06263
2.4	03332	03659	03995	04340	04694	05058
2.5	02543	02842	03150	03467	03793	04128
2.6	01966	02238	02520	02811	03110	03419
2.7	01548	01797	02054	02320	02596	02880
2.8	01247	01475	01710	01955	02208	02470
2.9	01031	01239	01456	01680	01914	02156
3.0	00875	01066	01265	01472	01688	01912
3.1	00760	00936	01120	01311	01511	01719
3.2	00674	00836	01007	01184	01370	01564
3.3	00607	00758	00916	01081	01255	01436
3.4	00554	00694	00842	00996	01158	01328
3.5	00510	00641	00779	00924	01076	01235
3.6	00473	00596	00725	00861	01004	01154
3.7	00441	00557	00678	00806	00941	01083
3.8	00413	00522	00636	00757	00885	01019
3.9	00388	00491	00599	00713	00834	00961
4.0	00366	00463	00565	00674	00788	00909

Table B.1 (Cont'd)

$\Delta = 0.3$

y \ λ	0.	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	01000	01000	01000	01000	01000	01000
0.2	03921	03922	03923	03923	03924	03925
0.3	08478	08482	08486	08490	08493	08497
0.4	14200	14212	14223	14235	14246	14258
0.5	20497	20523	20550	20576	20602	20629
0.6	26738	26788	26838	26889	26939	26990
0.7	32332	32417	22501	32586	32671	32756
0.8	36800	36928	37057	37186	37316	37446
0.9	39816	39997	40179	40361	40543	40727
1.0	41234	41473	41713	41953	42195	42437
1.1	41077	41375	41675	41976	42279	42583
1.2	39513	39869	40227	40587	40948	41312
1.3	36815	37222	37632	38045	38460	38878
1.4	33307	33757	34211	34667	35127	35591
1.5	29329	29810	30296	30785	31279	31777
1.6	25190	25690	26195	26706	27221	27742
1.7	21148	21655	22168	22688	23213	23744
1.8	17395	17898	28408	18925	19448	19979
1.9	14054	14544	15041	15546	16059	16579
2.0	11187	11656	12134	12619	13113	13615
2.1	08804	09248	09700	10160	10630	11108
2.2	06879	07294	07717	08150	08592	09043
2.3	05363	05747	06141	06543	06956	07377
2.4	04194	04548	04912	05284	05666	06059
2.5	03308	03633	03967	04311	04665	05028
2.6	02646	02944	03251	03567	03893	04229
2.7	02156	02429	02711	03002	03302	03613
2.8	01794	02044	02303	02571	02848	03135
2.9	01525	01755	01993	02241	02497	02763
3.0	01324	01535	01755	01984	02222	02469
3.1	01170	01366	01569	01782	02002	02232
3.2	01051	01232	01421	01618	01824	02039
3.3	00955	01123	01300	01484	01676	01877
3.4	00876	01033	01198	01371	01551	01739
3.5	00810	00957	01112	01273	01443	01620
3.6	00753	00891	01037	01189	01348	01516
3.7	00704	00834	00970	01114	01265	01423
3.8	00660	00782	00911	01047	01190	01340
3.9	00621	00736	00858	00987	01122	01265
4.0	00585	00695	00810	00932	01061	01197

Table B.1 (Cont'd)

$\Delta = 0.4$

y \ λ	0.	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	01003	01003	01003	01003	01004	01004
0.2	03947	03948	03949	03950	03950	03951
0.3	08563	08567	08571	08575	08579	08583
0.4	14393	14404	14416	14428	14439	10451
0.5	20848	20875	20901	20928	20955	20982
0.6	27295	27346	27397	27448	27499	27551
0.7	33131	33217	33304	33390	33476	33563
0.8	37861	37992	38123	38255	38387	38520
0.9	41138	41323	41509	41695	41882	42069
1.0	42797	43042	43288	43535	43782	44031
1.1	42844	43151	43459	43769	44080	44393
1.2	41434	41802	42171	42542	42915	43291
1.3	38833	39255	39679	40106	40536	40969
1.4	35365	35832	36303	36777	37255	37736
1.5	31371	31872	32378	32888	33403	33922
1.6	27169	27692	28221	28755	29294	29838
1.7	23028	23560	24099	24644	25195	25752
1.8	19149	19679	20216	20761	21312	21871
1.9	15667	16185	16711	17245	17786	18336
2.0	12652	13151	13657	14173	14697	15229
2.1	10124	10596	11078	11569	12069	12579
2.2	08060	08504	08957	09420	09892	10374
2.3	06416	06829	07251	07684	08126	08579
2.4	05131	05513	05905	06307	06719	07142
2.5	04143	04495	04858	05230	05612	06005
2.6	03393	03717	04050	04394	04748	05113
2.7	02826	03123	03431	03748	04076	04414
2.8	02397	02671	02955	03248	03552	03865
2.9	02072	02324	02586	02858	03139	03430
3.0	01822	02055	02298	02550	02811	03082
3.1	01627	01843	02068	02302	02545	02798
3.2	01471	01671	01881	02099	02327	02564
3.3	01343	01530	01726	01930	02143	02365
3.4	01237	01412	01595	01787	01987	02196
3.5	01146	01310	01483	01663	01851	02048
3.6	01068	01222	01384	01554	01732	01918
3.7	00998	01144	01297	01457	01625	01802
3.8	00937	01074	01219	01371	01530	01697
3.9	00882	01012	01149	01293	01444	01603
4.0	00832	00955	01085	01223	01366	01517

Table B.1 (Cont'd)

$\Delta = 0.5$

y \ λ	0.0	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	01007	01007	01007	01007	01007	01007
0.2	03973	03974	03975	03976	03977	03978
0.3	08651	08654	08657	08661	08665	08669
0.4	14587	14599	14611	14622	14634	14646
0.5	21202	21230	21258	21285	21312	21339
0.6	27860	27912	27964	28016	28016	28120
0.7	33946	34033	34120	34208	34296	34384
0.8	38944	39078	39212	39346	39481	39616
0.9	42491	42681	42871	43062	43253	43444
1.0	44402	44653	44905	45159	45413	45668
1.1	44664	44980	45297	45616	45936	46257
1.2	43419	43798	44179	44562	44947	45334
1.3	40925	41362	41801	42243	42688	43135
1.4	37504	37990	38479	38971	39467	39967
1.5	33502	34025	34552	35083	35619	36160
1.6	29244	29791	30343	30901	31464	32033
1.7	25005	25564	26129	26700	27278	27863
1.8	21001	21560	22126	22699	23279	23867
1.9	17379	17926	18481	19045	19618	20198
2.0	14215	14743	15280	15827	16382	16947
2.1	11536	12040	12553	13075	13607	14149
2.2	09330	09804	10288	10783	11288	11802
2.3	07554	07996	08449	08913	09388	09873
2.4	06148	06559	06981	07414	07858	08312
2.5	05054	05434	05825	06228	06641	07065
2.6	04209	04560	04922	05295	05679	06074
2.7	03560	03884	04219	04565	04921	05288
2.8	03062	03361	03670	03991	04322	04663
2.9	02675	02952	03239	03536	03844	04162
3.0	02372	02629	02896	03172	03459	03756
3.1	02033	02371	02619	02876	03144	03422
3.2	01938	02159	02390	02631	02882	03142
3.3	01777	01983	02199	02425	02660	02905
3.4	01639	01833	02036	02248	02469	02700
3.5	01522	01704	01895	02094	02303	02521
3.6	01419	01590	01770	01959	02156	02363
3.7	01329	01490	01660	01839	02026	02221
3.8	01248	01400	01561	01731	01908	02094
3.9	01174	01319	01472	01633	01802	01979
4.0	01109	01246	01391	01544	01705	01874

Table B.1 (Cont'd)

$\Delta = 0.6$

y \ λ	0.0	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	01010	01010	01010	01010	01010	01010
0.2	04000	04001	04002	04003	04003	04004
0.3	08736	08740	08744	08748	08752	08756
0.4	14783	14795	14807	14819	14831	14843
0.5	21563	21591	21618	21646	21673	21700
0.6	28435	28487	28540	28593	28646	28698
0.7	34774	34863	34952	35041	35131	35220
0.8	40049	40186	40323	40460	40597	40735
0.9	43877	44071	44265	44460	44655	44851
1.0	46049	46307	46566	46826	47086	47348
1.1	46537	46862	47189	47517	47846	48177
1.2	45469	47860	46254	46649	47046	47445
1.3	43094	43545	44000	44457	44917	45380
1.4	39731	40234	40741	41252	41767	42285
1.5	35728	36272	36820	37373	37931	38494
1.6	31417	31988	32565	31148	33736	34330
1.7	27086	27671	28263	28862	29478	30080
1.8	22959	23546	24141	24744	25354	25970
1.9	19192	19770	20357	20953	21557	22169
2.0	15877	16437	17007	17585	18174	18712
2.1	13046	13582	14128	14683	15249	15825
2.2	10692	11199	11716	12244	12783	13332
2.3	08777	09253	09739	10236	10745	11264
2.4	07247	07690	08145	08610	09087	09575
2.5	06040	06452	06875	07309	07755	08212
2.6	05097	05479	05871	06275	06690	07117
2.7	04362	04715	05080	05455	05842	06240
2.8	03789	04116	04454	04803	05163	05535
2.9	03338	03641	03955	04280	04616	04963
3.0	02980	03261	03554	03856	04170	04495
3.1	02690	02953	03225	03508	03802	04106
3.2	02452	02697	02952	03217	03493	03779
3.3	02253	02482	02721	02970	03229	03499
3.4	02083	02299	02523	02758	03002	03256
3.5	01937	02139	02351	02572	02803	03043
3.6	01808	01999	02199	02408	02626	02854
3.7	01694	01874	02063	02262	02469	02685
3.8	01591	01762	01942	02130	02327	02533
3.9	01499	01661	01832	02011	02198	02395
4.0	01415	01570	01732	01902	02081	02268

Table B.1 (Cont'd)

$\Delta = 0.7$

y \ λ	0.0	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	01013	01013	01013	01014	01014	01014
0.2	04026	04027	04028	04029	04030	04031
0.3	08824	08828	08832	08836	08840	08844
0.4	14982	14994	15006	15018	15030	15042
0.5	21929	21956	21983	22011	22039	22067
0.6	29017	29071	29125	29178	29232	29286
0.7	35618	35708	35798	35889	35980	36071
0.8	41177	41317	41457	41596	41737	41877
0.9	45294	45493	45692	45891	46091	46292
1.0	47739	48005	48271	48537	48804	49072
1.1	48335	48801	49137	49474	49812	50152
1.2	47586	47990	48396	48803	49213	49624
1.3	45341	45808	42278	46751	47227	47706
1.4	42045	42567	43093	43623	44157	44695
1.5	38048	38615	39186	39762	40342	40927
1.6	33692	34289	34891	35499	36114	36734
1.7	29269	29885	30506	31133	31767	32409
1.8	25022	25640	26266	26900	27541	28191
1.9	21114	21724	22343	22971	23608	24254
2.0	17645	18238	18841	19454	20077	20710
2.1	14658	15228	15808	16398	16999	17611
2.2	12153	12694	13246	13808	14382	14968
2.3	10095	10605	11126	11658	12201	12757
2.4	08436	08912	09400	09900	10412	10936
2.5	07112	07556	08012	08479	08959	09451
2.6	06044	06477	06902	07338	07787	08248
2.7	05239	05622	06017	06424	06843	07274
2.8	04587	04942	05309	05689	06080	06484
2.9	04067	04397	04739	05093	05459	05837
3.0	03646	03955	04275	04606	04949	05303
3.1	03305	03593	03892	04202	04523	04856
3.2	03019	03290	03571	03862	04164	04477
3.3	02781	03034	03297	03571	03856	04151
3.4	02578	02814	03061	03319	03588	03868
3.5	02397	02621	02855	03099	03353	03618
3.6	02238	02451	02673	02903	03144	03396
3.7	02099	02300	02510	02729	02958	03197
3.8	01974	02164	02363	02571	02789	03017
3.9	01859	02041	02231	02429	02637	02854
4.0	01758	01930	02110	02299	02497	02705

Table B.1 (Cont'd)

$\Delta = 0.8$

y \ λ	0.0	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	01017	01017	01017	01017	01017	01017
0.2	04053	04054	04055	04056	04057	04057
0.3	08912	08916	08920	08924	08928	08932
0.4	15182	15194	15206	15218	15231	15243
0.5	22297	22325	22353	22381	22409	22438
0.6	29610	29664	29718	29773	29827	29882
0.7	36476	36568	36660	36752	36845	36938
0.8	42329	42471	42614	42757	42900	43043
0.9	46746	46949	47152	47356	47561	47766
1.0	49477	49748	50020	50293	50567	50842
1.1	50453	50797	51142	51488	51836	52186
1.2	49773	50189	50607	51027	51450	51874
1.3	47667	48151	48637	49126	49618	50113
1.4	44449	44991	45537	46686	46640	47198
1.5	40469	41058	41652	42251	42855	43464
1.6	36073	36696	37324	37959	38600	39247
1.7	31567	32210	32859	33516	34181	34852
1.8	27199	27848	28505	29171	29845	30527
1.9	23147	23791	24443	25105	25777	26458
2.0	19523	20151	20789	21437	22096	22765
2.1	16378	16983	17599	18225	18863	19512
2.2	13717	14294	14882	15481	16092	16715
2.3	11513	12058	12615	13183	13764	14357
2.4	09717	10229	10753	11288	11837	12398
2.5	08271	08749	09240	09743	10259	10788
2.6	07115	07561	08019	08490	08974	09471
2.7	06193	06608	07036	07476	07930	08396
2.8	05455	05842	06242	06653	07078	07515
2.9	04862	05223	05596	05981	06379	06789
3.0	04379	04716	05064	05425	05799	06185
3.1	03980	04296	04622	04961	05312	05676
3.2	03647	03942	04249	04568	04899	05241
3.3	03363	03641	03930	04230	04542	04866
3.4	03119	03381	03653	03937	04232	04539
3.5	02905	03153	03410	03679	03958	04249
3.6	02717	02951	03195	03449	03715	03991
3.7	02549	02770	03002	03244	03496	03759
3.8	02398	02608	02828	03058	03299	03550
3.9	02261	02461	02671	02890	03120	03359
4.0	02137	02328	02528	02737	02956	03185

Table B.1 (Cont'd)

$\Delta = 0.9$

y \ λ	0.0	0.01	0.02	0.03	0.04	0.05
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	01020	01020	01020	01020	01020	01020
0.2	04080	04081	04082	04083	04084	04084
0.3	09001	09005	09009	09013	09017	09021
0.4	15385	15397	15409	15421	15433	15446
0.5	22671	22699	22728	22756	22785	22813
0.6	30211	30266	30321	30376	30431	30486
0.7	37349	37443	37537	37631	37725	37819
0.8	43505	43650	43795	43940	44086	44232
0.9	48231	48439	48647	48855	49064	49274
1.0	51258	51536	51815	52095	52376	52658
1.1	52496	52850	53205	53561	53919	54279
1.2	52030	52459	52890	53323	53758	54196
1.3	50078	50577	51079	51585	52094	52606
1.4	46944	47508	48075	48645	49219	49797
1.5	42991	43604	44222	44845	45473	46106
1.6	38560	39212	39869	40531	41200	41875
1.7	33976	34649	35329	36017	36712	37415
1.8	29492	30173	30863	31562	32270	32986
1.9	25296	25975	26663	37361	28068	28785
2.0	21515	22180	22855	23541	24237	24944
2.1	18210	18852	19505	20170	20846	21534
2.2	15390	16004	16630	17268	17918	18580
2.3	13033	13616	14211	14818	15438	16071
2.4	11097	11646	12207	12782	13369	13970
2.5	09524	10038	10565	11106	11660	12228
2.6	08253	08734	09228	09736	10257	10792
2.7	07229	07679	08142	08618	09107	09611
2.8	06403	06823	07256	07702	08162	08635
2.9	05730	06123	06529	06947	07379	07825
3.0	05178	05546	05926	06319	06726	07145
3.1	04721	05065	05422	05791	06174	06570
3.2	04333	04657	04993	05341	05702	06076
3.3	04004	04308	04624	04953	05294	05648
3.4	03717	04004	04303	04614	04937	05273
3.5	03466	03737	04020	04315	04622	04941
3.6	03245	03501	03769	04049	04340	04644
3.7	03045	03289	03544	03810	04088	04377
3.8	02866	03098	03341	03595	03859	04135
3.9	02703	02925	03157	03399	03651	03915
4.0	02556	02767	02988	03220	03461	03714

Table B.2

THE FUNCTION $y^2 e^{-y^2} \psi_1(\lambda, \Delta; y)$

	$\Delta = 0.4$			$\Delta = 0.8$		
$y \backslash \lambda$	0.2	0.4	0.6	0.2	0.4	0.6
0.0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	01004	01005	01006	01018	01019	01020
0.2	03963	03979	03995	04070	04086	04102
0.3	08641	08719	08798	08992	09072	09153
0.4	14627	14864	15103	15426	15672	15921
0.5	21386	21933	22490	22862	23437	24021
0.6	28328	29387	30472	30706	31829	32979
0.7	34879	36685	38552	38348	40282	42280
0.8	40540	43340	46264	45230	48259	51419
0.9	44943	48966	53217	50909	55305	59946
1.0	47866	53300	59118	55082	61082	67498
1.1	49246	56216	63790	57610	65387	73823
1.2	49157	57712	63161	58505	68152	78783
1.3	47786	57894	69261	57908	69430	82347
1.4	45389	56945	70197	56051	69368	84580
1.5	42256	55094	70129	53221	68180	85611
1.6	38675	52585	69245	49721	66108	85617
1.7	34906	49654	67740	45838	63405	84795
1.8	31162	46507	65802	41820	60302	83343
1.9	27604	43317	63594	37867	57001	81444
2.0	24339	40211	61251	34124	53662	79259
2.1	21423	37278	58878	30683	50407	76920
2.2	18878	34572	56552	27592	47317	74527
2.3	16693	32116	54324	24864	44440	72154
2.4	14840	29913	52222	22487	41800	69853
2.5	13282	27953	50262	20434	39399	67653
2.6	11975	26216	48446	18667	37228	65572
2.7	10880	24676	46770	17149	35271	63616
2.8	09957	23310	45223	15840	33506	61782
2.9	09175	22093	43796	14708	31911	60066
3.0	08505	21003	42477	13721	30466	58460
3.1	07937	20023	41254	12855	29151	56956
3.2	07423	19135	40117	12089	27950	55543
3.3	06978	18328	39057	11406	26848	54214
3.4	06582	17588	38064	10793	25832	52961
3.5	06227	16909	37132	10239	24893	51778
3.6	05906	16281	36256	09735	24020	50657
3.7	05615	15698	35428	09274	23207	49594
3.8	05348	15156	34646	08851	22447	48583
3.9	05103	14651	33904	08461	21736	47621
4.0	04877	14177	33200	08101	21067	46703

Table B.2 (Cont'd)

$\Delta = 1.6$

y \ λ	0.0	0.2	0.4	0.6
0.0	0.00000	0.00000	0.00000	0.00000
0.1	01044	01045	01046	01047
0.2	04272	04289	04306	04323
0.3	09641	09725	09811	09896
0.4	16858	17121	17387	17656
0.5	25421	26044	26676	27319
0.6	34678	35909	37169	38459
0.7	43912	46055	48268	50552
0.8	52427	55815	59347	63028
0.9	59629	64587	69815	75324
1.0	65082	71896	79172	86932
1.1	68542	77424	87041	97439
1.2	69958	81023	93191	1.06544
1.3	69454	82710	97536	14068
1.4	67287	82635	1.00118	19953
1.5	63803	81048	01084	24237
1.6	59384	78257	00652	27043
1.7	54406	74589	0.99082	28543
1.8	49204	70357	96641	28939
1.9	44053	65840	93587	28444
2.0	39159	61265	90145	27259
2.1	34657	56805	86507	25567
2.2	30621	52579	82820	23525
2.3	20775	48660	79194	21259
2.4	24009	45082	75702	18870
2.5	21384	41852	72390	16433
2.6	19154	38958	69280	13999
2.7	17263	36372	66380	11607
2.8	15659	34066	63686	09278
2.9	14293	32006	61887	07026
3.0	13123	30161	58870	04858
3.1	12114	28502	56718	02775
3.2	11235	27004	54717	00778
3.3	10463	25645	52852	0.98862
3.4	09780	24406	51109	97025
3.5	09171	23272	49477	95263
3.6	08624	22229	47945	93571
3.7	08130	21266	46503	91945
3.8	07682	20375	45144	90383
3.9	07272	19548	43861	88879
4.0	06897	18777	42646	87431

Table B.3

EIGENFUNCTIONS $y^2 e^{-y^2} W_n(y)$

$\Delta = 0.2$

y \ n	0	1	2	3	4
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	+ 00996	+ 00992	+ 00987	+ 00982	+ 00977
0.2	03892	03814	03738	03663	03588
0.3	08376	08003	07640	07288	06947
0.4	13959	12855	11808	10815	09876
0.5	20036	17563	15289	13206	11303
0.6	25971	21360	17289	13716	10597
0.7	31183	23655	17333	12078	07762
0.8	35210	24119	15352	08556	+ 03411
0.9	37753	22715	11673	+ 03843	- 01444
1.0	38698	19685	06913	- 01137	05705
1.1	38101	15468	+ 01831	05476	08504
1.2	36159	10617	- 02840	08486	09407
1.3	33167	05691	06526	09829	08478
1.4	29464	+ 01175	08891	09537	06188
1.5	25392	- 02576	09862	07947	03236
1.6	21257	05366	09590	05573	- 00331
1.7	17305	07147	08377	02964	+ 01973
1.8	13712	07998	06595	- 00586	03375
1.9	10583	08076	04606	+ 01248	03839
2.0	07962	07584	02704	02403	03534
2.1	05841	06727	- 01092	02898	02732
2.2	04181	05688	+ 00128	02857	01732
2.3	02921	04611	00938	02457	00776
2.4	01993	03600	01381	01876	+ 00021
2.5	01328	02714	01535	01261	- 00470
2.6	00865	01981	01485	00713	00706
2.7	00550	01401	01314	+ 00285	00742
2.8	00342	00962	01087	- 00010	00649
2.9	00208	00642	00852	00183	00495
3.0	00124	00417	00638	00261	00330
3.1	00072	00264	00458	00274	00187
3.2	00041	00162	00317	00249	00080
3.3	00023	00097	00211	00205	- 00010
3.4	00012	00057	00136	00158	+ 00029
3.5	00007	00033	00085	00115	00045
3.6	00003	00018	00052	00080	00047
3.7	00002	00010	00031	00053	00041
3.8	00001	00005	00018	00034	00033
3.9	00000	00003	00010	00021	00024
4.0	00000	00001	00005	00012	00016

Table B.3 (Cont'd)

$\Delta = 0.4$

y \ n	0	1	2	3	4
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	+ 01003	+ 00998	+ 00993	+ 00988	+ 00983
0.2	03940	03863	03786	03710	03635
0.3	08530	08153	07787	07431	07085
0.4	14291	13173	12110	11101	10147
0.5	20616	18102	15785	13659	11714
0.6	26851	22147	17981	14317	11114
0.7	32387	24679	18183	12769	08311
0.8	36727	25333	16287	09248	+ 03898
0.9	39543	24045	12601	+ 04442	- 01104
1.0	40693	21037	07739	- 00712	05567
1.1	40217	16749	+ 02476	05271	08579
1.2	38307	11745	- 02425	08508	09659
1.3	35260	06607	06352	10044	08840
1.4	31429	+ 01849	08938	09885	06580
1.5	27173	- 02148	10084	08354	03583
1.6	22819	05162	09926	05970	- 00583
1.7	18633	07130	08766	03297	+ 01838
1.8	14807	08120	06981	- 00826	03352
1.9	11461	08290	04948	+ 01110	03903
2.0	08646	07846	02979	02356	03647
2.1	06360	07002	- 01291	02922	02862
2.2	04564	05950	+ 00001	02926	01850
2.3	03197	04845	00873	02546	00868
2.4	02186	03797	01363	01967	+ 00079
2.5	01460	02872	01547	01340	- 00442
2.6	00953	02102	01515	00774	00702
2.7	00608	01492	01352	00327	00753
2.8	00379	01027	01125	+ 00015	00667
2.9	00231	00687	00886	- 00171	00514
3.0	00137	00447	00666	00258	00347
3.1	00080	00283	00480	00277	00200
3.2	00046	00175	00333	00254	00088
3.3	00025	00105	00223	00211	- 00014
3.4	00014	00062	00144	00163	+ 00027
3.5	00007	00035	00090	00119	00045
3.6	00001	00020	00055	00083	00047
3.7	00001	00011	00033	00055	00042
3.8	00000	00006	00019	00035	00033
3.9	00000	00003	00010	00022	00025
4.0	00000	00002	00006	00013	00017

Table B.3 (Cont'd)

$\Delta = 1.6$

y\n	0	1	2	3	4
0.0	0.00000	0.00000	0.00000	0.00000	0.00000
0.1	+ 01042	+ 01037	+ 01032	+ 01027	+ 01022
0.2	04244	04164	04085	04005	03927
0.3	09500	09102	08711	08329	07957
0.4	16423	15213	14050	12941	11885
0.5	24400	21617	19021	16620	14409
0.6	32678	27355	22573	18323	14573
0.7	40469	31565	23926	17469	12079
0.8	47059	33631	22733	14082	07368
0.9	51891	33276	19138	08771	+ 01475
1.0	54631	30586	13720	+ 02543	- 04294
1.1	55183	25965	07336	- 03460	08740
1.2	53671	20036	+ 00933	08240	11080
1.3	50402	13523	- 04642	11152	11109
1.4	45800	07124	08790	11994	09169
1.5	40340	+ 01415	11222	10988	05985
1.6	34488	- 03210	11961	08652	- 02422
1.7	28651	06556	11273	05643	+ 00752
1.8	23152	08617	09575	- 02593	03020
1.9	18212	09526	07327	+ 00013	04181
2.0	13955	09510	04950	01890	04317
2.1	10422	08832	02767	02960	03691
2.2	07590	07748	- 00980	03303	02649
2.3	05393	06480	+ 00324	03096	01512
2.4	03740	05198	01152	02553	+ 00516
2.5	02532	04014	01572	01870	- 00210
2.6	01674	02994	01682	01197	00636
2.7	01081	02161	01586	00627	00798
2.8	00682	01512	01374	+ 00202	00771
2.9	00421	01027	01116	- 00075	00635
3.0	00254	00678	00860	00226	00458
3.1	00150	00436	00633	00284	00287
3.2	00086	00272	00447	00281	00149
3.3	00049	00166	00305	00246	- 00051
3.4	00027	00098	00200	00197	+ 00009
3.5	00014	00057	00127	00148	00039
3.6	00008	00032	00079	00105	00048
3.7	00004	00018	00047	00072	00046
3.8	00002	00009	00027	00047	00038
3.9	00001	00005	00015	00029	00029
4.0	00000	00003	00009	00018	00021

Biographical Note

The author was born in Cádiz, Spain in 1929. He took his elementary studies in Colegio de San Felip Neri and graduated as Bachiller at the University of Sevilla in 1946. He attended the Escuela Naval Militar and graduated as an Officer of the Spanish Navy in 1951. After serving on board during two years, he took three years of postgraduate studies in the Escuela de Estudios Superiores at the Astronomical Observatory of the Spanish Navy obtaining a diploma in 1956. In March 1957, he was married to the former Margara Lastra in Puerto de Santa María, Spain. Shortly after he entered as a graduate student in the Massachusetts Institute of Technology obtaining his Master of Science degree in 1958. Since then he has been engaged in his doctoral studies.