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THE THERMAL NEUTRON MILNE PROBLEM

January 1968

A thesis submitted to the University of St. Andrews
in partial fulfillment of the requirements for the degree of
Doctor of Philosophy

A condensed version of Chapters 3,4 and 5 of this thesis
has been accepted for publication as two separate articles
in The British Journal of Applied Physics.

* * *



DECLARATION

I hereby declare that this thesis is based on research carried out by me, that it is my own composition and that it has not previously been presented for a higher degree.

STATEMENT

I certify that Michael J. Lancefield, having spent the required period of three terms in actual attendance as a research student in the Department of Theoretical Physics of the United College of St. Salvator and St. Leonard in the University of St. Andrews, has subsequently spent two years in full-time research at the Theoretical Physics Division, A.E.R.E. Harwell, that he has fulfilled the conditions of Ordinance No. 12 and Ordinance No. 16 of the University Court of St. Andrews and that he is qualified to submit the accompanying thesis in application for the degree of Doctor of Philosophy.

Research Supervisor

HIGHER STUDY AND RESEARCH

From 1961-1964 I studied at the University of St. Andrews and followed a course leading to the degree of Bachelor of Science with Upper Second Class Honours in Physics with Theoretical Physics. From October 1964 I spent three terms as a research student in the Department of Theoretical Physics of the University of St. Andrews and the following two years at the Atomic Energy Research Establishment, Harwell. During that time I was engaged in research on the subject of this thesis.

I was admitted as a research student under Ordinance General No. 12 of the University Court of St. Andrews on October 1st, 1964 and subsequently admitted as a candidate for the degree of Doctor of Philosophy under Ordinance No. 16 on October 1st, 1965.

Since October 1st 1967, I have held a post as Research Associate at the Brookhaven National Laboratory, U.S.A.

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ABSTRACT

This thesis is concerned with the Thermal Neutron Milne Problem; more precisely it is a study of the stationary neutron distribution in a moderating half-space sustained by a source of neutrons at a large distance from the boundary which is in thermal equilibrium with the medium. Special emphasis is given to the effects of anisotropic scattering and neutron capture. We shall determine the extrapolation length, the asymptotic flux far from the boundary and the distortion caused in the flux by the presence of the boundary.

In a non-capturing medium the energy dependence of the asymptotic flux is known to take the form of a Maxwellian distribution while the spatial dependence involves the extrapolation length. When neutrons are captured as well as scattered the asymptotic angular flux takes the form:

$$\Psi_{\text{asy}}(z, \mu, E) = \left[g(E, -\mu) e^{z/L} + a g(E, \mu) e^{-z/L} \right] M(E)$$

where a is closely related to the extrapolation length and an eigenvalue equation exists for the determination of L and $g(E, \pm\mu)$. The existence and numerical values of these eigenvalues and eigenfunctions is a problem in itself - the diffusion length problem - and numerical results are presented for a number of moderators.

A semi-analytical approach, involving Green's functions, is adopted which makes maximum use of the known or obtainable solutions to some monoenergetic problems in order to investigate the extrapolation length and transient flux. Basically the homogeneous transport equation for the angular flux $\Psi(z, \mu, E)$ is transformed into an inhomogeneous integral equation for the integrated flux $\Psi_0(z, E)$ in terms of the one-speed Milne solutions and the associated half-space Green's functions. Then a variational principle can be written down which estimates the extrapolation length or, in a capturing medium, the parameter a . Then by iterating a simple trial function one can determine the emergent angular distribution.

Results are obtained and compared with other exact solutions for some simple scattering models and with experimental results for a water moderator. For all these excellent agreement is found generally except for a slight discrepancy in the emergent spectra at grazing angles to a water surface for low energies - a discrepancy which could be removed by improving the trial function.

A prescription is given for obtaining, rather simply, a good first approximation to the extrapolation length in the Milne problem with anisotropic scattering and/or neutron capture. Lastly the possible extension of this Green's function method to more complex problems is discussed.

CHAPTER 1

INTRODUCTION

§1.1 The Milne Problem Defined

Milne's problem is concerned with the determination of the radiation emerging from the plane surface of a semi-infinite, scattering and possibly also absorbing medium in which there is a plane source of radiation parallel to the surface at a large distance from it. In the context of neutron transport theory we treat the problem of the energy spectrum of thermal neutrons emerging from the plane surface of a moderating medium in which we shall consider separately the effects of anisotropic scattering, neutron capture and fission. A stationary, that is time independent, distribution of neutrons is sustained by a source at infinity which, for simplicity, we shall assume to emit neutrons in thermal equilibrium with the moderator. A vacuum is assumed to exist outside the moderator so that we have the boundary condition at the interface that no neutrons return to the medium.

This geometry provides the simplest example by which one can study how boundaries and discontinuities distort the infinite medium neutron distributions. Besides determining the flux and emergent angular distribution we hope to obtain some insight into the physical processes which affect the neutron spectrum at the boundary. Finally we are able to determine the extrapolation length, a parameter which provides a boundary condition for an approximation widely used in reactor physics - the one-group diffusion approximation.

Such is the importance of the extrapolation length in the application of diffusion theory that we shall explain the general procedure involved. In a complex problem each boundary is considered separately. For each kind of boundary the simplest possible problem involving that kind of boundary is solved as exactly as possible and at least without using the diffusion approximation. That is, for a plane boundary we should solve the Milne problem already described and determine the extrapolation length (perhaps by the very accurate variational principle to be described later). Thus one can determine the precise form of the neutron flux far from the boundary, referred to as the asymptotic flux, in terms of the extrapolation length: in other words the extrapolation length implies a boundary condition on the asymptotic flux. In more complex problems the interference between different boundaries is neglected and in solving the diffusion equation the boundary conditions obtained from these simplified problems are used. Of course this plan cannot always be strictly adhered to but the relevance of a highly accurate determination of the extrapolation length for a semi-infinite medium with a plane boundary is manifest.

Experimentally this ideal situation will be difficult to achieve: the moderator will be of finite size and the source is unlikely to be in thermal equilibrium with the moderator. All the same it is realised to a fair approximation at the outer surface of an unshielded reactor.

A typical experimental arrangement is shown schematically in Figures 1.I and 1.II. A Cockcroft-Walton generator delivers a short burst of fast (\sim MeV) neutrons which diffuse through the medium, often water, and are eventually thermalised. After a sufficient waiting time the cadmium chopper opens to allow a short burst of neutrons leaking at a particular angle from the moderator surface to enter the 3 metre evacuated flight path where they are analysed into different energies. For other angles the slab is rotated while the source is maintained on a line perpendicular to the water surface.

It may be shown (Kallfelz 1967) that for a sufficiently large moderator with $1/v$ type absorption Milne problem conditions are attained if one waits for a sufficiently long time. To ensure that this is so and thermalisation is complete spectra are measured at different delay times even though theoretical estimates of the thermalisation times are available. In this way we can be doubly sure that the neutron distribution is not source dependent. In the same way measurements are made for different sizes of slab and it is found that a slab of approximate dimensions $15 \times 30 \times 30$ cms. is large enough to be sure that other boundaries in no way influence the neutron distribution at the surface we are interested in. However, it is found that without the neutron chopper to guarantee complete thermalisation a "slowing down" component is apparent in the high energy tail of the distribution (Sinclair and Williams 1965) although, of course, this high energy tail could be reduced by increasing the size of the slab.

Parallel emission must be considered a special case experimentally and cannot be measured with the set-up described above. Another arrangement is used which has an extraction channel a few centimetres wide and only a few millimetres deep in the water surface (see Figure 1.II). This step is a perturbation of the ideal situation which might be serious since the transient flux close to the surface dies away quite rapidly with increasing distance from the surface and furthermore the angular dependence of the spectra is expected to be quite strong for angles close to grazing incidence. In the experiments of Kallfelz (1967) it has been demonstrated that the difference in the results of measurements for 2mm and 4mm steps was negligible and could therefore justifiably be extrapolated to zero penetration depth.

In this way we believe the experimental arrangement to be an adequate representation of the ideal situation envisaged in the theory.

However it is not essential that the neutrons be taken from the actual moderator surface. In an earlier experiment Sinclair et al (1963) immersed a cadmium disc in a tank of water to act as a perfectly absorbing surface (see Figure 1.III). The neutrons were extracted by means of a probe tube from an aluminium "window" at the centre of the cadmium disc. The angular dependence of the neutron distribution at this surface could be determined by rotating the disc while keeping the probe tube fixed. Cadmium is transparent to neutrons having energies greater than about 2eV and this effect permits the normalisation of the neutron spectra at various angles with respect to each other. Otherwise a separate flux monitor is required

which would perturb the ideal Milne problem conditions.

§1.2 The Transport Equation

A mathematical description of the Milne problem is achieved through a linear Boltzmann equation (Williams 1966, p.14) which may be written quite generally as:

$$\frac{1}{v} \frac{\partial}{\partial t} \Psi(\underline{r}, \underline{\Omega}, E, t) + \underline{\Omega} \cdot \nabla \Psi(\underline{r}, \underline{\Omega}, E, t) + \left[\Sigma_s(E) + \Sigma_a(E) \right] \Psi(\underline{r}, \underline{\Omega}, E, t) = \int_{\underline{\Omega}'} d\Omega' \int_0^\infty dE' \Sigma(E' \rightarrow E; \underline{\Omega}' \rightarrow \underline{\Omega}) \Psi(\underline{r}, \underline{\Omega}', E', t) + S(\underline{r}, \underline{\Omega}, E, t) \quad (1.1)$$

where $\Psi(\underline{r}, \underline{\Omega}, E, t)$ is the neutron flux per unit energy interval per unit solid angle at position \underline{r} at time t and $S(\underline{r}, \underline{\Omega}, E, t)$ is a source term. $\Sigma(E' \rightarrow E; \underline{\Omega}' \rightarrow \underline{\Omega})$ is the scattering kernel while $\Sigma_s(E)$ and $\Sigma_a(E)$ (taken to be independent of position) are the total cross-sections for scattering and absorption respectively.

$$\Sigma_s(E) = \int_{\underline{\Omega}'} d\Omega' \int_{\underline{\Omega}} d\Omega \int_0^\infty dE' \Sigma(E \rightarrow E', \underline{\Omega} \rightarrow \underline{\Omega}') \quad (1.2)$$

and the subscript s will usually be dropped. We shall also refer to the mean free path $\ell(E)$ where

$$\ell^{-1}(E) = \Sigma_s(E) + \Sigma_a(E) \quad (1.3)$$

and it will normally be clear from the context whether or not $\Sigma_a(E)$ is zero.

We shall assume that the scattering kernel depends only on the scattering angle $\text{Cos}^{-1} \mu_0$ between $\underline{\Omega}$ and $\underline{\Omega}'$, that is on $\underline{\Omega} \cdot \underline{\Omega}' = \mu_0$. This is valid for all practical cases except for extruded graphite which has macroscopic anisotropy. Then the scattering kernel is conveniently expanded in terms of the Legendre polynomials:

$$\Sigma(E' \rightarrow E; \mu_0) = \frac{1}{4\pi} \sum_{n=0}^{\infty} (2n+1) \Sigma_n(E' \rightarrow E) P_n(\mu_0) \quad (1.4)$$

and throughout, as in (1.4), we adopt the notation that the n'th Legendre moment of a function $f(\underline{r}, \mu, E)$ is given by:

$$f_n(\underline{r}, E) = \int_{-1}^{+1} f(\underline{r}, \mu, E) P_n(\mu) d\mu \quad (1.5)$$

although for notational convenience we sometimes drop the subscript for the zero'th moment. We now consider the thermal neutron Milne problem in plane geometry for which there is a plane source in thermal equilibrium with the moderator at a large distance from the boundary. In that case substituting (1.4) into (1.1), specialising to plane geometry and using the addition theorem of Legendre polynomials (Davison 1957, p241) the transport equation becomes:

$$\begin{aligned} \mu \frac{\partial}{\partial z} \Psi(z, \mu, E) + \frac{1}{\ell(E)} \Psi(z, \mu, E) \\ = \frac{1}{2} \sum_{n=0}^{\infty} (2n+1) P_n(\mu) \int_0^{\infty} dE' \Sigma_n(E' \rightarrow E) \times \Psi_n(z, E') \end{aligned} \quad (1.6)$$

where μ is the cosine of the angle between the direction of motion

of the neutron and the positive z axis. For isotropic scattering only the first term of the Legendre expansion in (1.6) is non-zero while in treating anisotropic scattering it is usually sufficient to truncate the series after the first few terms. In writing (1.6) we have implicitly ignored the possibility of fission but we shall return to this in Chapter 6.

Since no neutrons can be scattered back into the medium from the vacuum region $z < 0$ the boundary condition at the interface will be:

$$\Psi(0, \mu, E) = 0 \quad 0 < \mu \leq 1 \quad . \quad (1.7)$$

Simply stated, the thermal neutron Milne problem involves a solution of the transport equation (1.6) with the boundary condition (1.7) but in order to obtain actual numerical results we must specify the scattering kernel. In practice, as long as there exists a procedure for evaluating the first few Legendre moments $\Sigma_n(E^{\dagger} \rightarrow E)$ we are in a position to attempt a solution of (1.6) either numerically or semi-analytically. An exact analytical solution only becomes possible if we make some drastic simplifying assumptions about the form of the scattering kernel. In the following chapters we shall make much use of a number of exact solutions obtained in this way.

In the early work on neutron transport theory a number of exact and good approximate solutions were derived in "one-speed theory", also referred to as monoenergetic theory and most commonly, but erroneously, as one-velocity theory. This approximation which is discussed in detail

by Davison (1957, Chap.4) and Tait (1964, Chap.3) is obtained, as the name suggests, if one assumes all the neutrons to have the same speed. For time independent problems this approximation may also be obtained by imposing the less restrictive conditions that the total cross-sections be independent of energy and that $\Sigma_0(E' \rightarrow E)$ be independent of E' . Thus it is sometimes called the constant cross-section approximation. These are very severe restrictions but ones which permit exact solutions to a large number of problems and we shall make maximum use of some of these solutions in dealing with the energy dependent Milne problem.

Generally the moments $\Sigma_n(E' \rightarrow E)$ may be calculated for each moderator from a quantum mechanical theory of scattering which has been reviewed by Williams (1966, Appendix IV) and is discussed further below. It has been shown that this quantum mechanical treatment of the scattering is fully consistent with the classical derivation of the transport equation. However all the transfer cross-sections calculated in this way have a general property of great importance, namely that they satisfy the condition of detailed balance.

This is essentially a necessary condition for the establishment of statistical equilibrium between neutrons and moderator which means that in an infinite, non-capturing medium there will be an equilibrium distribution of neutrons with a Maxwellian distribution in energy. It is derived ultimately from the transformation properties under time-reversal and space-reflection of the equations of motion which govern the scattering of

neutrons by the moderator atoms. In the present context it implies that:

$$M(E') \Sigma(E' \rightarrow E; \underline{\Omega}' \rightarrow \underline{\Omega}) = M(E) \Sigma(E \rightarrow E'; -\underline{\Omega} \rightarrow -\underline{\Omega}') \quad (1.8)$$

where $M(E)$ is the Maxwellian distribution at temperature T :

$$M(E) = \frac{E}{(kT)^2} \exp \left\{ -E/kT \right\} \quad (1.9)$$

and k is Boltzmann's constant. [see also (Williams 1966, Chap.1)].

The scattering kernels most often used may be conveniently divided into two distinct types which we shall call "mathematical" and "physical" models. Under the first heading we include those models which, while not representing a real physical moderator, are postulated for their mathematical convenience and can be made to satisfy certain important constraints. For example the often used separable kernel of Corngold et al (1963) given by:

$$\Sigma_0(E' \rightarrow E) = \Sigma_s(E) \Sigma_s(E') M(E) / \int_0^\infty M(E) \Sigma_s(E) dE \quad (1.10)$$

integrates over energy to give the correct total cross-section and furthermore satisfies the detailed balance condition (1.8) in the form:

$$M(E') \Sigma_0(E' \rightarrow E) = M(E) \Sigma_0(E \rightarrow E') \quad (1.11)$$

Sometimes called the amnesia kernel (Williams 1966, p.129) it virtually casts neutrons into thermal equilibrium with the moderator after a single

collision. Its prime advantage is that it enables one to obtain exact solutions in some cases to many energy dependent problems for which we were previously only able to obtain a solution in the one-speed approximation: for example with this scattering kernel exact solutions and numerical results for the energy dependent Milne problem have been obtained by the Wiener-Hopf technique (Williams 1964a; Arkuszewski 1967). This method relies on some results from complex variable theory. Basically one rearranges the transport equation so that each side of the equation is analytic in overlapping half-spaces in complex space: by analytic continuation and Liouville's theorem each part must be equal to a constant. Such a separation permits a solution in closed form. Exact solutions obtained by this approach for the separable kernel serve as standards against which the accuracy of approximate methods for more general kernels can be assessed. (see Chapters 4 and 5).

The "physical" models attempt a more realistic description of the scattering and are based on a knowledge of the atomic motions of the neutron scatterers. We give here but a brief and incomplete description of the problem of deriving the appropriate scattering kernels and refer the reader to Williams' book (Williams 1966, Chap. 2) for further details.

The magnitude of the scattering cross-sections is governed by the correlated motions of the atomic scatterers as represented by a space-time correlation function $G(\underline{r}, t)$ - this has been discussed in detail by Van Hove (1954). However the experimental and mathematical difficulties in determining $G(\underline{r}, t)$ are formidable and the alternative is to construct models which reproduce the general features of the scattering while reducing the

numerical difficulties. For this reason it is convenient to express the scattering kernel $\Sigma(E' \rightarrow E; \mu_0)$ in terms of a scattering law $S(\alpha, \beta)$ which is a function only of the energy transfer β and the momentum transfer α (Egelstaff and Schofield 1962):

$$\Sigma(E' \rightarrow E; \mu_0) = \frac{\Sigma_f}{4\pi} \left(\frac{A+1}{A}\right)^2 \cdot \left(\frac{E}{E'}\right)^{1/2} \exp\left\{-\frac{\beta}{2}\right\} S(\alpha, \beta) . \quad (1.12)$$

Here Σ_f is the free atom cross-section and A is the mass of the atoms in units of the neutron mass. Since the scattering law depends only on α and β it is clear that the separable kernel (1.10) cannot possibly represent a physical moderator.

Probably the simplest model to have some physical validity is the monatomic or free gas model. Because of the simplicity of the physical assumptions involved - no intermolecular forces, no internal structure - analytical expressions may be derived for $S(\alpha, \beta)$ and consequently for the first two moments of the scattering kernel (Kuščer and Ribarič 1958). Computer codes are available which generate $\Sigma_0(E' \rightarrow E)$ and $\Sigma_1(E' \rightarrow E)$ for the monatomic gas at any number of specified values of E and E' . Even for this model the analytic expressions are somewhat involved and for more complicated moderators analytic expressions are not generally available.

In that case one often considers the time transform of the scattering law, $I(\alpha, t)$ given by:

$$S(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} I(\alpha, t) \exp(i\beta t) dt \quad (1.13)$$

with the additional approximation:

$$I\left(\alpha, t + \frac{i}{2}\right) = \exp\left[-\alpha w(t)\right] \quad (1.14)$$

where $w(t)$ is a real function of t related to the mean square displacement of the scattering atom after time t . The imaginary time dependence of (1.14) is a quantum mechanical feature introduced by Schofield (1960) to ensure that the detailed balance condition is satisfied. This approximation is equivalent to the assumption that the self correlation function of the scattering atoms is a gaussian function of position and for this reason it is often referred to as the "Gaussian Approximation".

Experimentally it is usually only possible to determine $S(\alpha, \beta)$ over a restricted range of α and β . However it is possible to show that $w(t)$ may be obtained from $S(\alpha, \beta)$ in the limit of small α : then by means of the Gaussian Approximation one can rederive the scattering law for all values of α and β and hence compute the transfer cross-section $\Sigma_n(E^i \rightarrow E)$. The function $w(t)$ is itself closely related to the function $\rho(\beta)$ which for crystals is the phonon frequency distribution and for liquids and other moderators includes the diffusive and vibrational properties. (Egelstaff and Schofield 1962).

Thus we are faced with two alternatives within the limitations of the Gaussian Approximation. One can postulate the correct form for $w(t)$ based

on a precise knowledge of the function for large and small t and a reasonable interpolation for intermediate times and in this way evaluate $S(\alpha, \beta)$. Such a procedure was originally used to derive one model for water, namely the effective width model: a judicious choice of $w(t)$ once again permitted an analytic form for $S(\alpha, \beta)$ - (see Egelstaff and Schofield 1962). On the other hand one might equally well postulate the form of $\rho(\beta)$ whose shape will be fairly well established from scattering experiments. Nelkin (1960a) used this formulation in obtaining $S(\alpha, \beta)$ and hence $\Sigma_n(E' \rightarrow E)$ from a model for water which has become known as "Nelkin's model". For both these cases codes have been written which evaluate the first few moments of the scattering kernel at specified values of E and E' .

§1.3 A Review of the Green's Function Approach

This thesis is therefore concerned with a theoretical study of the thermal neutron Milne problem described in the preceding two sections. The simplest version of the problem, assuming isotropic scattering and no neutron capture has already been solved by Schofield (1963) with a variational method and reviewed in some detail by Tait (1964). Here we shall extend this approach to include anisotropic scattering and capture, concluding with a brief study of the effects of fission and finite geometries.

The technique adopted is to express the flux in the energy dependent problem in terms of the corresponding one-speed solution which is already well known: as a result some new one-speed, half-space Green's functions are introduced. A variational principle for the extrapolation length or a

closely related quantity may be written down and the angular distribution of emergent neutrons determined by iterating the trial function. Besides the Green's function technique which we shall describe in subsequent chapters there have been few analytical approaches to the problem which have not been restricted to particular scattering models. However Nelkin (1960b) has also employed a variational method for a general isotropic kernel which Kladnik and Kuscer (1961) have extended to include linearly anisotropic scattering while Conkie (1960) has used a purely P_1 approximation in which the angular flux, instead of being treated exactly, is expanded in a Legendre series and truncated after the second term. Prior to the present work the last two named were the only works to have included linearly anisotropic scattering whether for "mathematical" or "physical" kernels. For water moderators, at least, it is essential to account for anisotropic scattering.

Conkie's treatment is dominated by the thermalisation aspects of the problem while, on the other hand, the variational methods of Nelkin and of Kladnik and Kuscer give most emphasis to variations in the mean free path. The "Green's Function" method to be described here is sensitive both to variations in the mean free path and to the details of the scattering model [$\Sigma(E' \rightarrow E; \mu_0)$ and $\ell(E)$ are closely connected physically but mathematically they can be considered separately]. Furthermore this method has the advantage that in the case of no neutron capture it reduces to the correct limits for "constant (transport) mean free path" and for "no energy exchange".

In the next section we discuss briefly the relationship between neutron transport theory and radiative transfer theory. The remaining chapters are devoted to various aspects of the thermal neutron Milne problem.

The asymptotic spectrum far from the boundary which generally varies slowly over distances of the order of the mean free path is considered in Chapter 2. In the limit of no capture the form of the asymptotic flux is easily determined but when there is neutron capture we are faced with an eigenvalue problem presenting its own computational difficulties. Certain features of this are discussed in Chapter 2. We have already mentioned that the "Green's function" approach relies on some results from one-speed theory: in Chapter 3 we gather together those results which will be required in treating the capture-free, energy dependent Milne problem with anisotropic scattering which is then discussed in terms of a variational principle in Chapter 4. The main interest here lies in the transient flux which generally decays fairly rapidly with increasing distance from the boundary as well as the emergent angular distribution and the extrapolation length. In Chapter 4, too, we present the results of a number of computations based on the preceding theory which are critically compared with some experimental results for a water moderator and the results of other methods for simple scattering kernels. Chapter 5 deals with the effect of capture both on the one-speed solutions and, of course, on the energy dependent Milne problem itself. Again a comparison of the numerical results is made with results obtained by other methods. Finally in Chapter 6 we give an outline of the possible extension of the "Green's Function" method to more complex problems.

§1.4 Connection between Neutron Transport and Radiative Transfer Theory

Neutron transport theory has close connections through the Boltzmann equation with many branches of physics but the closest is undoubtedly with the theory of radiative transfer in stellar atmospheres. Indeed, many of the problems of neutron transport theory were effectively solved by astrophysicists even before the neutron was discovered. Direct analogues of the neutron flux, current and other parameters of neutron transport theory appear in the astrophysical literature and have been compared by Kourganoff (1952).

The Milne problem was first defined in terms of radiative transfer and a knowledge of the analogue of the emergent angular distribution of neutrons accounts for the phenomenon of limb darkening in the sun. That is the edges of the sun appear darker than the rest of the surface because of the deviation from the asymptotic solution at points close to the surface. It is well-known (Stewart et al 1966) that there is a direct equivalence between one-speed neutron transport and monochromatic radiative transfer and this equivalence extends, for time independent problems, to the constant cross-section approximation mentioned earlier and the "grey case" in radiative transfer which implies an absorption coefficient which is independent of frequency. Moreover it has recently been shown that this equivalence may also be extended to some special models in energy dependent neutron transport and non-grey radiative transfer (Stewart et al 1966). Despite the physical dissimilarity a mathematical equivalence can be established between the separable kernel described briefly in §1.2 and the uniform line-blanketing model of radiative transfer. A discussion of the latter model is outside the scope of this introduction.

The point we wish to make in a non-rigorous way is that the analogy between the Milne problem in neutron transport and radiative transfer is extremely close. We should not, therefore, be surprised if the variational principle which we shall derive for the thermal neutron Milne problem can also be usefully adapted to the corresponding problem in radiative transfer theory.

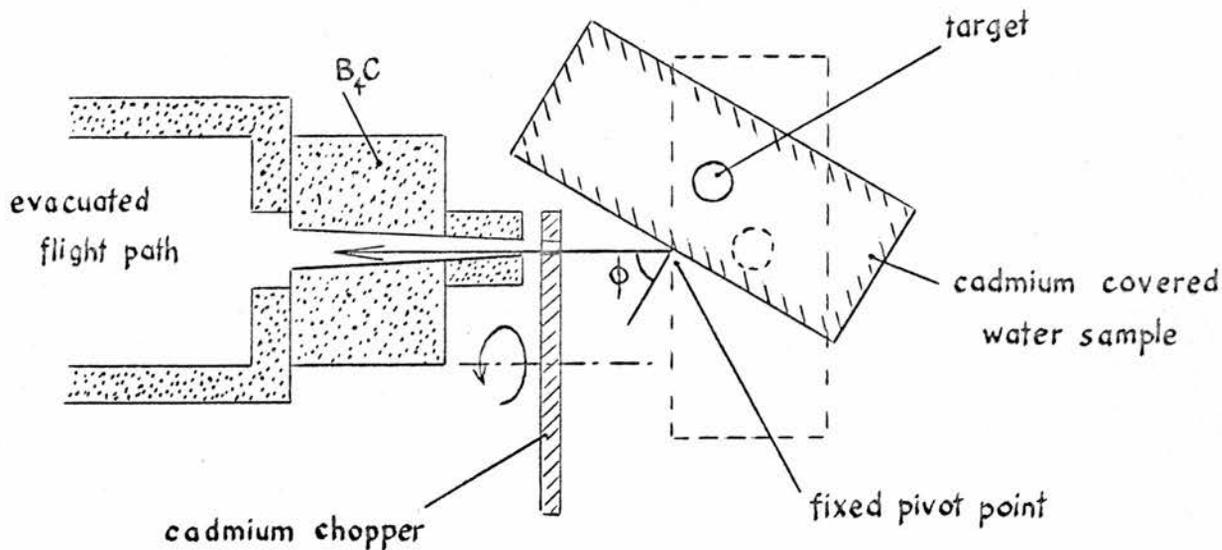


FIG. 1·I

Set-up for measuring angular dependent leakage spectra

$$\phi < 90$$

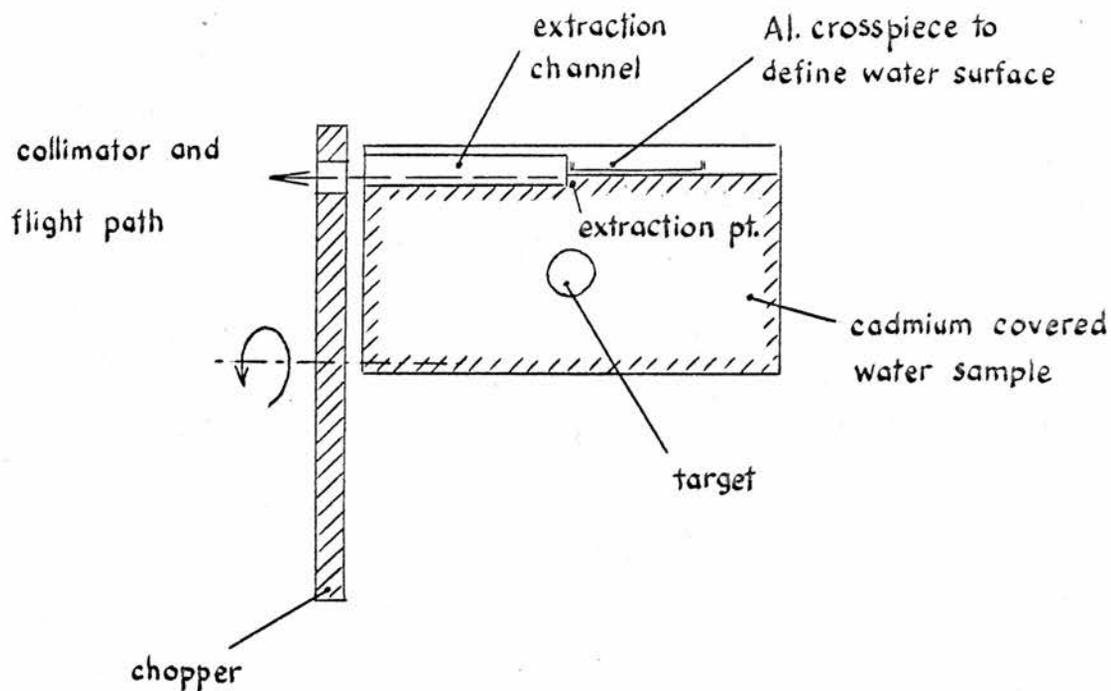


FIG. 1·II

Assembly for measuring the leakage spectra at the grazing angle

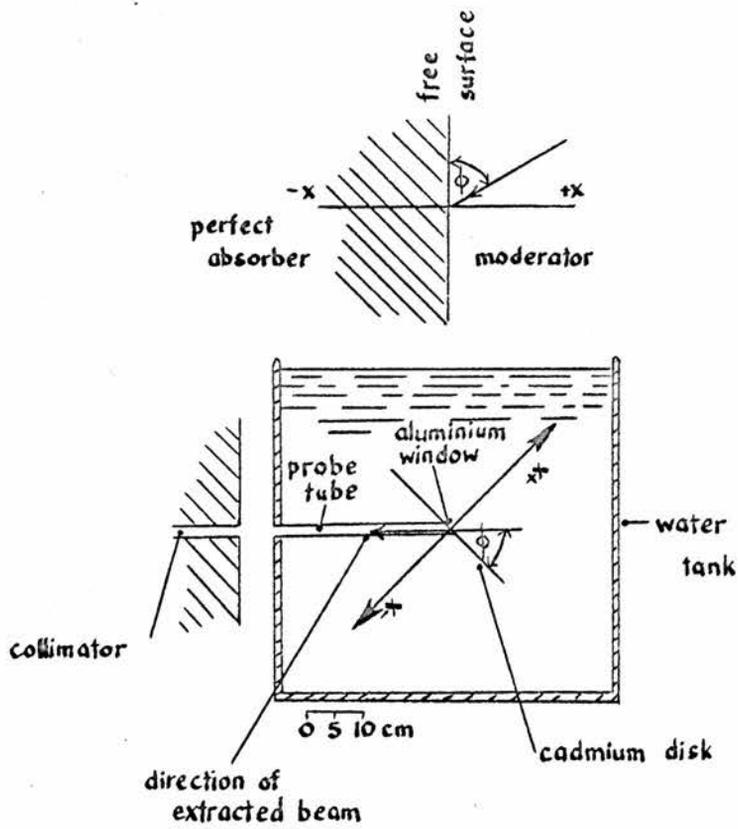


FIG. 1·III

Measurement of neutron spectrum near to a plane absorber

CHAPTER 2

INFINITE MEDIUM SOLUTIONS OF THE TRANSPORT EQUATION

§2.1 Introduction

The first step in any study of the Milne problem is the determination of the asymptotic flux far from the boundary. This leads to a discussion of the existence and properties of various eigen-solutions of the transport equation. Not only is this an essential part of the problem in its own right but it gives us valuable insight into the nature of general solutions of transport problems.

So, for the remainder of this chapter, we shall ignore the boundary and emphasise only the infinite medium solutions of the time independent transport equation. This is often referred to as the diffusion length problem for reasons which will become clear later. Looked at in another way it is concerned with the evolution in space of a distribution of neutrons incident upon the face of a semi-infinite medium in which our interest lies in points far from the boundary, where we expect the flux to be decaying exponentially with distance.

Furthermore this approach permits a review of "Case's method" which expresses the solutions to more general problems in terms of an expansion in the elementary solutions of the infinite medium equation and incidentally introduces many of the concepts of subsequent chapters.

Thus in §2.2 we consider the number and existence of eigen-solutions of the infinite medium equation in the simplest case of one-speed theory and isotropic scattering: we shall discuss the asymptotic solution both with and without capture. This will lead quite naturally to a discussion of "Case's method of elementary solutions" and the possibility of a solution to the Milne problem by this approach. In §2.3 we extend these considerations to the energy dependent problem and mention the effects of anisotropic scattering. Paragraph §2.4 deals with the theoretical predictions that under certain conditions no asymptotic equilibrium distribution may be possible and the implications of this for experiment.

Until the present work and that of other workers at about the same time little was known quantitatively about the eigen-solutions of the transport equation: therefore in §2.5 we present some numerical results for the free gas and water moderators with both isotropic and anisotropic scattering. Then in §2.6 we give quantitative meaning to the limits above which no equilibrium distribution exists (see §2.4). Finally in an appendix the numerical methods are described.

§2.2 One-speed Eigen-solutions and Case's Method

In introducing the eigenvalues and eigenfunctions of the thermal neutron transport equation we look first at the one-speed equation with isotropic scattering. As we mentioned in Chapter 1 this may be derived from (1.6), with only the first term in the Legendre expansion non-zero, by assuming all the neutrons to have the same energy E or alternatively

by assuming all the total cross-sections to be energy independent and $\Sigma_0(E' \rightarrow E)$ to be independent of E' . Whichever conditions we choose to impose the result is the much simpler transport equation:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{l} \right] \rho(z, \mu, l, L) = \frac{c}{2l} \rho_0(z, l, L) \quad (2.1)$$

where $\rho(z, \mu, l, L)$ is the one-speed directional neutron flux, $c = l/l_s$, and

$$l_s = 1/\Sigma_s; \quad l = 1/(\Sigma_s + \Sigma_a) \quad (2.2)$$

When all the neutrons have the same energy l will be the mean free path at that energy (i.e. $l=l(E)$). The significance of the functional parameter L will become apparent from the following remarks.

We look for solutions of (2.1) which are separable in space and angle, having the form:

$$\rho(z, \mu, l, L) = e^{-z/L} \rho(\mu, l, L) \quad (2.3)$$

with $\rho_0(l, L)$ normalised to unity. Inserting (2.3) into (2.1) we find that $\rho(\mu, l, L)$ satisfies:

$$\left[-\frac{\mu}{L} + \frac{1}{l} \right] \rho(\mu, l, L) = \frac{c}{2l} \quad (2.4)$$

Provided $L > l$ we can divide both sides of (2.4) by $\left[-\frac{\mu}{L} + \frac{1}{l} \right]$ and integrate over angle to obtain an equation for L :

$$c^{-1} = \frac{L}{2\ell} \ln \left[\frac{L + \ell}{L - \ell} \right] \quad (2.5)$$

or

$$\frac{\ell}{L} = \text{Tanh} \left(\frac{\ell}{cL} \right) .$$

Equation (2.5) has just two solutions $\pm L_0$ (Davison 1957, p.53) where the quantity L_0 is called the diffusion length. Besides this solution for $L > \ell$ there is also an infinite set of 'singular' solutions for $L \leq \ell$. In this range there exists some value of μ for which $\left[-\frac{\mu}{L} + \frac{1}{\ell} \right]$ is zero. In that case the solutions have the form (Case 1960; see also Dirac 1958, pp.61 and 195):

$$\rho(\mu, \ell, L) = \frac{c}{2\ell} P \frac{1}{\left[-\frac{\mu}{L} + \frac{1}{\ell} \right]} + \lambda(\ell, L) \delta \left(-\frac{\mu}{L} + \frac{1}{\ell} \right) \quad (2.6)$$

where $\lambda(\ell, L)$ is determined by the normalisation and " P " indicates that in integrations over μ the principal part should be taken. For the rigorous justification of (2.6) see (Case and Zweifel 1967).

This set of solutions has a number of important properties (Case 1960). Firstly any two solutions $\rho(\mu, \ell, L)$ and $\rho(\mu, \ell, L')$ are orthogonal; that is:

$$\int_{-1}^{+1} \mu \rho(\mu, \ell, L) \rho(\mu, \ell, L') d\mu = 0 \quad \text{for } L \neq L' \quad (2.7)$$

and for $L=L'$ the integral (2.7) is equal to a constant determined by the normalisation. Secondly, the functions $\rho(\mu, \ell, \pm L_0)$ and $\rho(\mu, \ell, L)$ for

$-\ell \leq L \leq \ell$ form a complete set defined in the interval $-1 \leq \mu \leq 1$. Thus we can express any function $\eta(\mu, \ell)$ as a linear combination of these elementary solutions:

$$\eta(\mu, \ell) = A_{+L_0}(\ell) \rho(\mu, \ell, +L_0) + A_{-L_0}(\ell) \rho(\mu, \ell, -L_0) + \frac{1}{\ell} \int_{-\ell}^{\ell} A(\ell, L) \rho(\mu, \ell, L) dL \quad (2.8)$$

and the coefficients may be determined with recourse to the orthogonality relationships. These theorems are proved in Case's paper for a wide range of functions $\eta(\mu, \ell)$.

Lastly there is the very important and powerful "partial range completeness theorem". This may be defined formally in the following way: if α, β are two real numbers such that $-1 \leq \alpha < \beta \leq 1$ then

- (a) if $\alpha \neq -1$ and $\beta \neq 1$ the functions $\rho(\mu, \ell, L)$ for $\ell\alpha \leq L \leq \ell\beta$ are complete for functions $\eta(\mu, \ell)$ defined in the interval $\alpha \leq \mu \leq \beta$;
- (b) if $\alpha = -1$ (or $\beta = +1$) the set of functions $\rho(\mu, \ell, L)$ for $\ell\alpha \leq L \leq \ell\beta$ is complete when supplemented by $\rho(\mu, \ell, -L_0)$ [or $\rho(\mu, \ell, +L_0)$].

So, for instance, we can write down the solution to the one-speed Milne problem: a solution is required in the range $0 \leq z \leq \infty$ subject to the boundary conditions:

$$(i) \quad \rho(0, \mu, \ell, L) = 0 \quad 0 < \mu \leq 1 \quad (2.9)$$

$$(ii) \quad \lim_{z \rightarrow \infty} \rho(z, \mu, \ell, L) = e^{z/L_0} \rho(\mu, \ell, -L_0) \quad (2.10)$$

The complete solution may then be written down as:

$$\rho(z, \mu, \ell, L) = e^{z/L_0} \rho(\mu, \ell, -L_0) + A_{+L_0}(\ell) e^{-z/L_0} \rho(\mu, \ell, +L_0) + \frac{1}{\ell} \int_0^\ell A(\ell, L) \rho(\mu, \ell, L) e^{-z/L} dL \quad (2.11)$$

while the boundary condition (i) implies that, from (2.11):

$$-\rho(\mu, \ell, -L_0) = A_{+L_0}(\ell) \rho(\mu, \ell, +L_0) + \frac{1}{\ell} \int_0^\ell A(\ell, L) \rho(\mu, \ell, L) dL . \quad (2.12)$$

Applying the "partial range completeness theorem" to (2.12) we are able to find the coefficients $A_{+L_0}(\ell)$ and $A(\ell, L)$ and hence completely solve the problem.

Before becoming embroiled in the further complications of energy dependent theory we shall take this opportunity to emphasise some of the conclusions which may be drawn even on the basis of one-speed theory. One advantage of the normal mode expansion method is that it has a fairly direct physical interpretation. Another is that it is possible to extend the theory, in principle at least, to take account of anisotropic scattering and energy dependence (Mika 1961; Zelazny 1966), and there is no distinction between problems with and without capture. It might be asked, therefore, why we seek a variational solution of the thermal neutron Milne problem when a ready-made solution already exists in terms of the singular eigenfunctions of the infinite medium transport equation.

The main disadvantage of Case's method is that even for one-speed problems it yields expressions for the flux, angular distribution and extrapolation length which are, at best, unwieldy. Although the energy dependent Milne problem can be solved formally by this approach for the separable kernel (Mika 1965) and in a multigroup version of this method for more general kernels (Zelazny 1966) it is quite unsuitable for convenient numerical computation. This is illustrated by the wealth of papers on theoretical aspects of Case's method and the contrasting dearth of numerical results contained in them. On the other hand the variational method lends itself readily to fairly accurate numerical computations.

It is evident from the above considerations that the diffusion length L_0 plays a fundamental rôle in neutron transport theory and that an accurate determination of it will be an essential part of the complete solution of the Milne problem. We shall learn in the next section that one effect of energy exchange may be to introduce other eigenvalues analogous to L_0 at discrete values of L greater than the maximum value of the mean free path ℓ_{\max} and less than L_0 . In a later section we shall report on calculations in which all the discrete eigenvalues (L_n) are investigated for certain moderators.

Finally we should note the effect of neutron capture on the form of the asymptotic solution. The one-speed flux may be written in the form:

$$\rho(z, \mu, \ell, L) = \rho_{\text{asy}}(z, \mu, \ell, L) - \rho_{\text{tr}}(z, \mu, \ell, L) \quad (2.13)$$

where

$$\rho_{\text{asy}}(z, \mu, \ell, L) = e^{z/L_0} \rho(\mu, \ell, -L_0) + A_{+L_0}(\ell) e^{-z/L_0} \rho(\mu, \ell, +L_0) \quad (2.14)$$

and $\rho_{\text{tr}}(z, \mu, \ell, L)$ is given in terms of the singular eigenfunctions corresponding to the eigenvalues $-\ell \leq L \leq \ell$. Thus, from (2.4), we see that:

$$\rho_{\text{asy}}(z, \mu, \ell, L) = \frac{c}{2\ell} \left[e^{z/L_0} \left/ \left(\frac{\mu}{L_0} + \frac{1}{\ell} \right) + A_{+L_0}(\ell) e^{-z/L_0} \left/ \left(-\frac{\mu}{L_0} + \frac{1}{\ell} \right) \right. \right]. \quad (2.15)$$

Therefore besides L_0 we also have to determine A_{+L_0} which, as we shall see in Chapter 5, is closely related to the extrapolation length for those problems which consider neutron capture. However when the capture becomes small L_0 becomes infinite and c tends towards $1 + O\{\ell/L_0\}$ so that expanding the terms in (2.15) to first order in $1/L_0$ we find:

$$\rho_{\text{asy}}(z, \mu, \ell, L) = \zeta(\ell) \left[z - \mu\ell + \xi(\ell) \right] \quad (2.16)$$

where $\zeta(\ell)$ is a normalising factor and $\xi(\ell)$ is related to A_{+L_0} . Thus the complete solution to the no-capture problem is a linear combination of the two solutions " $z - \mu\ell$ " and a constant. This form of solution implies that the flux becomes negative at some point in the medium: the paradox is resolved because it is not possible to obtain a steady state

solution if there is a plane source in a non-capturing, infinite medium. Integrating (2.16) over angle we find that $\xi(\ell)$ is the linear extrapolation length (or the extrapolated end-point) for the one-speed, capture-free Milne problem with isotropic scattering: that is at a distance $\xi(\ell)$ from the boundary, outside the medium, the asymptotic flux falls to zero. We make this distinction between the form of the asymptotic flux for the situations with and without capture since we shall treat each problem separately in subsequent chapters. Similar remarks apply to the energy dependent counterpart.

In this section, on the basis of one-speed theory, we have introduced many of the concepts relevant also to the energy dependent diffusion length problem and the thermal neutron Milne problem. In the following section we consider some of these in more detail.

§2.3 Elementary Solutions of the Energy Dependent Problem

In considering the energy dependent problem we treat first the no-capture case for which we expect an infinite diffusion length and the associated neutron distribution to be Maxwellian. With isotropic scattering the transport equation (1.6) is:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \Psi(z, \mu, E) = \frac{1}{2} \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi(z, E'). \quad (2.17)$$

As before we adopt the ansatz that:

$$\Psi(z, \mu, E) = e^{-z/L} \Psi_L(\mu, E) \quad (2.18)$$

with the result that $\Psi_L(\mu, E)$ satisfies:

$$\left[-\frac{\mu}{L} + \frac{1}{\ell(E)} \right] \Psi_L(\mu, E) = \frac{1}{2} \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi_L(E') \quad (2.19)$$

For L greater than the maximum value of the mean free path ℓ_{\max} discrete solutions exist which satisfy the eigenvalue equation:

$$\Psi_L(E) = \frac{L}{2} \ln \left[\frac{L + \ell(E)}{L - \ell(E)} \right] \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi_L(E') \quad (2.20)$$

with the boundary conditions that for $E \rightarrow 0, \infty$ the flux $\Psi_L(E)$ is zero. For liquids the maximum value of the mean free path will be that for large E given by the inverse of the free atom cross-section. For solid moderators ℓ_{\max} may occur at low energies below the Bragg cut-off.

One solution of (2.20) occurs for L infinite with $\Psi_L(E) = M(E)$. However one might also expect discrete solutions $L_n (n=1, 2, \dots)$. At the time this research was begun knowledge of the existence and number of these solutions was rudimentary and confined to the monatomic gas moderator of atomic mass A .

In the limit of large atomic mass the number of roots becomes large: simple expressions for evaluating the eigenvalues exist in this case based on the assumption that the total scattering cross-section $\Sigma_s(E)$ approaches a constant (Ferziger and Leonard 1963). In particular:

$$L_1 = \left(1 + \frac{1}{A} \right) \left(\frac{A}{6} \right)^{\frac{1}{2}} \ell_{\max} \quad (2.21)$$

L_1 is called the thermalisation length and represents the distance within the medium which the neutron distribution requires to relax to equilibrium. Hutchinson (1965) has found that for $A < 3$ no solutions other than L_0 exist and for $A = 3$ the existence of a thermalisation length at $L_1 = 1.005 \ell_{\max}$ was still rather doubtful due to the uncertainties inherent in the numerical methods. For $A \geq 4$ at least two eigenvalues exist. A somewhat improved version of Hutchinson's numerical method has confirmed these conclusions and the calculations have been extended to take account of anisotropic scattering (see §2.5).

A quantity related to L_1 is the rethermalisation length encountered in experiments with differentially heated stacks. Ideally two half-spaces in contact are maintained at different temperatures and the rethermalisation length in each medium is a measure of the distance required to establish equilibrium. It has been suggested without much justification that if L_1 does not exist then neither will the rethermalisation length (Williams 1966a). This is not self-evident. Recent experimental results to test for the existence of a rethermalisation length are inconclusive (Goddard et al 1967).

For $L \leq \ell(E) \leq \ell_{\max}$ there will again be a continuum of singular solutions given by:

$$\Psi_L(\mu, E) = \frac{1}{2} P \frac{1}{\left(-\frac{\mu}{L} + \frac{1}{\ell(E)}\right)} \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi_L(E') + S_L(E) \delta\left(-\frac{\mu}{L} + \frac{1}{\ell(E)}\right) \quad (2.22)$$

where $S_L(E)$ is an arbitrary function. Although our understanding of the rôle played by the continuum spectrum has improved in recent years it is probably true to say that no simple physical interpretation of these solutions has yet been given. Orthogonality and completeness theorems may be obtained for the energy dependent problem but it is doubtful whether they have much practical value in the sense of finding numerical results (Zelazny 1966; Zweifel and Inönü 1967). In any case our main interest lies in the existence or otherwise of the discrete solutions.

We have so far restricted our attention to a capture-free medium where we saw that one solution was given by $L = \infty$ with $\Psi_L(E) = M(E)$. When capture is introduced this eigenfunction will be displaced from a Maxwellian distribution and the eigenvalue L will, in general, assume some finite value L_0 called the thermal neutron diffusion length (an exception to this rule is discussed in the next section). There will also be a corresponding negative eigenvalue $-L_0$ and again we might expect other discrete eigenvalues $L_n > l_{\max}$. Even now there exist no general theorems about the number and existence of discrete eigenvalues for the diffusion length problem and little work has been done along these lines. By contrast a complementary problem in time dependent theory relating to the number of time decay constants has received a great deal of attention (Williams 1966, p158). Usually however one or more pairs of discrete eigenvalues exist on the real axis above l_{\max} . The pair of largest eigenvalues ($\pm L_0$) is simple (except for a non-capturing medium when the pair merges at infinity) and corresponds to a unique pair of

non-negative eigenfunctions $\Psi_{\pm L_0}(\mp\mu, E)$ which we shall meet in another guise in Chapter 5. According to Kuscer (1967), the principle of detailed balance and the fact that the capture cross-section is non-negative indicate that all the discrete eigenvalues L_n are real and that none are embedded in the continuum.

Our calculations of the discrete eigenvalues L_n are based on the B_n approximation which is derived as follows. With anisotropic scattering the transport equation is:

$$\left[-\frac{\mu}{L} + \frac{1}{\ell(E)} \right] \Psi_L(\mu, E) = \frac{1}{2} \sum_{p=0}^{\infty} (2p+1) \int_0^{\infty} dE' \Sigma_p(E' \rightarrow E) \Psi_{L_p}(E') P_p(\mu) \quad (2.23)$$

where it is clear that $\Psi_{L_p}(E)$ represents the p 'th Legendre moment of the angular flux corresponding to an eigenvalue L . Dividing by $\left[-\frac{\mu}{L} + \frac{1}{\ell(E)} \right]$ and integrating over angle we obtain a set of coupled equations in the various angular moments of the flux:

$$\Psi_{L_m}(E) = \frac{1}{2} \sum_{p=0}^{\infty} (2p+1) \int_0^{\infty} dE' \Sigma_p(E' \rightarrow E) \Psi_{L_p}(E') \int_{-1}^{+1} \frac{P_p(\mu) P_m(\mu) d\mu}{\left[-\frac{\mu}{L} + \frac{1}{\ell(E)} \right]} \quad (2.24)$$

These equations are valid whether there is capture or not and form the basis of the B_n approximation in which the series on the right is truncated after $p=n$. Thus if $\Sigma_p(E' \rightarrow E) = 0$ for $p > n$ the solution is exact.

It is often the case that the first few moments of the scattering kernel are sufficient to represent anisotropic scattering. The B_n approximation may be contrasted with the P_n approximation in which one truncates a Legendre series expansion of $\Psi_L(\mu, E)$ after the n 'th term; that is one approximates the solution to an exact equation. In the B_n method one finds the exact solution (by dividing (2.23) throughout by $\left[-\frac{\mu}{L} + \frac{1}{\ell(E)}\right]$) to an approximate equation. In an infinite medium the B_n approximation is to be preferred.

We have calculated L_n for water and the free gas moderators ($A=1$ to 12) in the B_0 and B_1 approximations assuming no neutron capture (see §2.5) and also in the B_0 approximation with the no-capture restriction removed. Calculations have also been carried out by others (e.g. Wood 1965) in the B_n , P_n and diffusion approximations. In the last named approximation, which may only be used when the spatial curvature in the flux is not too great, the current is assumed to be given by:

$$\Psi_1(z, E) = D(E) \frac{\partial}{\partial z} \Psi_0(z, E) \quad (2.25)$$

where $D(E)$ is the diffusion coefficient. Of these approximations only the B_n theory predicts the true singular behaviour of the transport equation for while the B_n approximation correctly predicts a lower limit of ℓ_{\max} for the discrete eigenvalues, diffusion theory predicts a limit point of $\ell_{\max}/\sqrt{3}$ and the P_n approximations only tend to the proper limit as $n \rightarrow \infty$. For example P_3 theory predicts a limit point of $\ell_{\max}/\sqrt{1.96}$. These limits are obtained by expanding the coefficient:

$$\Lambda(\ell(E), L) = \frac{L}{2} \ln \left[\frac{L + \ell(E)}{L - \ell(E)} \right] \quad (2.26)$$

in powers of $1/L$ and retaining terms up to $(1/L)^2$ in the diffusion approximation and up to the fourth power in P_3 theory. Thus while all three approaches may predict results which are in substantial agreement for $L_n \gg \ell_{\max}$ there may be significant differences for L_n close to the limit point.

In our numerical computations we shall determine the eigenvalues L_n which occur above ℓ_{\max} . In any numerical calculation we would also expect to find discrete eigenvalues below ℓ_{\max} but these will be ignored. When the energy mesh or number of energy points in the numerical integration is improved the eigenvalues above ℓ_{\max} will converge to a particular value (although another eigenvalue may appear above the limit point) but those below ℓ_{\max} will simply redistribute themselves according to the energy mesh and may move appreciably - they are of course an attempt to represent the continuum (Williams 1966, p185). If an infinite number of energy points could be taken the true discrete spectrum would be given and below ℓ_{\max} the eigenvalues would close together to form a continuous line. From this kind of argument it is not difficult to see that if a particularly heavy weighting is given to one of the eigenvalues below ℓ_{\max} a true asymptotic relaxation might, erroneously, be supposed by an experimenter. A very recent paper by Corngold and Durgun (1967) puts this sort of discussion on a far more rigorous basis.

§2.4 Critical Absorption Theorem

We now wish to investigate the effect on the eigenvalues of increasing absorber concentration. In the first place it is clear that L_0 cannot be less than l_{\max} . With the exception of the non-physical case of constant scattering and capture cross-sections (Corngold 1964, 1966) and Leonard (1965) have shown through the "maximum absorption theorem" that this limiting value is reached for some finite concentration of absorber and that for stronger absorption the diffusion length does not exist; that is the asymptotic flux no longer has a truly exponential decay with distance. Consequently all the higher eigenvalues ($L_n < L_0$) disappear too. Physically this is not surprising since if the capture is strong one would expect that a typical neutron has a strong probability of being captured before it has had sufficient collisions to bring it into thermal equilibrium. Thus the decay of the flux is dominated more strongly by the rate of neutron capture than by the decay to an equilibrium distribution. In brief, the spectrum is distorted by capture more rapidly than it regains equilibrium by scattering.

If the absorption law has the form $\exp(-cE)$ it is possible that the maximum absorption theorem will be violated since then the flux will be so hardened towards higher energies that it no longer "sees" the absorption and huge changes in absorber concentration are required to alter the eigenvalues by even a small amount. However for absorption laws of the form $1/v$, e^{-av} and e^{-av}/v the theorem is undoubtedly valid, (Corngold 1966).

Corngold's proof is restricted to isotropic scattering but it is unlikely that the relaxation of this condition will affect the conclusions.

We have determined the critical absorber concentration for the free gas and water moderators in both the B_0 and B_1 approximations (see §2.6). It is evident from the remarks at the end of the preceding section that it is essential that we use B_n theory, and not P_n or diffusion theory, since we are in effect determining the absorber concentration which leads to a diffusion length an infinitesimal amount greater than the limit point l_{\max} . Other approximations are seriously in error in this region as we can see from the results of Wood (1965).

It should be emphasised that our calculations do not provide a proof that the spatial eigenvalues disappear. The numerical procedures are limited to a restricted energy range and it could be argued that in this case the hardening of the spectrum, which occurs for the absorption laws usually considered where there is a preferential absorption of slower neutrons, is severe at arbitrary high energies outside the domain under consideration. Of course such an effect is extremely unlikely except for very rapidly varying absorption laws. Within the limitations set by the restricted energy range inherent in any computational procedure we feel that the method described in Appendix §2A.1 for calculating the critical absorption concentration is more reliable than the extrapolative procedure suggested by Wood (1964, 1965). The diffusion length is determined by Wood for various absorber concentrations and the results are extrapolated to find the absorption for which $L_0 = l_{\max}$. However if the diffusion length approaches

l_{\max} very slowly for increasing absorber concentrations this method may be extremely inaccurate unless L_0 is evaluated at a number of points very close to l_{\max} .

The most obvious experimental ramification of the preceding arguments is that the measured diffusion length must lie above l_{\max} . Several experiments have been analysed in this context and the suggestion made that an asymptotic mode did not in fact exist (Corngold and Michael 1964). The most interesting experiments would be those conducted with crystal moderators in which there is elastic coherent scattering and consequently a Bragg cut-off in the scattering cross-section at about 0.001 eV below which $\Sigma_s(E)$ is very small. Those few neutrons having energies below the Bragg cut-off have very long mean free paths and control the approach of the entire distribution to equilibrium. If they are not "seen" by the experimenter the full distribution will behave almost as though l_{\max} were evaluated in the range $E \gtrsim 0.001$ eV and the measured diffusion length will appear to be smaller than l_{\max} . Supposedly asymptotic modes for $L < l_{\max}$ can also be explained in terms of peaks in the continuum distribution of eigenfunctions (Corngold and Durgun 1967).

During 1967 another associated problem has attracted some attention (Williams 1967). It has been shown that the diffusion length in a block of material of finite transverse dimensions ceases to exist when the transverse dimensions are sufficiently small. If the system is decreased in size still further it is found that the transverse flux shape changes continually along the axis of the system. For water the

minimum dimensions for L_0 to exist are about 3 cms. square but for graphite and beryllium it is more than a metre square. Thus for the last two materials a fairly large block is required for the diffusion length to exist.

§2.5 Numerical Values for L_n in the B_0 and B_1 Approximations

In this section we discuss the number and numerical values of the eigenvalues L_n for (i) the monatomic gas model of atomic mass A assuming no neutron capture and (ii) the Nelkin model for water with oxygen accounted for as an isotropically scattering free gas of mass $A=16$ and appropriate cross-sections for scattering and absorption taken from Hughes and Schwartz (1958). In this case the absorption follows the $1/v$ law. Both moderators were assumed to be at a temperature of 300°K . We mention here only the results of the calculations and reserve a description of the numerical techniques for an appendix.

(i) The Monatomic Gas of Atomic Mass A

In the B_0 approximation, that is with isotropic scattering, Hutchinson (1965) has evaluated the eigenvalues when there is no neutron capture for gases of mass $A=1,2,3,4,6,8$ and 12 . The numerical method is given in an appendix and the results are shown in Figure 2.I and Table 2.I: also shown are the heavy gas results for L_1 described in §2.3. The comparison suggests that Hutchinson's values may be in error because, instead of converging with increasing mass, the results tend to diverge. We found that this was primarily due to the choice of mesh in the numerical integrations over energy: therefore a few of Hutchinson's calculations were repeated with an improved energy mesh and these results

too are shown in Figure and Table 2.I. Even with the few points plotted it is clear that the computed values are now compatible with the heavy gas results.

The more important conclusions that may be drawn from these calculations are unaltered. For $A < 3$ no thermalisation length exists. For $A = 3$ Hutchinson predicted a thermalisation length ($L_1 = 1.005 \ell_{\max}$) so close to the limit point that one might doubt its existence: with the improved energy mesh we find $L_1 = 1.037 \ell_{\max}$ thus confirming its presence. For $A \geq 4$ the number of eigenvalues increases steadily. It should be remarked that the difference between our results and those of Hutchinson is quite noticeable for L_n close to ℓ_{\max} : indeed for $A = 8, 12$ an additional eigenvalue appears just above the limit point which was not there previously.

These computations bear out the results of Williams (1966a) who was able to predict the existence or otherwise of a thermalisation length by the W.K.B. method. By means of a synthetic kernel which is exact for the proton gas model (Cadilhac 1964) the usual integro-differential form of the transport equation may ultimately be converted to a second order differential equation to which the W.K.B. method may be applied. In contrast to the variational and other methods the W.K.B. method is particularly suited to an accurate study of the higher eigenvalues. Thus Williams too is able to predict a thermalisation length for the gas of mass $A = 3$ without being able to specify its value and no thermalisation length for $A = 1, 2$. He suggests that as A increases so will the number of eigenvalues but implies that for finite mass there will be a finite number.

Including anisotropic scattering through the B_1 approximation but retaining the assumption of no capture the equations (2.24) become:

$$\begin{aligned} \Psi_{L_0}(E) &= \Lambda(\ell(E), L) \int_0^\infty dE' \Sigma_0(E' \rightarrow E) \Psi_{L_0}(E') \\ &\quad + 3L \left[-1 + \frac{\Lambda(\ell(E), L)}{\ell(E)} \right] \int_0^\infty dE' \Sigma_1(E' \rightarrow E) \Psi_{L_1}(E') \\ \Psi_{L_1}(E) &= L \left[-1 + \frac{\Lambda(\ell(E), L)}{\ell(E)} \right] \int_0^\infty dE' \Sigma_0(E' \rightarrow E) \Psi_{L_0}(E') + \frac{3L^2}{\ell(E)} \\ &\quad \times \left[-1 + \frac{\Lambda(\ell(E), L)}{\ell(E)} \right] \int_0^\infty dE' \Sigma_1(E' \rightarrow E) \Psi_{L_1}(E') \quad (2.27) \end{aligned}$$

and again the numerical method of solution is described in the Appendix. Only the free gases of atomic mass 1 to 4 were considered since it is for low mass numbers that the effect of anisotropic scattering should be most significant. Furthermore we know that even in the B_0 approximation the errors for $A=8, 12$ will show a marked increase compared with those for the lower mass numbers due mainly to the difficulty in integrating $\Sigma_0(E' \rightarrow E)$ accurately over energy to give $\Sigma_s(E)$ - see Appendix §2A.1. In the B_1 approximation this type of error will be still more accentuated. The results are presented in Figure 2.II and Table 2.II which show that the most interesting effect due to anisotropic scattering is that a thermalisation length appears above the limit point for $A=1$ and 2 while for $A=3$ the thermalisation length is now well established.

In both B_0 and B_1 approximations the thermalisation length is seen to increase linearly with increasing mass, at least for the small mass numbers. This effect could probably be explained in terms of a small mass expansion of the scattering kernel or possibly by means of a synthetic kernel such as the separable kernel or the secondary model, used to such good effect by Williams (1966a), which is exact for the proton gas. However it does not seem to be a point of great physical interest and will not be mentioned again.

So far we have only been concerned with eigenvalues determined for the case of zero capture: as part of the calculations in Chapter 5 the diffusion length L_0 has been evaluated in the B_0 approximation for a monatomic gas with $1/v$ type capture. The results are given in Tables 5.I to 5.IV where the absorber concentration is prescribed by the parameter β :

$$\Sigma_a(E) = \beta \left(\frac{kT}{E} \right)^{1/2} ; \quad \ell_{\max} = 1 \quad (2.28)$$

and we consider both the full monatomic gas kernel and the separable kernel representation. For the latter model the eigenvalues are given as the roots of:

$$V(L) = 1 - \hat{C} \left\{ \frac{L}{2} \ln \left[\frac{L + \ell(E)}{L - \ell(E)} \right] \right\} = 0 \quad (2.29)$$

where the integral operator \hat{C} is defined by:

$$\hat{C} \{f(E)\} = \int_0^{\infty} \frac{M(E) f(E)}{\ell^2(E)} dE \quad / \quad \int_0^{\infty} \frac{M(E)}{\ell(E)} dE \quad . \quad (2.30)$$

Fairly simple analytic expressions for $\ell(E)$ exist for the monatomic gas with the result that the roots are determined rather easily (Arkuszewski 1967). The values of L_0 which we have determined are the result of a direct numerical computation without making use of this simplification: they are seen to be in good agreement with Arkuszewski's results throughout. It is to be expected therefore that the corresponding numbers for the full kernel will be equally accurate since the computations were consistent. The results obtained numerically by Wood (1965) in the B_0 approximation for the proton gas are very slightly low but this may be due to the fact that only 25 energy points were used: some convergence tests with 35 energy points (Wood 1964) appear to bear this out.

Wood (1964, 1965) has also calculated L_0 and L_1 for other gas moderators with finite capture in the diffusion and P_3 approximations. They only confirm the general conclusion that neither of these approximations is sufficient to accurately determine the eigenvalues L_n if the absorption is strong or L_n is close to the limit point ℓ_{\max} .

(ii) The Nelkin Model for Water

We have performed similar calculations in the B_0 and B_1 approximations for a water moderator. We found that no thermalisation length exists either for unpoisoned water or when capture is neglected.

In the B_0 approximation we found the diffusion length to be 2.43 cms. and the introduction of anisotropic scattering through the B_1 approximation does not greatly alter this result ($L_0 = 2.81$ cms.). This is in excellent agreement with the experimental value of 2.82 cms. obtained by Besant and Grant (1966) which is one of the most recent measurements of L_0 . Earlier measurements tended to give a somewhat lower value (~ 2.78 cms.) but showed a spread from about 2.71 cms. to 2.87 cms. Thus it appears that first order anisotropic scattering may be sufficient in determining the diffusion length in water, at least when the scattering is described by Nelkin's model.

Honeck (1962) too has evaluated L_0 in the B_n approximations up to B_3 for "Nelkin water" in which there is a variable amount of absorber poison. Repeating the calculation for a number of absorber concentrations he reports the coefficients α_1 , α_2 and α_3 in an expansion of the form:

$$\frac{1}{L_0} = \alpha_1\beta - \alpha_2\beta^2 + \alpha_3\beta^3 \quad (2.31)$$

where three terms are found to be adequate even for quite high absorption. In this way he finds for the pure water moderator

Approximation:	B_0	B_1	B_2	B_3
Diffusion length L_0 (cms)	2.43	2.80	2.80	2.80

confirming that the B_1 approximation is adequate to determine L_0 for water. It was only because Honeck did not consider very high absorber concentrations that he was able to accurately estimate the diffusion length before the full mathematical complexity of the diffusion length problem was fully appreciated.

More detailed calculations of L_0 for a water moderator with a number of different poisons have been made by Goyal and Ghatak (1966): although a comparison is made with B_0 transport theory their results are generally from diffusion theory with anisotropic scattering accounted for in calculating the diffusion coefficient $D(E)$. Since there is doubt as to the validity of diffusion theory especially for high absorption and non- $1/v$ type capture we shall not discuss their results further.

In concluding this section we shall mention one other method of estimating eigenvalues of the transport equation: this is a variational principle formulated by Schofield (unpublished) which may be especially useful if the scattering is peculiarly anisotropic. In summary the method is as follows; the transport equation with anisotropic scattering is written:

$$\left[-\frac{\mu}{L} + \frac{1}{\ell(E)} \right] \Psi_L(\mu, E) = \int_{-1}^{+1} d\mu' \int_0^{\infty} dE' \Sigma(E' \rightarrow E; \mu_0) \Psi_L(\mu', E'). \quad (2.32)$$

For convenience it is assumed that $\ell(E)$ is a monotonically increasing function of energy which tends to unity for large E with the result that we may adopt $\ell(E)$ as the independent variable instead of E . Then (2.32) may be written as:

$$\left[-\frac{\mu}{L} + \frac{1}{\ell} \right] \Psi_L(\mu, \ell) = \int_{-1}^{+1} d\mu' \int_0^1 d\ell' \Sigma(\ell' \rightarrow \ell; \mu_0) \Psi_L(\mu', \ell'). \quad (2.33)$$

Since the adjoint flux $\Psi_L^+(\mu, \ell)$ is simply given by

$$\Psi_L(\mu, \ell) = M(\ell) \psi_L(\mu, E); \quad \Psi_L^+(\mu, \ell) = \psi_L(\mu, \ell) \quad (2.34)$$

for the capture-free problem it may be easily verified that if (2.33) is satisfied the functional $\mathcal{L}\{\tilde{\Psi}(\mu, \ell)\}$ has a stationary value with

$\tilde{\Psi}(\mu, \ell) = \psi(\mu, \ell)$ and $\mathcal{L}\{\psi(\mu, \ell)\} = L_n$ where:

$$\mathcal{L}\{\tilde{\Psi}(\mu, \ell)\} = \frac{\int_0^1 d\ell M(\ell) \int_{-1}^{+1} d\mu \tilde{\Psi}^2(\mu, \ell)}{\int_0^1 d\ell M(\ell) \int_{-1}^{+1} d\mu \left[\frac{1}{\ell} \tilde{\Psi}^2(\mu, \ell) - \int_0^1 d\ell' \int_{-1}^{+1} d\mu' \Sigma(\ell' \rightarrow \ell; \mu_0) \tilde{\Psi}(\mu, \ell) \tilde{\Psi}(\mu', \ell') \right]} \quad (2.35)$$

For a trial function it is suggested that a function having the correct angular dependence for isotropic scattering should be chosen, namely:

$$\tilde{\Psi}(\mu, \ell) = \left[\ln \left| \frac{L+\ell}{L-\ell} \right| \right]^{-1} \frac{\Psi_L(\ell)}{\frac{L}{\ell} - \mu} \quad (2.36)$$

Substituting (2.36) into (2.35) and doing the variation with respect to $\tilde{\Psi}_L(\ell)$ one eventually obtains a second order iterative process for determining L_n for an arbitrary anisotropic scattering kernel.

§2.6 Critical Absorption in the B_0 and B_1 Approximations

Having discussed in some detail the numerical values of L_n for monatomic gas and water moderators we now come to consider quantitatively the critical absorber concentrations above which these discrete eigenvalues disappear into the continuum below l_{\max} . We restrict attention to $1/v$ type capture which, however, is representative of a wide class of real absorbers and for which there is no doubt that the diffusion length will finally vanish (Corngold 1966). The absorber concentration is again defined by the parameter β given by (2.28) and the associated quantity β_c indicates the critical value. The numerical method is almost identical with that used in §2.5 and is discussed in the Appendix.

In Table 2.III and Figure 2.III the critical absorption parameters β_c for each of the eigenvalues L_n are shown for the monatomic gas moderators in the B_0 approximation: Table 2.IV and Figure 2.IV show the corresponding results in the B_1 approximation. The two circled results do not appear to be genuine roots and are probably the result of the numerical procedures. Wood (1965) has predicted $\beta_c = 0.31$ for the diffusion length of the proton gas which is fractionally lower than our result (0.317) but this is probably due to the smaller number of energy points used by Wood. It is worth remarking that Wood determined β_c by extrapolating a curve of β versus L_0 back to $L_0 = l_{\max}$. The three values of $1/L_0$ closest to $1/l_{\max}$ were 0.8245, 0.9136 and 0.9689; this hardly seems sufficient points close to the limit point to be able to predict β_c with any degree of accuracy bearing in mind that it is the precise behaviour of L_0 as a function of β close to l_{\max} which is still in doubt.

A more useful comparison may be made with the results of Arkuszewski (1967) for the separable kernel in which only a single discrete eigenvalue L_0 exists - see Table 2.V. In this case β_c is determined from (2.29) by setting $V(1) = 0$. It is seen that while the critical absorption for the full kernel is not substantially different from that of the separable kernel for $A=1,2$ there is a marked difference for larger mass numbers ($A=8,12$). The increasing though still small error in β_c for the higher mass numbers (with the separable kernel) is probably caused by the inadequacy of the trapezium rule integration procedure in integrating accurately over the increasingly sharp discontinuity in $\Sigma_0(E' \rightarrow E)$ at $E=E'$ in evaluating the total scattering cross-section.

As we might expect, linear anisotropy in the scattering increases the diffusion length and consequently β_c (Table 2.IV), but while there is the expected large increase in β_c for $A=1$ the difference soon diminishes for $A \geq 2$.

The results for water are generally in excellent agreement with those of Arkuszewski (1967) and Honeck (1962) but disagree somewhat with those of Wood (1967). All these results are tabulated in Table 2.VI. Arkuszewski's values of β_c for water in the separable kernel representation are identical with our own. Honeck's results are quoted by Arkuszewski and are presumably obtained from the series expansion (2.31) by setting $L_0 = l_{\max}$ and solving for β_c ; they too are in good agreement. The value of β_c for water with the Selengut-Goertzel approximation for anisotropic scattering which has been ascribed to Wood by Arkuszewski has

been misquoted (Wood 1967). Wood has only found β_c for water assuming isotropic scattering on the basis of the effective width model. We can only suppose that the two values listed in Table 2.VI were obtained by adjusting the parameters in the effective width model (this model is discussed further in the Appendix). The fact remains that both show a marked disagreement with the present calculations on the basis of Nelkin's model which we must assume to be fairly accurate because of the generally good agreement with all other calculations. We believe that the fault must lie in the use of the effective width model.

Once again Honeck's results in the B_3 approximation when compared with the present B_1 calculations affirm that linearly anisotropic scattering describes the scattering process.

We are also interested in the behaviour of the flux as the absorption is increased. When there is no capture the diffusion length is infinite and the flux Maxwellian: as the $1/v$ type absorption concentration is increased the flux hardens in the sense that the peak moves towards higher energies. In Figure 2.V we have drawn the flux compared with a Maxwellian energy distribution for the monatomic gases of masses $A=1$ and 12 when the absorber concentration is close to its critical value. The slight bump in the curve for $A=12$ is probably caused by numerical effects. Clearly there is a shift further away from a Maxwellian distribution as the mass increases. Subsequently Arkuszewski (1967) has shown that for high A and $1/v^n$ type capture where $n \geq 4$ this shift may be quite large - and in those cases it might be necessary to retain higher energies in any numerical procedures.

APPENDIX

§2A.1 Numerical Methods

In this appendix we outline the numerical methods employed in calculating the eigenvalues and critical absorber concentrations described elsewhere in this chapter. The calculations were done on the I.B.M. 7030 ("Stretch") computer at A.W.R.E. Aldermaston. Throughout the work checks on the accuracy and consistency of the computer programmes were maintained wherever possible (e.g. $l(E)$ was compared with an analytic expression for the monatomic gas moderator and L_0 was compared with an analytic expression, valid for small capture) but the final test is in the comparison with other calculations and experiments. We believe that the results already quoted and those given in later chapters fully demonstrate the precision of the numerical approximations and solutions.

The appendix is divided into three parts. The first considers more fully the models which eventually lead to the scattering kernels $\Sigma_n(E^{\dagger} \rightarrow E)$: the second describes the general method of solution and the last part illustrates the general method by treating in more detail the problems of the present chapter.

(a) The Scattering Models

In Chapter 1 we mentioned that the first few angular moments of the scattering kernel $\Sigma_n(E^{\dagger} \rightarrow E)$ are generally evaluated at specified values of E and E^{\dagger} from computer codes specially written for that purpose. But these codes are based on models which attempt to represent

in a fairly straightforward way the scattering processes which take place in the moderator in which we are interested. In this thesis we are concerned only with the free gas and water moderators - and require only the first two angular moments.

In the free gas model there are no intermolecular forces and since there can therefore be no correlation between the positions of the scattering atoms there is no interference scattering. In fact the only internal structure is spin. The scatterers are assumed to be in thermal equilibrium with the medium and therefore have a Maxwellian distribution in velocity. As we have already mentioned it is because of the simplicity of this model that analytic expressions for the first two moments $\Sigma_0(E' \rightarrow E)$ and $\Sigma_1(E' \rightarrow E)$ may be derived (Kuščer and Ribarić 1958) and these are incorporated in a code SCAT (Hutchinson and Schofield 1967) which also deals with other moderators. Although the analytic expressions are rather involved for a gas of atomic mass $A \neq 1$ a much simpler result for $\Sigma_0(E' \rightarrow E)$ is obtained for the proton gas (Williams 1966, p27). The monatomic gas provides, in a sense, a standard against which we can measure the effects of chemical binding. With some adjustment of the parameters (mass and maximum mean free path) it has even been used to represent a water moderator.

Nelkin (1960a) has considered the scattering of neutrons from a particle of mass A whose dynamical behaviour can be represented by a sum of harmonic oscillator normal modes with appropriate weights and applied this to a water moderator. The motion of hydrogen atoms in water is treated in terms of the H_2O molecule as the basic dynamical unit.

Hindered translation is ignored and the translational motion is that of a free gas of mass $A=18$. Otherwise it is assumed that the atomic motions can be described in terms of vibrations and hindered rotations. The vibrations are assumed to be spatially isotropic while the hindered rotation is treated as a torsional oscillation of a single frequency.

This model, the Nelkin model for water, has been embodied in the GAKER computer code (Honeck 1961) modified for the I.B.M. 7030 (Stretch) computer which predicts $\Sigma_0(E^i \rightarrow E)$ and $\Sigma_1(E^i \rightarrow E)$ at a number of specified energy points. The oscillations are looked upon as δ -functions in frequency and the parameters involved, for example the weights associated with the δ -functions and their position in the frequency range, may be chosen to some extent to fit the measured mean free path or spectra. The chosen set of parameters provides a fairly accurate representation of $l(E)$ and the adopted energy points are those in common use, a decision dictated by custom but apparently justified by the fact that GAKER is very sensitive to the choice of energy mesh and for this particular mesh is well tested for trapezium rule integration (Beyster and Neill 1967): $l(E)$ is predicted accurately up to about 3 eV.

Hutchinson and Schofield (1967) point out an unexplained error in GAKER, namely that $E \cdot \Sigma_0(E \rightarrow E)$ is not monotonically increasing with energy as it ought to be. This is presumably caused by the numerical procedures in GAKER rather than the model itself - and we shall continue to use the code since, for the leakage spectra with which we shall be most concerned, it is the correct form of $l(E)$ which is of prime importance.

Broadly speaking the Nelkin model has been extremely successful in predicting scattering cross-sections and neutron spectra and although improvements have been made to the basic model recently we expect this simple model to be quite adequate for our purposes.

Amongst the more important improvements Koppel and Young (1964) have taken account of the anisotropy of the molecular vibrations while Haywood (1967) has suggested a kernel in which the hindered rotations and low energy vibrations are represented by a continuous frequency spectrum. At low energies diffusive effects become more important but, so far, few models have taken this into account. In that case the δ -function in the frequency spectrum which represents free translation would become a distribution, over a range of frequencies, having a specified width.

It has been suggested that by a suitable choice of the width of this distribution we might describe a suitable model for the scattering of neutrons by water molecules, ignoring all the other vibrations and rotations of the molecule (Williams 1966; p49ff): this is commonly called the effective width model. Unfortunately, with such a model, there will be a singularity in the forward scattering ($E=E'$) which makes calculations in B_n theory difficult to perform although there is a fortuitous cancellation if we restrict ourselves to calculations within the P_n approximations (Hutchinson and Schofield 1967). Some recent calculations of β_c in the B_0 approximation (Wood 1967) show marked disagreement with results obtained by other authors (see Table 2.VI) using the Nelkin model. It may be that in using the effective width model the singularity in the forward direction was not adequately accounted for.

(b) The Point Method

Generally we require the solution of an equation having the form:

$$\phi(E) = \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \phi(E') + S(E) \quad (2A.1)$$

where $\phi(E)$ is the flux and $S(E)$ is a source term. We shall describe here one method of solving equations having the general form (2A.1) which is commonly referred to as the "point method".

One attempts to calculate the flux ϕ_i at a set of specified energies E_i and then use an interpolation formula to estimate $\phi(E)$ at intermediate energies. Thus we write:

$$\phi(E) = \sum_i a_i(E) \phi_i \quad (2A.2)$$

so that (2A.1) becomes:

$$\phi_i = \sum_j \phi_j \Sigma_{ji} + S_i \quad (2A.3)$$

where $S_i = S(E_i)$ and

$$\Sigma_{ji} = \int_0^{\infty} a_j(E') \Sigma_0(E' \rightarrow E_i) dE' . \quad (2A.4)$$

The simplest interpolation procedure possible is linear interpolation between neighbouring energies; in that case:

$$\begin{aligned}
a_i &= \frac{E_{i+1} - E}{E_{i+1} - E_i} && \text{for } E_i < E < E_{i+1} \\
&= \frac{E - E_{i-1}}{E_i - E_{i-1}} && \text{for } E_{i-1} < E < E_i \\
&= 0 && \text{otherwise .}
\end{aligned} \tag{2A.5}$$

The points E_i have to be chosen so that the interpolation can be expected to give a good representation of the flux between the points and typically so that any required reaction rate is accurately given by the approximation:

$$\int_0^{\infty} dE \Sigma(E) \phi(E) = \sum_i \phi_i \int_0^{\infty} a_i(E) \Sigma(E) dE \tag{2A.6}$$

where $\Sigma(E)$ is the appropriate cross-section. A modified form of the point method is adopted here which avoids the necessity of evaluating integrals like (2A.4). Instead of interpolating between values of ϕ_i as in (2A.2) and evaluating the scattering term exactly one uses an integration formula; that is one approximates an integral over energy by:

$$\int dE f(E) = \sum_i f(E_i) w_i \tag{2A.7}$$

where w_i are the weights associated with the energy points E_i which are appropriate to the integration procedure chosen. The equations to be solved are then:

$$\phi_i = \sum_j \phi_j w_j \Sigma_0(E_j \rightarrow E_i) + S_i \quad (2A.8)$$

Great care must be taken over the choice of points and integration formula in particular to cope with the singularity in the gradient of $\Sigma_0(E' \rightarrow E)$ for a gas at $E=E'$. We use the weights associated with the trapezium rule:

$$w_j = \frac{1}{2} (E_{j+1} - E_{j-1}) \quad (2A.9)$$

with slight modifications to (2A.9) at the end-points of the range of integration.

We should emphasise that this approach is distinct from the well known "group method" in which one attempts to approximate the flux in an interval E_g^+, E_g^- by:

$$\phi_g(E) = w_g(E) \phi_g; \quad \phi_g = \int_{E_g^-}^{E_g^+} \phi(E) dE \quad (2A.10)$$

$w_g(E)$ is assigned by an inspired guess based on a knowledge of the rough shape of the flux, in contrast to the point method where one attempts to find ϕ_i at E_i and then interpolates at intermediate energies.

(c) The Point Method in the Determination of L_n and β_c

As an example of the point method in action we now describe the determination of L_n for the monatomic gas moderator by means of a computer programme originally written by Hutchinson (1965) which has not been published elsewhere: this programme requires only minor modifications for our present purposes.

The transport equation to be solved is given by the eigenvalue equation (2.20) except that the limits of integration are restricted to E_0, E_1 such that the contribution to the integral from energies above and below these limits may be neglected. We then consider $\Psi_L(E)$ as a list of M numbers ϕ_i evaluated at energies E_i , $\Sigma_0(E^i \rightarrow E)$ as a matrix $\Sigma_0(E_j \rightarrow E_i)$ and introduce quadrature weight factors w_j so that (2.20) may be rewritten as a set of M coupled linear equations:

$$\phi_i = \frac{L}{2} \ln \left| \frac{L + \ell_i}{L - \ell_i} \right| \sum_{j=1}^M w_j \Sigma_0(E_j \rightarrow E_i) \phi_j \quad i=1,2,\dots,M \quad (2A.11)$$

where $\ell_i = \ell(E_i)$. An eigenvalue is obtained when the determinant of (2A.11) is zero, that is:

$$\left| \left| \delta_{ij} - \frac{L}{2} \ln \left| \frac{L + \ell_i}{L - \ell_i} \right| \Sigma_0(E_j \rightarrow E_i) w_j \right| \right| = 0 \quad (2A.12)$$

where δ_{ij} is a Kronecker δ -symbol. The eigenvalue is, in fact, determined by finding two values of L (say L and $L+\epsilon$ where ϵ is arbitrarily small) such that the value of the determinant has opposite sign. Supplying two 'first guesses' for the eigenvalue the determinant is evaluated in each case and a Wegstein extrapolative procedure used to determine L_n : ϵ is chosen to be about $10^{-5} \ell_{\max}$ in order to ensure numerical convergence of the procedure. This method has already been applied in finding the roots of transcendental equations (Wegstein 1958) but it is readily adapted to this problem also. The advantages of the Wegstein procedure are that the rate of convergence is fast and convergence is induced even if a normal iterative procedure diverges. Furthermore one only needs to evaluate the determinant at each iteration

not, as in Newton's method, the derivative as well. Consequently it is fairly straightforward to programme.

In order to evaluate the components of the determinant and hence the determinant itself we require $\Sigma_0(E_j \rightarrow E_i)$, w_j and l_i . The first of these, the scattering kernel, has already been discussed in this appendix. Before specifying an integration formula through the weights w_j we must comment on the evaluation of the mean free path. It might be supposed that, for the monatomic gas at least, this is best calculated from the analytic formula for $l(E)$. That this is not the case is easily seen by considering equation (2.20) for the diffusion length: when there is no capture L_0 is infinite, (2.20) becomes:

$$\frac{\Psi_{L_0}(E)}{l_S(E)} = \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi_{L_0}(E') \quad (2A.13)$$

and we know that the solution of this is $\Psi_{L_0}(E) = M(E)$ because of the detailed balance condition (1.11). However in these computations the right hand side of (2A.13) is calculated numerically. To satisfy the detailed balance condition it is essential that the left hand side (i.e. $l_S(E)$) be calculated by the same method of quadrature. That is to say "in-scatter" and "out-scatter" from a particular energy interval must be estimated in the same way, otherwise spurious "source" and "capture" terms arise.

A trapezium rule integration procedure was adopted with about 70 points at approximately equal intervals on a logarithmic energy scale between 10^{-3} and 3 eV. The choice of upper limit is determined to some

extent by the condition that for no upscattering $E \gg kT$ and is supported by a recent article (Bollacasa and Goldman 1967) which shows that the customary upper limit of about 0.6 eV is, in many cases, too low.

For the kernel (M.M.R. Williams in a private communication to P. Hutchinson)

$$\begin{aligned} \Sigma_0(E^t \rightarrow E) &= \frac{1-e^{-E}}{E^t} & E^t > E \\ &= \frac{e^{-E}(e^{E^t}-1)}{E^t} & E^t < E \end{aligned} \quad (2A.14)$$

which is chosen mainly for its simplicity, $\Sigma_s(E)=1$ and the eigenvalues are given by the roots of:

$$\frac{L}{2} \ln \left(\frac{L+1}{L-1} \right) = N \quad N = 1, 2, \dots \quad (2A.15)$$

When $N=1$, $L_0=\infty$ and when $N=2$, $L_1=1.04$. Hutchinson was unable to find the thermalisation length and it was thought that this was due to the restricted energy range: on increasing the energy range to 10 eV he found $L_1=1.013$ which still implies a 3% error. However we were later able to show that the cause of the trouble was not so much the restricted energy range as errors in the calculated mean free path. Although Hutchinson had chosen points which were approximately equally spaced on a logarithmic energy scale there were a number of points at which the distances between neighbouring points changed fairly abruptly. The effect of this was a sharp drop in the mean free path at those energies: this is clearly seen in Figures 2.VI and 2.VII where we have compared Hutchinson's results with the exact values of

$\ell(E)$ obtained from the analytic expressions for $A=1$ and 12 . We were able to show that by choosing equally spaced points on a logarithmic scale throughout the energy range $\ell(E)$ was more accurately predicted and better agreement was obtained for L_n . For example with the improved energy mesh the thermalisation length for William's simple kernel (2A.14) becomes 1.045 . It is found that the errors introduced by an inappropriate choice of energy points were most serious in predicting those eigenvalues which lie very close to ℓ_{\max} and especially so for higher mass numbers, as we might expect from Figures 2.VI and 2.VII.

Rather similar calculations were performed in the B_1 approximation.

In order to determine the critical absorption parameter β_c we perform rather similar calculations except that now L_n is set equal to ℓ_{\max} and β_c is effectively treated as the eigenvalue. That is we vary the absorption β until, for concentrations differing by some arbitrarily small amount, the determinant (2A.12) has opposite sign - the same iterative procedure may be adopted. This is basically the method employed at a later date by Arkuszewski (1967) for the separable kernel.

In all the calculations mentioned so far either 70 or 80 energy points were used between 10^{-3} and $1-10$ eV although such a large number of points may not be essential. On the other hand for 20-30 energy points over a similar energy range we found non-physical roots appearing which disappeared as the number was increased. In any case when this work was begun the behaviour of L_n close to ℓ_{\max} as β increased and the behaviour of the flux at high energies were not known precisely and it was

thought that it might be necessary to include energies up to about 10 eV which would require a fairly large number of mesh points. By supposing a high energy flux of the form $E^{q(E)} M(E)$ where $q(E)$ is a slowly varying function of energy it is possible to show analytically, since we know the form of $\Sigma_0(E^i \rightarrow E)$ for the monatomic gas, that energies higher than 10 eV would not contribute significantly to the term on the right hand side of (2.20) for $1/v$ type absorber. Similar order-of-magnitude arguments were concluded in the B_1 approximation also.

Typical times taken to calculate an eigenvalue in the B_0 and B_1 approximations were 2 minutes and 8 minutes respectively.

Lastly we mention the method of determining the eigenfunctions associated with the diffusion length close to l_{\max} when $\beta \approx \beta_c$ which are shown for the monatomic gases ($A=1,12$) in Figure 2.V. The method of finding L_n which we have described is incapable of determining the eigenvalues exactly if only because of rounding errors: nevertheless the inverse of the associated matrix will be almost singular. Thus the problem is ill-conditioned as far as the determination of the eigenfunctions is concerned and without care serious errors may occur. It is easily seen how this happens: consider, in the usual matrix notation, the difference in the solution of $Ax=b$ where A is a square matrix and x, b are column vectors and of $(A+\delta A)(x+\delta x) = b+\delta b$. This may be expressed as:

$$\delta x = (A + \delta A)^{-1} (\delta b - \delta A \cdot x) \quad (2A.16)$$

with the result that if A is nearly singular small errors in the components of the matrix or the solving process may have a serious effect (Fox 1964).

Computer programmes have been written which solve ill-conditioned problems such as this but we choose, instead, to avoid the difficulty in the following way. The ill-conditioning is simply removed by replacing any one of the linear equations (2A.11) by a normalisation condition - in our case

$$\int_0^{\infty} dE \Psi_{L_n}(E) = 1 \quad (2A.17)$$

and solving the resultant set of well-conditioned linear equations. This final step is achieved with another standard computer programme by pivotal condensation with row interchange followed by back substitution.

The methods which have been described in this appendix are also applicable with only minor modifications to a number of other problems which we shall meet in this thesis.

Atomic Mass (A)	Eigenvalues	Heavy Gas Approx.-(2.21)	Hutchinson-Lancefield	
			Original calculation	+ improved energy mesh
1	None	o	o	o
2	None	o	o	o
3	L ₁	o	1.005	1.037
4	L ₁	1.020	1.059	n.c.o.
6	L ₁	1.167	1.173	n.c.o.
	L ₂	n.c.o.	1.020	n.c.o.
8	L ₁	1.297	1.284	n.c.o.
	L ₂	n.c.o.	1.0815	n.c.o.
	L ₃	n.c.o.	o	1.015→1.025
12	L ₁	1.532	1.485	1.560
	L ₂	n.c.o.	1.209	1.223
	L ₃	n.c.o.	1.057	1.098
	L ₄	n.c.o.	o	1.035

TABLE 2.1

Spatial eigenvalues L_n ($n \geq 1$) of the infinite medium transport equation in units of l_{\max} for the monatomic gas of atomic mass A in the B_0 approximation

$$\Sigma_a(E) = 0 \quad \therefore \quad L_0 = \infty$$

o = no eigenvalue predicted. n.c.o. = no eigenvalue calculated.

Thermalisation Length	← Atomic Mass(A) →			
	1	2	3	4
B ₀ Approximation	None	None	1.037	(1.059)
B ₁ Approximation	1.058	1.111	1.164	1.219

TABLE 2. II

The thermalisation length L_1 in units of l_{\max} for the monatomic gas of atomic mass A in the B₀ and B₁ approximations.

$$\Sigma_a(E) = 0 \quad \therefore \quad L_0 = \infty$$

The figure in parentheses is taken from Hutchinson (1965).

Atomic Mass A	← β_c →				
	L_0	L_1	L_2	L_3	L_4
1	0.317	o	o	o	o
2	0.362	o	o	o	o
3	0.389	0.058	o	o	o
4	0.410	0.125	o	o	o
6	0.442	0.218	0.072	o	o
8	0.472	0.281	0.141	0.04±.01	o
12	0.520	0.366	0.241	0.140	0.060

TABLE 2.III

The critical absorber concentration $\beta_c = (2.28)$ - for the disappearance of the discrete eigenvalues L_n of the monatomic gas of atom mass A calculated in the B_0 approximation.

o indicates that no such eigenvalue exists.

Atomic Mass A	← β_c for the disappearance of L_0, L_1 →				
	B_0 approximation			B_1 approximation	
	L_0	L_1		L_0	L_1
1	0.317	o		0.517	0.119
2	0.362	o		0.491	0.114
3	0.389	0.058		0.489	0.123
4	0.410	0.125		0.496	0.287

TABLE 2. IV

The critical absorber concentration $\beta_c - (2.28) -$ for the disappearance of the diffusion and thermalisation lengths for a monatomic gas of atomic mass A calculated in the B_0 and B_1 approximations.

o indicates that no such eigenvalue exists.

		β_c for the monatomic gass of mass A			
		A=1	A=2	A=8	A=12
Arkuszewski (1967)	: Separable kernel	0.3002	0.3370	0.3749	0.3800
Direct Computation in B_0 Approximation	: Separable kernel	0.300	0.337	0.372	0.376
	: True kernel	0.317	0.362	0.472	0.520

TABLE 2.V

The critical absorber concentration $\beta_c - (2.28) -$ calculated in the B_0 approximation, for the disappearance of the diffusion length L_0 for the monatomic gas of atomic mass A as represented by the separable kernel as well as the true kernel.

β_c for disappearance of L_0		Direct computation in B_0 or B_1 approximation
Honeck (1962): B_0 approx.	0.22	0.217 (B_0)
Honeck (1962): B_3 approx.	0.30	0.307 (B_1)
Arkuszewski (1967) : Separable kernel	0.20	0.200 (B_0)
Arkuszewski (1967) : Separable kernel for proton gas	0.30	0.300 (B_0)
Wood (1967) : (a)	0.30	0.217 (B_0)
Wood (1967) : (b)	0.25	0.217 (B_0)

TABLE 2. VI

The critical absorber concentration β_c -- (2.28) -- for the disappearance of the diffusion length L_0 for a water moderator. The results are normalised artificially to $l_{\max} = 1$. In fact $l_{\max} = 1.49$ cms. so that the figures given will be increased proportionally.

— THE SPATIAL EIGENVALUES L_n ($n \geq 1$), UNITS OF L_{\max} ←

⊙ HEAVY GAS

• HUTCHINSON (1965)

X HUTCHINSON-LANCEFIELD, IMPROVED ENERGY MESH

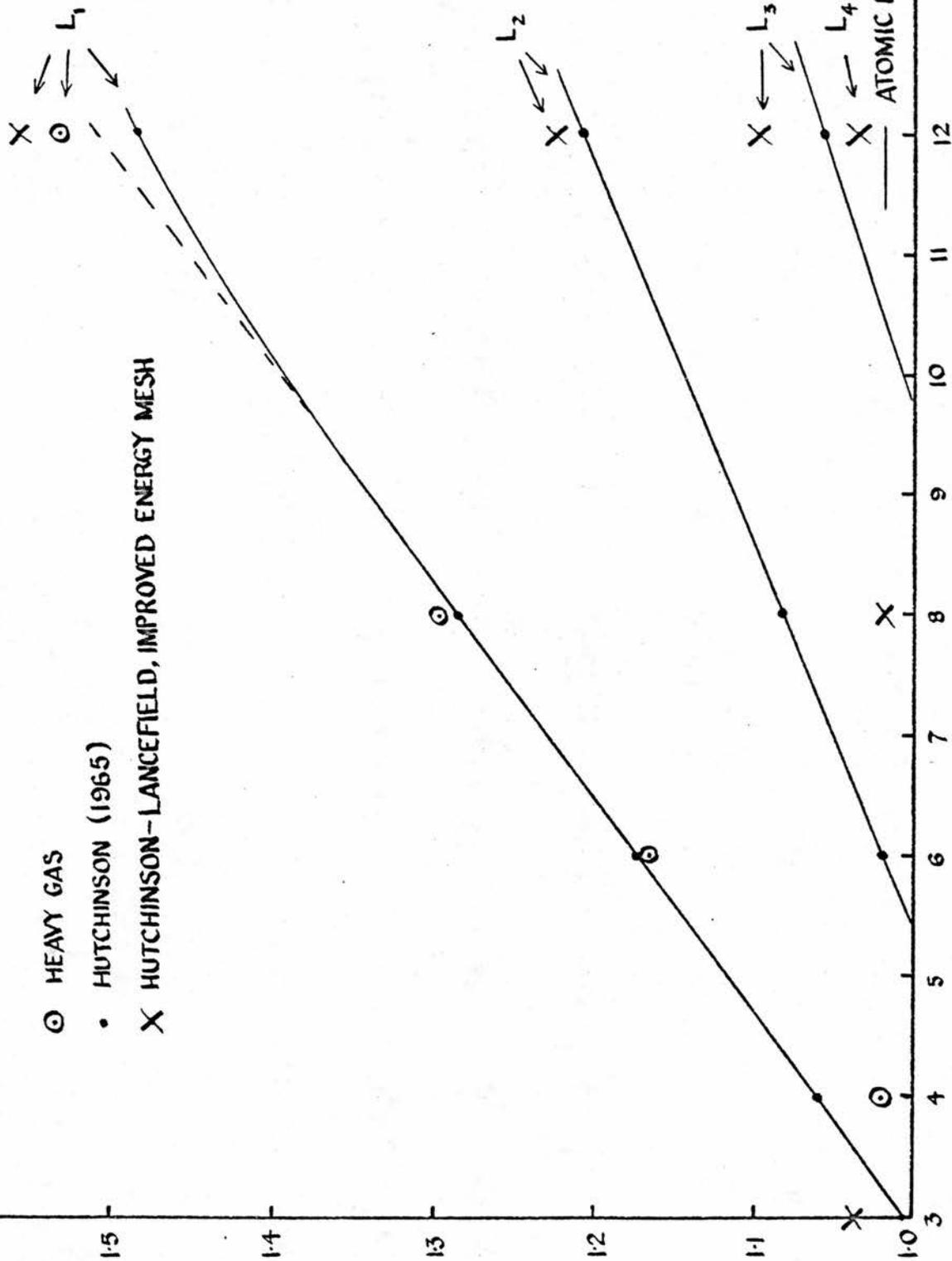


FIG. 2.1

The eigenvalues L_n in the B_0 approximation for the monatomic gas moderator. $\sum_a = 0 \therefore L_0 = \infty$

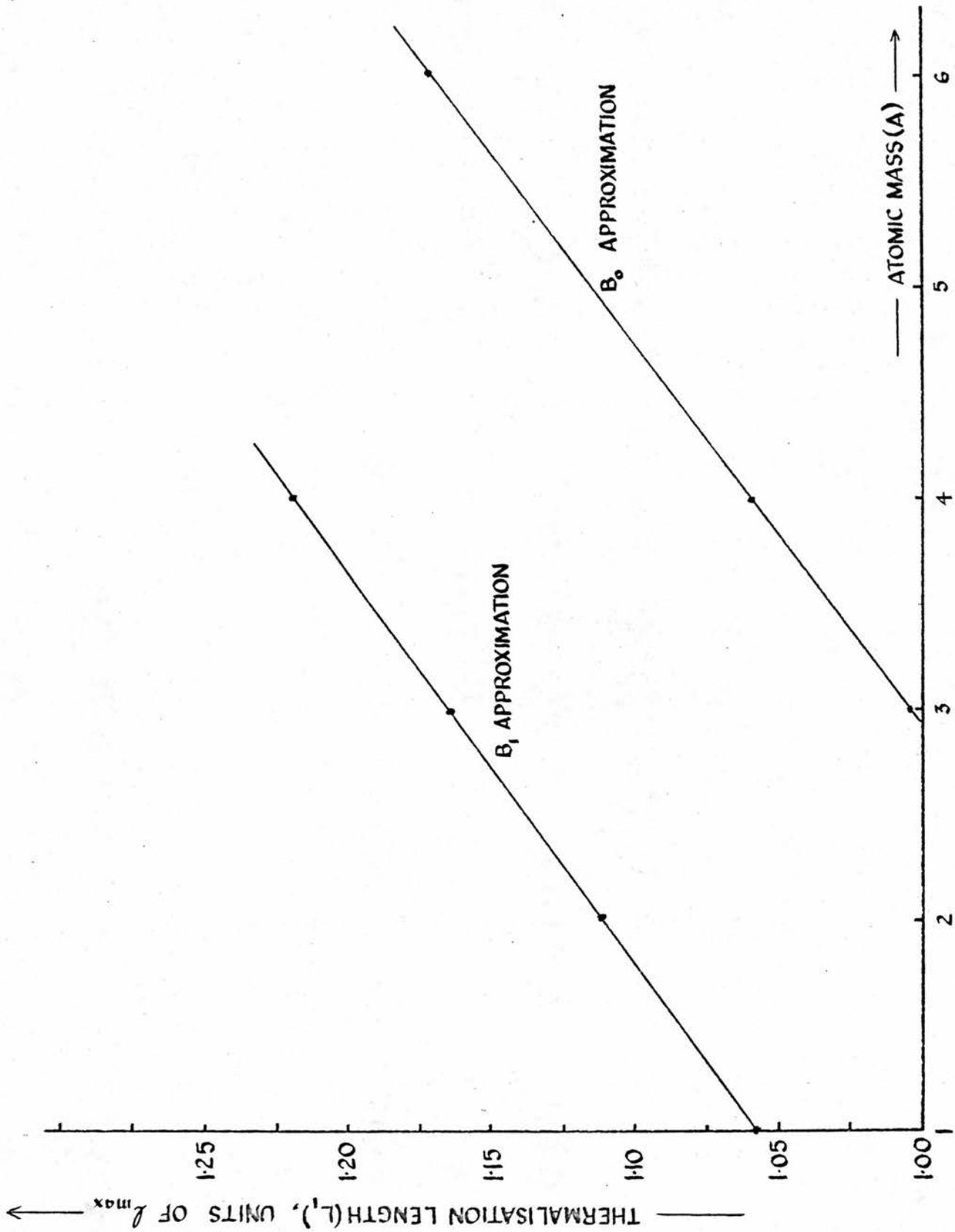


FIG.2:II

The thermalisation length in the B_0 and B_1 approximations for the monatomic gas moderator. $\sum_a^0 = 0 \therefore L_0 = \infty$

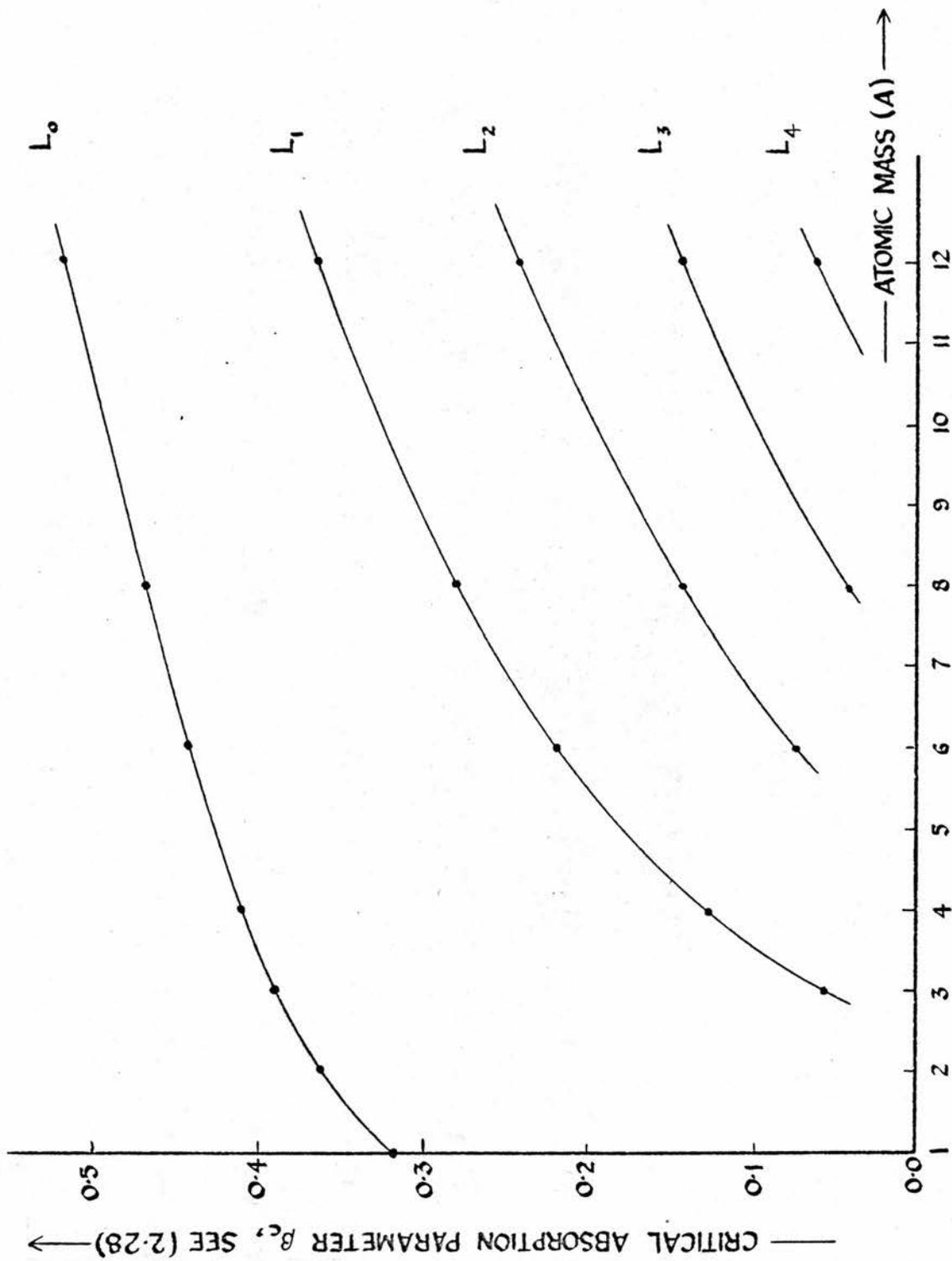


FIG.2.III

The critical absorber concentration for the disappearance of the discrete eigenvalues L_n for the monoatomic gas moderator: B_0 approximation

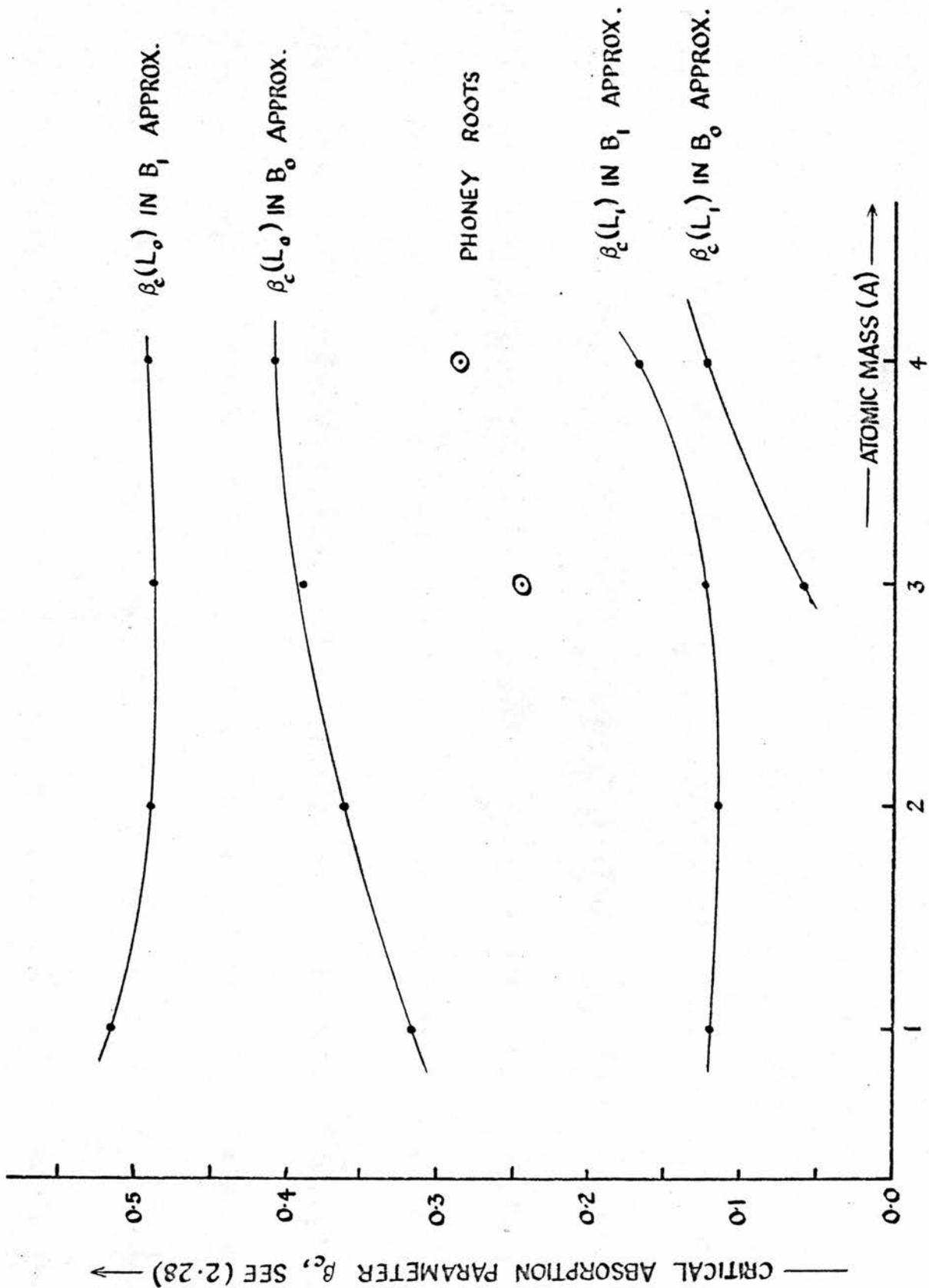


FIG. 2.4

The critical absorber concentration for the disappearance of the diffusion and thermalisation lengths for the monatomic gas moderator

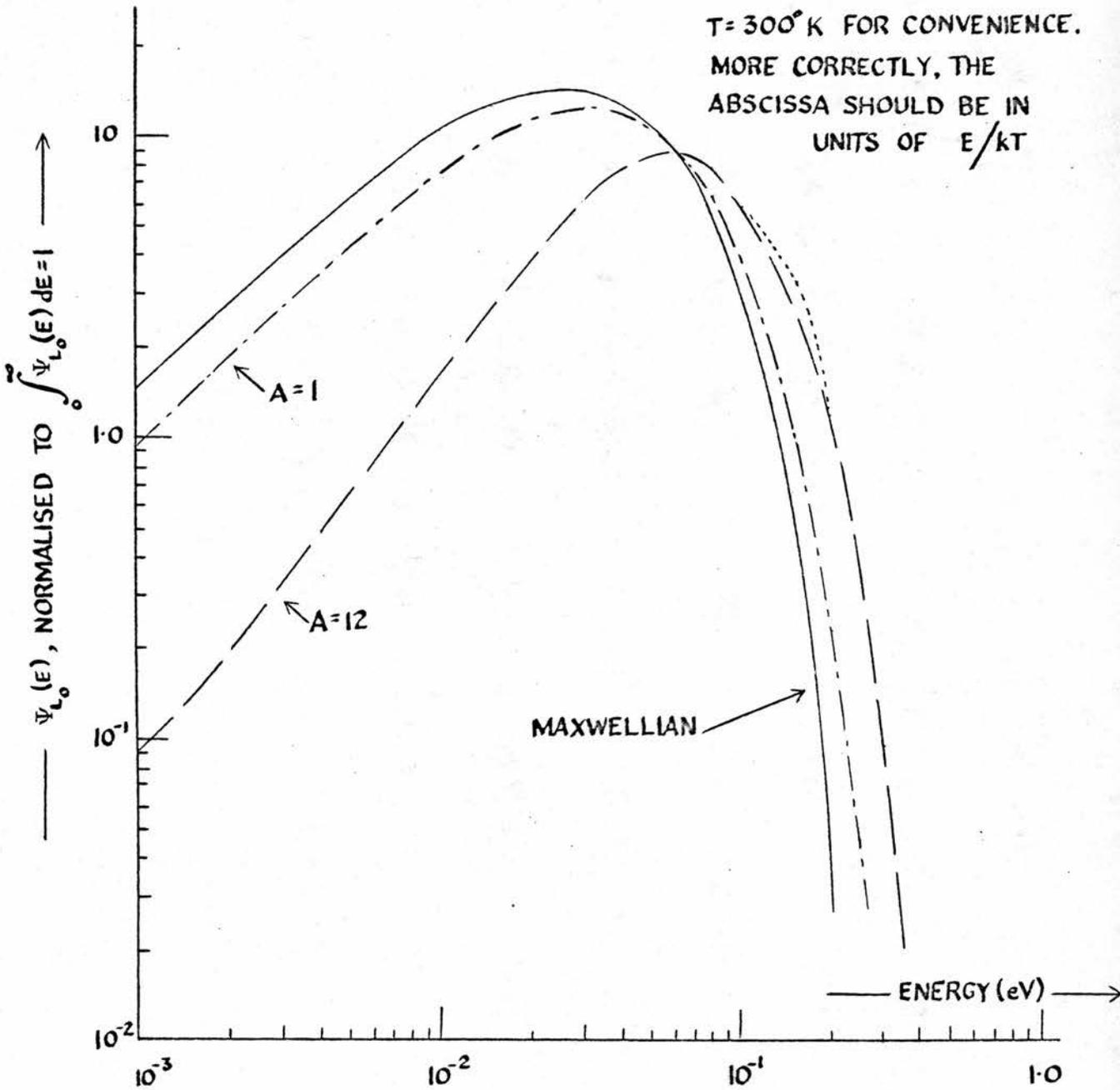


FIG. 2. ∇

The eigenspectrum $\Psi_{L_0}(E)$ close to critical absorption, that is $L_0 \gtrsim l_{\max}$

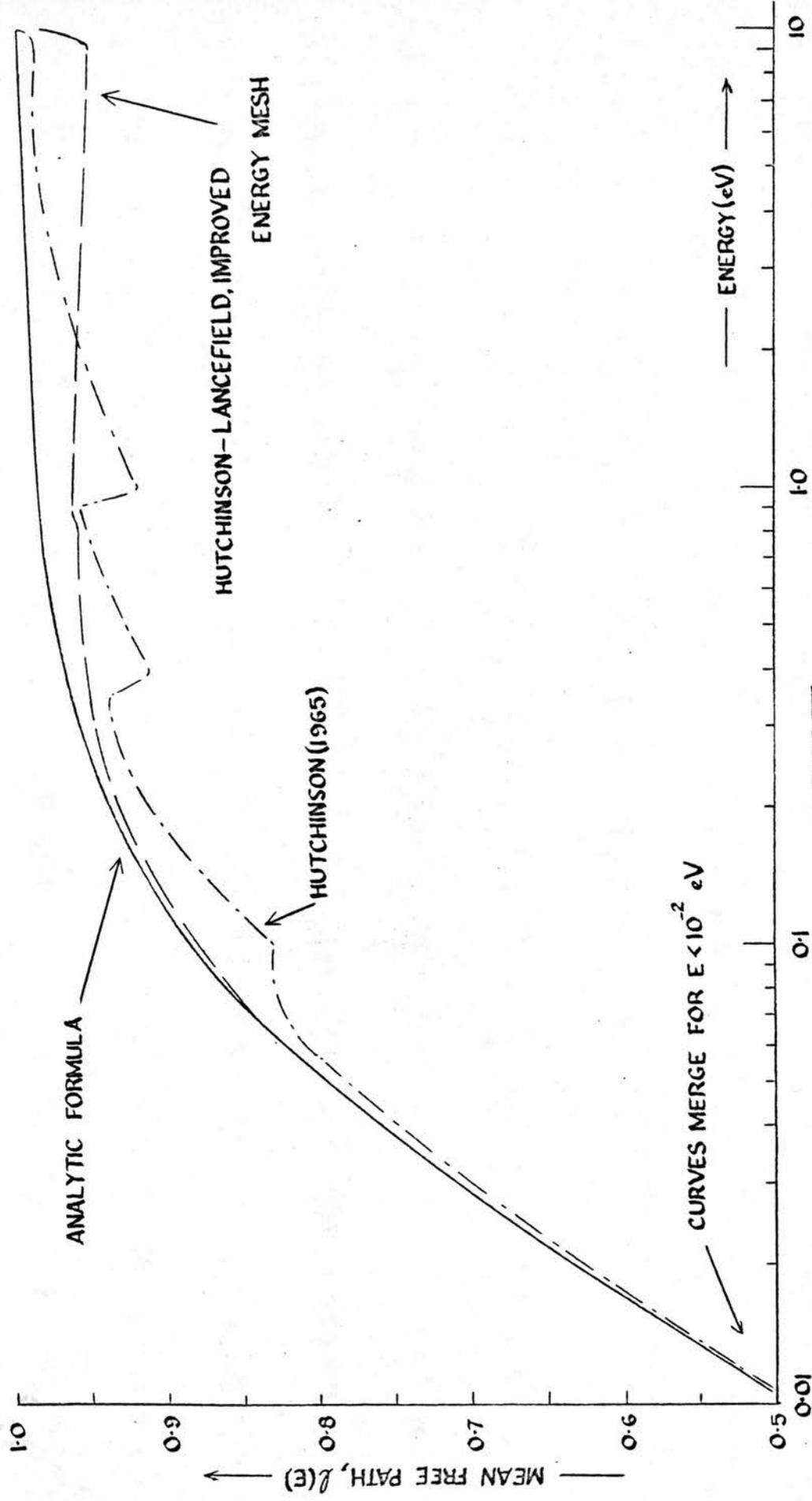


FIG. 2.VI

The mean free path for the proton gas moderator; $l_{\max} = 1$

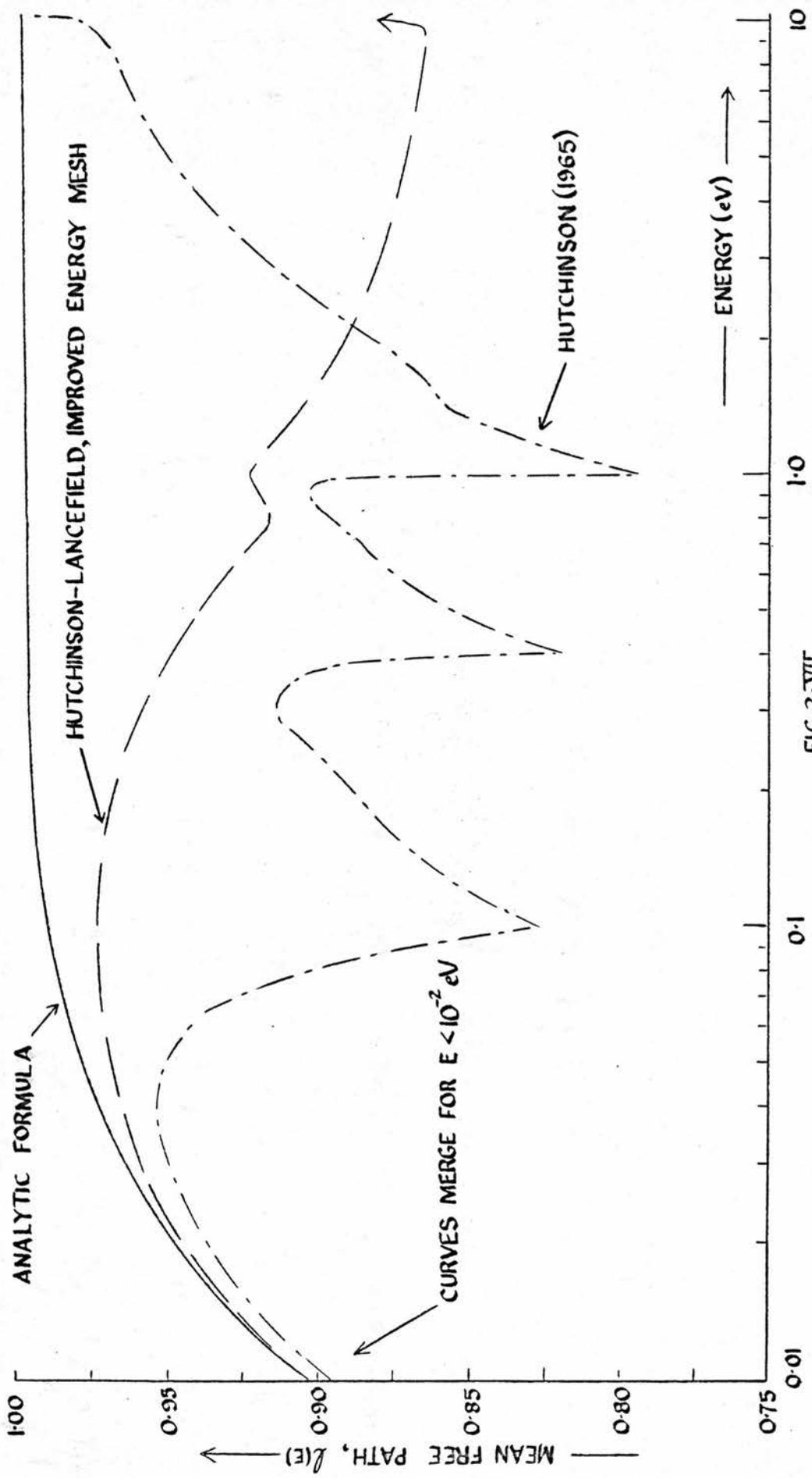


FIG. 2.VII

The mean free path for the monatomic gas moderator of atomic mass $A=12$; $l_{max}=1$

CHAPTER 3

THE ONE-SPEED MILNE PROBLEM AND ASSOCIATED GREEN'S FUNCTIONS

§3.1 Introduction

In Chapter 2 we discussed in some detail the asymptotic flux for the thermal neutron Milne problem, both with and without neutron capture. The remainder of this thesis is devoted to a study of the transient flux close to the plane boundary and its relationship to the asymptotic flux already determined. This is achieved through a variational principle which relies on a knowledge of some results from one-speed theory. We refer in particular to solutions of the one-speed Milne problem and the associated Green's functions, some of which are already known while others have not yet been explicitly stated. In this chapter we shall collect together those results which will be required.

It is not particularly surprising that many of the results which are available in one-speed theory have not been generalised to their energy dependent counterparts except through the multigroup approach. However the present treatment makes full use of these one-speed solutions in expressing, to first approximation, a quantity related to the extrapolation length as a weighted average over the corresponding one-speed parameter which is already known. The correction term may be expressed in terms of some one-speed Green's functions, is estimated by a variational principle and is generally found to be small. The fact remains that the one-speed solutions evidently play a leading part in this study.

With one exception we consider here only no-capture solutions so that this chapter may be looked upon as preparatory to the following chapter on the energy dependent Milne problem without capture. The restriction to capture-free media leads to much simpler expressions for the one-speed Milne solutions and Green's functions. This is a direct consequence of the fact that away from sources the transport equation conserves the neutron current for a non-capturing medium: this is true both for isotropic and anisotropic scattering. A discussion of the effect of capture on the solutions will be given in Chapter 5.

Exact and approximate solutions to the one-speed Milne problem with isotropic and linearly anisotropic scattering are reviewed in §3.2. In §3.3 expressions are obtained for various Green's functions on the assumption of isotropic scattering: a recursion relationship is developed by means of which one can derive fairly simple expressions for the first few angular moments of the Green's functions for isotropic and anisotropic sources in terms of the solution to the one-speed Milne problem. We arrive at the same results by an alternative approach in §3.4. There the treatment is rather more traditional but it does illustrate that certain integrals which often arise in neutron transport theory may be greatly simplified in some cases. Finally in §3.5 we present expressions, similar to those derived in §3.3, for the one-speed Green's function for an isotropic source assuming in this case linearly anisotropic scattering.

§3.2 The One-Speed Milne Problem

The one-speed, capture-free Milne problem with isotropic scattering has been solved exactly both by the Wiener-Hopf technique as described in a classic paper by Placzek and Seidel (1947) and by the normal mode expansion method first applied to neutron transport theory by Case (1960). This is typical of the state of affairs in which those problems already solved by one of these methods appear to be soluble by the other also. Although these treatments have been extended to energy dependent problems their practical success has not been particularly encouraging except for some simple scattering models. Even in the context of one-speed theory the resultant expressions for the flux and emergent angular distribution are somewhat unwieldy.

Of sufficient accuracy for our purposes is an approximate expression for the flux obtained by LeCaine (1947) whose method we shall now describe. The usual differential form of the transport equation without capture is:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{l} \right] \rho(z, \mu, l) = \frac{1}{2l} \rho_0(z, l); \quad l = l_s. \quad (3.1)$$

Integrating (3.1) over angle we find $\frac{\partial}{\partial z} \rho_1(z, l) = 0$ or in other words the current is constant (see §3.1) which is not surprising in a capture-free medium. (3.1) is transformed into an integral equation by rewriting it as:

$$\frac{\partial}{\partial z} \left[\mu e^{+z/\mu l} \rho(z, \mu, l) \right] = \frac{e^{z/\mu l}}{2l} \rho_0(z, l) \quad (3.2)$$

and integrating over z . This leads to the equations

$$\begin{aligned} \rho(z, \mu, l) &= (2\mu l)^{-1} \int_0^z dz' e^{(z'-z)/\mu l} \rho_0(z', l) \quad \mu > 0 \\ &= - (2\mu l)^{-1} \int_z^\infty dz' e^{(z'-z)/\mu l} \rho_0(z', l) \quad \mu < 0 \end{aligned} \quad (3.3)$$

where we have already invoked the boundary condition that there are no incident neutrons on the surface $z=0$. Integrating (3.3) over μ we find that:

$$\rho_0(z, l) = \frac{1}{2l} \int_0^\infty dz' E_1 \left(\frac{|z-z'|}{l} \right) \rho_0(z', l) \quad (3.4)$$

where $E_n(x)$ is the exponential integral

$$E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} dt \quad (3.5)$$

This alternative expression of the transport equation which has the boundary conditions built into it is commonly referred to as Milne's integral equation. LeCaine then makes the substitution

$$\rho_0(z, \ell) = z + q(z, \ell) \quad (3.6)$$

in (3.4) where limit $q(z)$ is the extrapolation length $\xi(\ell) = c\ell$ and $z \rightarrow \infty$

obtains an inhomogeneous integral equation for $q(z)$:

$$q(z, \ell) = \frac{1}{2\ell} \int_0^{\infty} dz' E_1\left(\frac{|z-z'|}{\ell}\right) q(z', \ell) + \frac{\ell}{2} E_3(z/\ell) \quad (3.7)$$

The solution of (3.7) minimises the functional (Davison 1957, p208)

$$\mathcal{L}[\tilde{q}(z, \ell)] = \frac{\int_0^{\infty} dz \tilde{q}(z, \ell) \left[\tilde{q}(z, \ell) - \frac{1}{2\ell} \int_0^{\infty} dz' \tilde{q}(z', \ell) E_1\left(\frac{|z-z'|}{\ell}\right) \right]}{\left[\int_0^{\infty} dz' \tilde{q}(z', \ell) E_3(z'/\ell) \right]^2} \quad (3.8)$$

and in that case

$$\mathcal{L}[q(z, \ell)] = \left[\frac{2}{\ell} \int_0^{\infty} dz q(z, \ell) E_3(z/\ell) \right]^{-1} \quad (3.9)$$

Now LeCaine has shown that the extrapolation length $c\ell$ is given by $\mathcal{L}[q] = \left(\frac{4c\ell}{3} - \frac{\ell}{2}\right)^{-1}$ so that for a suitable trial function $\tilde{q}(z, \ell)$ one may obtain an accurate estimate of (3.9) and hence of the extrapolation length. She chooses a trial function of the form:

$$\tilde{q}(z,l) = cl \left[1 - \alpha E_2(z/l) + \beta E_3(z/l) \right]$$

which is suggested by the fact that if the method of successive approximations is applied to (3.7) beginning with $\tilde{q}(z,l) = cl$ the next approximation is:

$$\tilde{q}(z,l) \doteq cl - \frac{1}{2} cl E_2(z/l) + \frac{l}{2} E_3(z/l) .$$

Minimising the functional (3.8) with respect to α and β one finds $\alpha \doteq 0.3429$ and $\beta \doteq 0.3157$ giving a value for the extrapolation length $c \doteq 0.71045$. Thus the approximate form of the flux given by LeCaine is:

$$\rho_0(z,l) \doteq z + cl - cl \left[\alpha E_2(z/l) - \beta E_3(z/l) \right] \quad (3.10)$$

where the normalisation is such that the current is given by:

$$\rho_1(z,l) = - l/3 . \quad (3.11)$$

This form of $\rho_0(z,l)$ predicts the extrapolation length correct to six figures and a maximum error in the emergent angular distribution of 0.3% which occurs for $\mu=0$ and which incidentally is reduced to 0.02% after one iteration (Davison 1957, p219).

In the corresponding problem with linearly anisotropic scattering (denoted hereafter by a superscript A) the flux satisfies the equation:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{l} \right] \rho^A(z, \mu, l_t) = \frac{1}{2l} \rho_0^A(z, l_t) + \frac{3}{2} \mu \Sigma_1 \rho_1^A(z, l_t) \quad (3.12)$$

and at large z it is easily seen (by substitution into (3.12)) to have the asymptotic form:

$$\rho^A(z, \mu, l_t) \sim \rho_{\text{asy}}^A(z, \mu, l_t) = \frac{1}{2} \left[z + cl_t - \mu l_t \right] \quad (3.13)$$

where l_t is the transport mean free path defined by:

$$l_t = \frac{l}{1 - \Sigma_1 l} \quad . \quad (3.14)$$

Hence

$$\rho_1^A(z, l_t) = -l_t/3 \quad . \quad (3.15)$$

It has been observed by Mark (1947) and again by Shure and Natelson (1964) that the solution of (3.12) may be written down in terms of $\rho(z, \mu, l)$: in fact:

$$\rho^A(z, \mu, l_t) = \frac{l_t}{l} \rho(z, \mu, l) + \frac{3}{2} \Sigma_1 \rho_1^A(z, l_t) z \quad (3.16)$$

For example, with LeCaine's approximate solution for $\rho_0(z, l)$:

$$\rho_0^A(z, l_t) \doteq z + cl_t - cl_t \left[\alpha E_2(z/l) - \beta E_3(z/l) \right] \quad . \quad (3.17)$$

§3.3 Green's functions with Isotropic Scattering

In this section we shall derive useful expressions for the one-speed half-space Green's functions appropriate to a medium which scatters neutrons isotropically and contains both isotropic and anisotropic sources. For the present we assume a capturing medium. Let us define the Green's function $\rho_m(z' \rightarrow z, \mu; \ell, L)$ for a $P_m(\mu)$ source at $z=z'$ through the equation:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell} \right] \rho_m(z' \rightarrow z, \mu; \ell, L) = \frac{c}{2\ell} \rho_{m0}(z' \rightarrow z; \ell, L) + \frac{P_m(\mu)}{2} \delta(z-z') \quad (3.18)$$

with the stipulation that the Green's function is bounded at infinity and satisfies the boundary condition that there are no incident neutrons on the surface $z=0$. The medium is assumed to have mean free path ℓ and multiplication c so that the diffusion length L is given by (2.5). Thus:

$$\rho_{mn}(z' \rightarrow z; \ell, L) = \int_{-1}^{+1} d\mu P_n(\mu) \rho_m(z' \rightarrow z, \mu; \ell, L) \quad (3.19)$$

represents the n 'th Legendre moment of the angular flux resulting from a $P_m(\mu)$ source at $z=z'$ in a medium having the properties described above. If there is no capture $c=1$ and the diffusion length becomes infinite: in that case we indicate that no neutrons are absorbed by excluding L from amongst the functional parameters for the one-speed flux and

Green's functions. Thus if there is no capture the Green's function would be denoted by $\rho_{mn}(z' \rightarrow z; l)$.

For an isotropic source $\rho_{00}(z' \rightarrow z; l, L)$ can be written in terms of $\rho_{q_0}(z, l, L)$ which is the flux due to a uniform distribution of isotropic sources of unit strength in a medium having the properties already described (Davison 1957, p85):

$$\rho_{00}(z' \rightarrow z; l, L) = (1-c)^{\frac{1}{2}} \rho_{q_0}^i(|z-z'|, l, L) + \frac{c(1-c)}{l} \int_0^{\min(z, z')} \rho_{q_0}^i(y, l, L) \rho_{q_0}^i(y+|z-z'|, l, L) dy \quad (3.20)$$

We shall make use of (3.20) in Chapter 5, but we expect that for a non-capturing medium (3.20) will be greatly simplified. Davison(1957, p80) has shown that:

$$\rho_{q_0}(z, l, L) = \frac{1}{c|j(0)|} \left[L \rho_0(z, l, L) - \int_0^z \rho_0(u, l, L) du - l|j(0)| \right] \quad (3.21)$$

where $j(z)$ is the source-free current. Thus we find that:

$$(1-c)^{\frac{1}{2}} \rho_{q_0}^i(z, l, L) = \frac{(1-c)^{\frac{1}{2}}}{c|j(0)|} \left[L \rho_0^i(z, l, L) - \rho_0(z, l, L) \right] \quad (3.22)$$

The no-capture limit is achieved by letting c tend to unity while L tends to infinity although this must be done with some care. As L becomes large, we see from (2.5) that:

$$(1-c)^{\frac{1}{2}} \rightarrow \frac{1}{\sqrt{3}} \left(\frac{\ell}{L} \right) .$$

Bearing in mind that in the no-capture limit $|j(0)| = \ell/3$ we obtain:

$$\lim_{c \rightarrow 1} (1-c)^{\frac{1}{2}} \rho_{q_0}^{\dagger}(z, \ell, L) = \sqrt{3} \rho_0^{\dagger}(z, \ell)$$

with the result that:

$$\begin{aligned} \rho_{00}(z' \rightarrow z; \ell) &= \sqrt{3} \rho_0^{\dagger}(|z-z'|, \ell) \\ &+ \frac{3}{\ell} \int_0^{\min(z, z')} \rho_0^{\dagger}(y, \ell) \rho_0^{\dagger}(y + |z-z'|, \ell) dy \end{aligned} \quad (3.23)$$

for the Green's function for an isotropic source in a non-capturing medium.

Knowing $\rho_{00}(z' \rightarrow z; \ell)$ one may construct a recursion equation for calculating $\rho_{mn}(z' \rightarrow z; \ell)$. The angular flux which results from a source of unit strength at z' emitting neutrons in a direction $\cos^{-1} \mu'$ with respect to the positive z axis in a non-capturing medium with isotropic scattering is determined by:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell} \right] \rho(z', \mu' \rightarrow z, \mu; \ell) = \frac{1}{2\ell} \rho_0(z', \mu' \rightarrow z; \ell) + \frac{1}{2} \delta(\mu - \mu') \delta(z - z') . \quad (3.24)$$

Multiplying by $P_m(\mu')$ $P_n(\mu)$, integrating over both the angular variables and using the identity:

$$\int_{-1}^{+1} P_m(\mu) P_n(\mu) d\mu = \frac{2\delta_{mn}}{2n+1} \quad (3.25)$$

where δ_{mn} is the Kronecker δ -symbol we find:

$$\begin{aligned} \int_{-1}^{+1} d\mu \int_{-1}^{+1} d\mu' P_m(\mu') P_n(\mu) \mu \frac{\partial}{\partial z} \rho(z', \mu' \rightarrow z, \mu; \ell) + \frac{\rho_{mn}(z' \rightarrow z; \ell)}{\ell} \\ = \frac{\rho_{m0}(z' \rightarrow z; \ell) \delta_{n0}}{\ell} + \frac{\delta(z-z') \delta_{nm}}{2n+1} \end{aligned} \quad (3.26)$$

By means of the recursion formula for Legendre polynomials:

$$(n+1) P_{n+1}(\mu) - (2n+1)\mu P_n(\mu) + n P_{n-1}(\mu) = 0 \quad (3.27)$$

equation (3.26) may be rewritten:

$$\begin{aligned} \frac{(n+1)}{2n+1} \frac{\partial}{\partial z} \rho_{m(n+1)}(z' \rightarrow z; \ell) + \frac{n}{2n+1} \frac{\partial}{\partial z} \rho_{m(n-1)}(z' \rightarrow z; \ell) + \frac{\rho_{mn}(z' \rightarrow z; \ell)}{\ell} \\ = \frac{\rho_{m0}(z' \rightarrow z; \ell) \delta_{n0}}{\ell} + \frac{\delta(z-z') \delta_{nm}}{2n+1} \end{aligned} \quad (3.28)$$

From the recursion relationship (3.28) we see, for example, that the current from an isotropic source at z' for which $n=m=0$ is given by:

$$\frac{\partial}{\partial z} \rho_{01}(z' \rightarrow z; l) = \delta(z - z') \quad . \quad (3.29)$$

Integrating (3.29) over z and imposing the boundary condition that

$\lim_{z \rightarrow \infty} \rho_{01}(z' \rightarrow z; l) = 0$ we obtain:

$$\rho_{01}(z' \rightarrow z; l) = \begin{cases} 0 & z > z' \\ -1 & z < z' \end{cases} \quad (3.30)$$

This result is in accord with the observation (Tait 1964, p88; Davison 1957, p210) that when the source is at infinity the Green's function may be written down in terms of the solution to the one-speed Milne problem; that is:

$$\lim_{z' \rightarrow \infty} \rho_{01}(z' \rightarrow z; l) = \frac{3}{l} \rho_1(z, l) = -1 \quad . \quad (3.31)$$

This is a particular case of the more general relationship:

$$\lim_{z' \rightarrow \infty} \rho_0(z' \rightarrow z, \mu; l) = \frac{3}{l} \rho(z, \mu, l) \quad (3.32)$$

just as the boundary condition $\lim_{z \rightarrow \infty} \rho_{01}(z' \rightarrow z; l) = 0$ is a particular

case of the more general boundary condition:

$$\lim_{z \rightarrow \infty} \rho_{mn}(z' \rightarrow z; l) = 0 \quad n \neq 0 \quad . \quad (3.33)$$

Applying the optical reciprocity theorem (Davison 1957, p48) which states that:

$$\rho(z', \mu' \rightarrow z, \mu; l) = \rho(z, -\mu \rightarrow z', -\mu'; l)$$

i.e.

$$\rho_{mn}(z' \rightarrow z; l) = (-1)^{m+n} \rho_{nm}(z \rightarrow z'; l)$$

(3.34)

we find that the flux from a $P_1(\mu)$ source is given by:

$$\rho_{10}(z' \rightarrow z; l) = \begin{cases} 1 & z > z' \\ 0 & z < z' \end{cases} \quad (3.35)$$

Proceeding as for the derivation of (3.30) with $n=0, m=1$ we then obtain:

$$\rho_{11}(z' \rightarrow z; l) = 0 \quad (3.36)$$

The simplicity of these Green's functions which may at first appear surprising deserves some comment. It arises because away from sources the transport equation without capture conserves the neutron current. Hence $\rho_{m1}(z' \rightarrow z; l)$ is constant for $z \lesseqgtr z'$. For $z > z'$ this constant must be zero to give no net source of neutrons at infinity; its value for $z < z'$ is determined by the discontinuity in the flux at $z=z'$ introduced by the source.

By means of the recursion formula (3.28) and applying the appropriate boundary conditions we are able to express some of the higher order Green's functions in terms of $\rho_0(z, l)$ and $\rho_{00}(z' \rightarrow z; l)$. For example it may be shown without much difficulty that:

$$\begin{aligned} \rho_{02}(z' \rightarrow z; l) &= \frac{3}{2l} \rho_0(z', l) - \frac{1}{2} \rho_{00}(z' \rightarrow z; l) & z > z' \\ &= \frac{3}{2l} \rho_0(z', l) - \frac{1}{2} \rho_{00}(z' \rightarrow z; l) + \frac{3}{2l} (z - z') & z < z' \end{aligned} \quad (3.37)$$

and by the optical reciprocity theorem:

$$\rho_{20}(z' \rightarrow z; l) = \rho_{02}(z \rightarrow z'; l) \quad (3.38)$$

while

$$\rho_{21}(z' \rightarrow z; l) = -\rho_{12}(z \rightarrow z'; l) = 0. \quad (3.39)$$

Finally

$$\begin{aligned} \rho_{22}(z' \rightarrow z; l) &= \frac{3z'}{4l} - \frac{3}{4l} \left[\rho_0(z, l) + \rho_0(z', l) \right] + \frac{1}{4} \rho_{00}(z' \rightarrow z; l) & z < z' \\ &= \frac{3z}{4l} - \frac{3}{4l} \left[\rho_0(z, l) + \rho_0(z', l) \right] + \frac{1}{4} \rho_{00}(z' \rightarrow z; l) & z > z' \end{aligned} \quad (3.40)$$

The Green's functions we have written down have a particularly simple form - higher order Green's functions will involve quadratures of $\rho_{00}(z' \rightarrow z; l)$ and are consequently more complex. Although they will not be required these higher order Green's functions could still be obtained from the recursion equation. In attempting to apply a similar recursion relationship to the corresponding problem with capture this difficulty arises for even the simplest, first order Green's functions and provides the major stumbling block to a straightforward extension of the theory for the thermal neutron Milne problem with

capture (see Chapter 5) to anisotropic scattering. We shall look at this problem in more detail in Chapter 6.

§3.4 Integral Equations for Green's Functions with Isotropic Scattering

In §3.3 we described one way of finding the Green's functions for anisotropic sources $\rho_{mo}(z' \rightarrow z; \ell)$ -- namely by integrating the transport equation to obtain $\rho_{om}(z' \rightarrow z; \ell)$ and then applying the optical reciprocity theorem -- and this is likely to be the simplest. The traditional method was suggested much earlier (Case et al 1953, p122; Davison 1957, p59) and permits a direct solution for $\rho_{mo}(z' \rightarrow z; \ell)$ itself without invoking the optical reciprocity theorem.

Basically the flux is considered to be made up of two parts: the flux of neutrons coming directly from the anisotropic source and the flux of neutrons which have had at least one collision. The latter may be regarded as the flux from a distributed system of isotropic sources. If $H_{mo}(z' \rightarrow z; \ell)$ is the flux of neutrons at z which have come directly from the $P_m(\mu)$ source at z' we may write quite generally:

$$\rho_{mo}(z' \rightarrow z; \ell) = \int_0^{\infty} dz^+ \rho_{oo}(z^+ \rightarrow z; \ell) H_{mo}(z' \rightarrow z^+; \ell) + H_{mo}(z' \rightarrow z; \ell). \quad (3.41)$$

Let us, for the present, be even more general and apply the ideas just outlined to the derivation of an integral equation for the Green's functions $\rho_{mn}(z' \rightarrow z; \ell)$: that is, we seek by this approach an equation for the angular flux, and hence the angular moments of the flux, due to a $P_m(\mu)$ source at $z=z'$. We therefore start with the transport equation:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{l} \right] \rho_m(z' \rightarrow z, \mu; l) = \frac{1}{2l} \rho_{mo}(z' \rightarrow z; l) + \frac{1}{2} P_m(\mu) \delta(z-z') \quad (3.42)$$

and write:

$$\rho_m(z' \rightarrow z, \mu; l) = \Lambda_m(z' \rightarrow z, \mu; l) + H_m(z' \rightarrow z, \mu; l) \quad (3.43)$$

where $\Lambda_m(z' \rightarrow z, \mu; l)$ is the angular flux of neutrons which have had at least one collision and $H_{mo}(z' \rightarrow z; l)$ which has already been defined is related to $H_m(z' \rightarrow z, \mu; l)$ in the usual way by:

$$H_{mo}(z' \rightarrow z; l) = \int_{-1}^{+1} d\mu H_m(z' \rightarrow z, \mu; l) \quad (3.44)$$

Thus $H_m(z' \rightarrow z, \mu; l)$ satisfies:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{l} \right] H_m(z' \rightarrow z, \mu; l) = \frac{1}{2} P_m(\mu) \delta(z-z') \quad (3.45)$$

and $\Lambda_m(z' \rightarrow z, \mu; l)$ is given by:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{l} \right] \Lambda_m(z' \rightarrow z, \mu; l) = \frac{1}{2l} \Lambda_{mo}(z' \rightarrow z; l) + \frac{1}{2l} H_{mo}(z' \rightarrow z; l) \quad (3.46)$$

Equation (3.46) resembles a one-speed Milne equation with an isotropic source $H_{mo}(z' \rightarrow z; l)/l$ and may therefore be written in terms of the Green's function $\rho_0(z' \rightarrow z, \mu; l)$ as

$$\Lambda_m(z' \rightarrow z, \mu; \ell) = \frac{1}{\ell} \int_0^{\infty} dz^+ H_{m0}(z' \rightarrow z^+; \ell) \rho_0(z^+ \rightarrow z, \mu; \ell); \quad (3.47)$$

hence, from (3.43):

$$\rho_m(z' \rightarrow z, \mu; \ell) = \frac{1}{\ell} \int_0^{\infty} dz^+ H_{m0}(z' \rightarrow z^+; \ell) \rho_0(z^+ \rightarrow z, \mu; \ell) + H_m(z' \rightarrow z, \mu; \ell) \quad (3.48)$$

giving

$$\rho_{mn}(z' \rightarrow z; \ell) = \frac{1}{\ell} \int_0^{\infty} dz^+ H_{m0}(z' \rightarrow z^+; \ell) \rho_{0n}(z^+ \rightarrow z; \ell) + H_{mn}(z' \rightarrow z; \ell). \quad (3.49)$$

In order to determine $H_{mn}(z' \rightarrow z; \ell)$ explicitly (3.45) is written in the form:

$$\mu \frac{\partial}{\partial z} \left[e^{z/\mu \ell} H_m(z' \rightarrow z, \mu; \ell) \right] = \frac{1}{2} P_m(\mu) \delta(z - z') e^{z/\mu \ell}. \quad (3.50)$$

For $\mu > 0$ we integrate (3.50) from 0 to z and impose the condition of no incoming neutrons at the surface $z=0$ while for $\mu < 0$ we integrate from z to ∞ under the constraint that the solution is bounded as $z \rightarrow \infty$. This gives $H_m(z' \rightarrow z, \mu; \ell)$: in order to evaluate the n 'th moment we simply multiply by $P_n(\mu)$ and integrate over angle. The result is:

$$H_{mn}(z' \rightarrow z; \ell) = \frac{1}{2} \int_0^1 d\mu \cdot \frac{P_m(\pm\mu) P_n(\pm\mu)}{\mu} \exp \left\{ - \left| \frac{z - z'}{\mu \ell} \right| \right\} \begin{array}{l} z > z' \\ z < z' \end{array}$$

(3.51)

Having obtained an integral equation for $\rho_{mn}(z' \rightarrow z; \ell)$ which is valid for all m and n let us now be more specific and consider two particular examples of (3.49) and (3.51) to illustrate that in certain circumstances these rather involved expressions can be greatly simplified, a fact which may have application in other problems in neutron transport theory. For $m=1$ and $n=0$ it is easily shown that (3.49) and (3.51) reduce to the single equation:

$$\begin{aligned} \rho_{10}(z' \rightarrow z; \ell) = \frac{1}{2\ell} \int_0^{\infty} dz^+ \rho_{00}(z^+ \rightarrow z; \ell) E_2\left(\frac{|z^+ - z'|}{\ell}\right) \text{sign}(z^+ - z') \\ + \frac{1}{2} E_2\left(\frac{|z - z'|}{\ell}\right) \text{sign}(z - z') \end{aligned} \quad (3.52)$$

where

$$\begin{aligned} \text{sign}(z - z') &= 1 & z > z' \\ &= -1 & z < z' \end{aligned} \quad (3.53)$$

while for $m=2$ and $n=0$ we obtain a similar equation:

$$\begin{aligned} \rho_{20}(z' \rightarrow z; \ell) = \frac{3}{2} \left\{ \frac{1}{2\ell} \int_0^{\infty} dz^+ \rho_{00}(z^+ \rightarrow z; \ell) E_3\left(\frac{|z^+ - z'|}{\ell}\right) + \frac{1}{2} E_3\left(\frac{|z - z'|}{\ell}\right) \right\} \\ - \frac{1}{2} \rho_{00}(z' \rightarrow z; \ell). \end{aligned} \quad (3.54)$$

Thus far we have produced integral equations for $\rho_{10}(z' \rightarrow z; \ell)$ and $\rho_{20}(z' \rightarrow z; \ell)$ - and all the other Green's functions - without recourse to the optical reciprocity theorem. We shall show also that one does not need to refer to the optical reciprocity theorem in order to evaluate (3.52) and (3.54) to provide simple expressions for

$\rho_{10}(z^+ \rightarrow z; \ell)$ and $\rho_{20}(z^+ \rightarrow z; \ell)$. The fact remains that both of these integral equations may also be obtained by writing down the integro-differential form of the transport equation for the appropriate source, following through the procedure outlined below equation (3.50) to produce a similar integral equation for $\rho_{om}(z^+ \rightarrow z; \ell)$; $m=1,2$ and then applying the optical reciprocity theorem. We have seen too that the final simple expressions for $\rho_{10}(z^+ \rightarrow z; \ell)$ and $\rho_{20}(z^+ \rightarrow z; \ell)$ may also be obtained by means of the optical reciprocity theorem.

There are a number of ways of evaluating the integrals appearing in (3.52) and (3.54): we shall mention one method which illustrates the important steps in the process. Let us assume for the moment that the solution of (3.52) is already known and consider instead the solution of (3.54) which represents the more general situation.

Within (3.54) we define:

$$\Pi(z^+, z; \ell) = \frac{1}{2\ell} \int_0^{\infty} dz^+ \rho_{00}(z^+ \rightarrow z; \ell) E_3\left(\frac{|z^+ - z^+|}{\ell}\right) \quad (3.55)$$

for which

$$\frac{\partial}{\partial z} \Pi(z^+, z; \ell) = \frac{1}{2\ell^2} \int_0^{\infty} dz^+ \rho_{00}(z^+ \rightarrow z; \ell) E_2\left(\frac{|z^+ - z^+|}{\ell}\right) \text{sign}(z^+ - z^+). \quad (3.56)$$

Integrating (3.56) between z^+ and X noting that we shall eventually consider the limit $X \rightarrow \infty$ we find:

$$\Pi(X, z; l) - \Pi(z', z; l) = \frac{1}{2l^2} \int_{z'}^X dz'' \int_0^\infty dz^+ \rho_{00}(z^+ \rightarrow z; l) E_2 \left(\frac{|z^+ - z''|}{l} \right) \text{sign}(z^+ - z'') \quad (3.57)$$

$$\begin{aligned} &= \frac{1}{l} \int_{z'}^X dz'' \rho_{10}(z'' \rightarrow z; l) \\ &\quad - \frac{1}{2l} \int_{z'}^X dz'' E_2 \left(\frac{|z'' - z|}{l} \right) \text{sign}(z'' - z) \end{aligned} \quad (3.58)$$

where we have used (3.52) to derive (3.58) from (3.57). Substituting for $\rho_{10}(z'' \rightarrow z; l)$ from (3.35) and taking the limit as $X \rightarrow \infty$

$$\begin{aligned} \lim_{X \rightarrow \infty} \Pi(X, z; l) - \Pi(z', z; l) &= \frac{z - z'}{l} + \frac{1}{2} E_3 \left(\frac{|z - z'|}{l} \right) \quad z > z' \\ &= \frac{1}{2} E_3 \left(\frac{|z - z'|}{l} \right) \quad z < z' \end{aligned} \quad (3.59)$$

$$\begin{aligned} \text{Now } \lim_{X \rightarrow \infty} \Pi(X, z; l) &= \lim_{X \rightarrow \infty} \left\{ \frac{1}{2l} \int_X^\infty dz^+ \rho_{00}(z^+ \rightarrow z; l) E_3 \left(\frac{z^+ - X}{l} \right) \right. \\ &\quad + \frac{1}{2l} \int_z^X dz^+ \rho_{00}(z^+ \rightarrow z; l) E_3 \left(\frac{X - z^+}{l} \right) \\ &\quad \left. + \frac{1}{2l} \int_0^z dz^+ \rho_{00}(z^+ \rightarrow z; l) E_3 \left(\frac{X - z^+}{l} \right) \right\} \end{aligned} \quad (3.60)$$

$$\text{i.e.} \quad \lim_{X \rightarrow \infty} \Pi(X, z; \ell) = \rho_0(z, \ell)/\ell, \quad (3.61)$$

and in reducing (3.60) to (3.61) we have used (3.32). Substituting (3.61) into (3.59) and (3.59) in turn into (3.54) we obtain the desired result (3.38). A similar procedure may be adopted to evaluate

$\rho_{10}(z^+ \rightarrow z; \ell)$ but in that case the term corresponding to $\lim_{X \rightarrow \infty} \Pi(X, z; \ell)$ is zero and the limiting process becomes redundant -

the difference depends on the existence or otherwise of a factor $\text{sign}(z^+ - z')$ in the integrand. We also have to invoke the integral equation for $\rho_{00}(z^+ \rightarrow z; \ell)$ given by Davison (1957, p84) with $c=1$.

§3.5 Green's Functions with Linearly Anisotropic Scattering

In general we do not expect to be able to account for anisotropic scattering in any simple way even for one-speed problems and in particular we expect that there will be no straightforward method for obtaining Green's functions for an anisotropically scattering medium. But an exception is the Green's function $\rho_{00}^A(z^+ \rightarrow z; \ell_t)$ for a non-capturing half-space which scatters neutrons with linear anisotropy.

For an isotropic source the flux satisfies the transport equation

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell} \right] \rho_0^A(z^+ \rightarrow z; \mu; \ell_t) = \frac{1}{2\ell} \rho_{00}^A(z^+ \rightarrow z; \ell_t) + \frac{3}{2} \mu \Sigma_1 \rho_{01}^A(z^+ \rightarrow z; \ell_t) + \frac{1}{2} \delta(z - z'). \quad (3.62)$$

Integrating (3.62) over angle we find that for $z \neq z'$ the current

$\rho_{01}^A(z^+ \rightarrow z; \ell_t)$ is constant and then integrating over z as in (3.29) to

(3.30) we see that:

$$\rho_{01}^A(z' \rightarrow z; l_t) = \rho_{01}(z' \rightarrow z; l) \cdot \quad (3.63)$$

The boundary condition at the interface is:

$$\rho_0^A(z' \rightarrow z, \mu; l_t) = 0 \quad 0 < \mu \leq 1 \quad (3.64)$$

while for large z'

$$\rho_0^A(z' \rightarrow z, \mu; l_t) = \frac{3}{l_t} \rho^A(z, \mu, l_t) \cdot \quad (3.65)$$

We have already remarked in §3.2 that the solution to problems with linearly anisotropic scattering may be expressed in terms of the solution to the corresponding problem with isotropic scattering as long as there is no neutron capture: in this case a solution which satisfies the boundary conditions is:

$$\begin{aligned} \rho_{00}^A(z' \rightarrow z; l_t) &= \rho_{00}(z' \rightarrow z; l) + 3\Sigma_1 \rho_{01}^A(z' \rightarrow z; l_t) z \\ &= \rho_{00}(z' \rightarrow z; l) - 3\Sigma_1 z \cdot \end{aligned} \quad z < z' \quad (3.66)$$

By the optical reciprocity theorem we have:

$$\rho_{00}^A(z' \rightarrow z; l_t) = \rho_{00}(z' \rightarrow z; l) - 3\Sigma_1 z' \quad z > z' \cdot \quad (3.67)$$

Alternatively we may treat (3.62) as a Milne equation with isotropic scattering and two sources: an isotropic source $\delta(z-z')$ and a $P_1(\mu)$ source $3\Sigma_1 \rho_{01}^A(z' \rightarrow z; l_t)$. Then we may express $\rho_{00}^A(z' \rightarrow z; l_t)$ as:

$$\rho_{00}^A(z' \rightarrow z; l_t) = \rho_{00}(z' \rightarrow z; l) + 3\Sigma_1 \int_0^\infty dz^+ \rho_{10}(z^+ \rightarrow z; l) \rho_{01}^A(z' \rightarrow z^+; l_t) .$$

(3.68)

Replacing $\rho_{01}^A(z' \rightarrow z^+; l_t)$ by (3.63) and (3.30) enables us to evaluate the integral appearing in (3.68) and leads to the result already obtained. For a $P_1(\mu)$ source $\rho_{10}^A(z' \rightarrow z; l_t)$ is again found by the optical reciprocity theorem and it is easily shown, by integrating the transport equation with a $P_1(\mu)$ source over angle and imposing the boundary condition, that $\rho_{11}^A(z' \rightarrow z; l_t) = 0$.

The results (3.66) to (3.68) are in agreement with those found by McCormick and Kuščer (1965) who extended Case's normal mode expansion method (Case 1960) to include linearly anisotropic scattering.

CHAPTER 4

THE THERMAL NEUTRON MILNE PROBLEM WITH ANISOTROPIC SCATTERING

§4.1 Introduction

In Chapter 1 we discussed the reasons for attempting a solution of the thermal neutron Milne problem and sketched the important steps in a variational method devised for the simplest case of isotropic scattering and no neutron capture (Schofield 1963; see also Tait 1964). We saw in Chapter 2 that in order to determine the infinite medium eigenvalues of the transport equation in agreement with experiment for a water moderator it was necessary to take account of anisotropic scattering. This holds true also for transient effects: to predict accurately the angular distribution of neutrons emerging from a plane water surface it is essential to include the effects of anisotropic scattering. In this chapter we show how these effects may be incorporated in Schofield's variational principle.

We are mainly interested in the extrapolation length and the emergent angular distribution of neutrons for a water moderator in which we expect neutron capture to play only a small part. In fact for most of the common, unpoisoned moderators the extrapolation length will be determined largely by chemical binding and anisotropic scattering. The capture can usually be neglected (Williams 1964c). For the remainder of this chapter we shall therefore assume a purely scattering medium.

For any light moderator such as water in order to expect reasonable agreement with experiment one must include anisotropic scattering since it is the energy dependence of the transport mean free path $\ell_T(E)$ rather than the scattering mean free path $\ell(E)$ which is predominant in determining the spatial dependence of the neutron distribution. This has been very elegantly demonstrated by Sinclair et al (1963). Since $\ell_T(E)$ is determined by $\ell(E)$ and the first moment of the scattering kernel $\Sigma_1(E' \rightarrow E)$ it is to be expected that linearly anisotropic scattering will be sufficient to describe the situation in water and other incoherently scattering moderators although for crystals with significant coherent scattering cross-sections higher order anisotropic scattering may be necessary. The situation is quite different if there is a large "slowing-down" component to the spectrum.

At the time this work was begun the theoretical treatment of Kladnik and Kušcer (1961) predicted the mean energy of the neutron distribution emitted perpendicularly to the surface to be about 18% greater than the mean energy of a Maxwellian distribution, a result in substantial agreement with experiments performed up to that time. However the theory is constrained to give a Maxwellian distribution at grazing angles to the surface. Other theoretical treatments, generally under the assumption of isotropic scattering and for free gas moderators, also suggested that at grazing angles the spectrum would be near-Maxwellian (Williams 1964a,b; Eisenhauer 1964). This conflicted

with the experimental results of Sinclair and Williams (1965) and of Kallfelz (Kallfelz and Reichardt 1965; Kallfelz 1966, 1967; Kallfelz and Beckurts 1967) who predicted a mean energy to the neutron distribution 5-10% greater than that of a Maxwellian. It is now known that the prediction of a near-Maxwellian spectrum at grazing angles depends largely on the scattering model chosen or the limitations of the method employed: indeed there is no good reason to expect a Maxwellian in general. With the theoretical treatment described in this chapter it is now possible to predict accurately the energy dependence of the emergent spectrum at all angles to the surface.

It may be asked what is the value of any analytical approach to this type of problem when there exist computer codes such as those based on the S_n method which can, in principle at least, solve the problem numerically. One answer is the practical one that a knowledge of the qualitative behaviour of the flux as a function of position and energy not only allows one to make a suitable choice of mesh points for such a calculation but also provides a standard for the comparison of various codes. Another is that even now it is very difficult to obtain from the results of purely numerical computation any feeling for the way in which boundaries and discontinuities affect the diffusion of thermal neutrons. Moreover there are inherent numerical difficulties in some of the codes which are avoided in an analytical approach: one such problem, encountered in the calculations of Eisenhauer (1964), is mentioned in §4.8. [Some of the remarks in this

paragraph were originally made by Schofield (1963) and are included for completeness only: complementary remarks have been made by Williams (1966,p309)].

While there have been other analytical approaches to this problem an exact solution is only possible when the scattering model is particularly simple. One such model is the separable kernel of Corngold, implying strong energy exchange, which has been described in §1.2 and which permits a solution by the Wiener-Hopf technique (Williams 1964a). This method of solution has recently been extended to a two-term degenerate kernel (Williams 1967) in which the first term corresponds to the one-term degenerate (or separable) kernel and thus ensures the correct total cross-section; the remaining terms allow a more realistic description of the energy transfer process by conserving the first energy moment of the kernel and have the same general form as the first term. The kernel satisfies the detailed balance condition. A solution for the separable kernel has also been obtained by "Case's method" (Mika 1965) which for half-space problems is entirely equivalent to the older Wiener-Hopf approach (Arkuszewski 1967). Although this method has been applied to a wide variety of problems in fairly simple geometries its practical success in other energy dependent problems has been rather limited. The diagonal or δ -function kernel implying no energy exchange also allows a solution by these methods

Eisenhauer (1964) obtained some numerical results for the proton gas moderator using the THERMOS computer code (Honeck 1961) which enabled Williams (1964b) to show that the separable kernel is a fairly close approximation to the true kernel for this particular moderator. Williams was then able to apply perturbation theory with the separable kernel results as the unperturbed solution.

Amongst other work which has not been restricted to particular scattering models nor restricted to isotropic scattering the variational and spherical harmonics methods figure prominently. Nelkin (1960b) has employed a variational technique for a general isotropic kernel which is simply an energy dependent version of LeCaine's variational principle for the one-speed Milne problem, described in §3.2. The differential form of the transport equation (2.17) with the boundary conditions appropriate to the Milne problem is rewritten as an integral equation, in the way that we described from (3.1) to (3.4) for the one-speed solution:

$$\Psi_0(z, E) = \frac{1}{2} \int_0^{\infty} dz' \int_0^{\infty} dE' E_1 \left(\frac{|z-z'|}{\ell(E)} \right) \Sigma_0(E' \rightarrow E) \Psi_0(z', E') \quad (4.1)$$

and in like manner it is found that the asymptotic flux has the form:

$$\Psi_0(z, E) \sim \Psi_{0, \text{asy}}(z, E) = (z+z_0) M(E) \quad (4.2)$$

where z_0 is the extrapolation length (to be calculated) which will be discussed in greater detail later. The subsequent steps in the estimation of z_0 are very similar to the procedure adopted by LeCaine except that the trial function for the flux has a much simpler form than that chosen in the one-speed problem. While LeCaine was able to represent the transient flux very accurately through the terms involving exponential integrals in (3.10) the corresponding terms in the energy dependent case lead to more complicated integrals and were not considered by Nelkin.

Kladnik and Kuscer (1961) have extended this variational principle still further by including anisotropic scattering and writing the functional in terms of the angular flux $\Psi(z, \mu, E)$ instead of the scalar flux $\Psi_0(z, E)$. The approach is similar to that given earlier by Nelkin and again the flux is approximated firstly by its asymptotic behaviour. An improved trial function is also adopted which associates the transient flux with a decaying spatial dependence of the form $\exp\{-z/\ell_{\max}\}$. Kladnik and Kuscer give most emphasis to the effect of variations in the mean free path to the virtual exclusion of thermalisation effects: the energy dependence of their trial function is predetermined so that the thermalisation model only enters into the calculation of the transport mean free path. Furthermore the form of the trial function determines that the emergent flux at grazing angles to the surface of the moderator will be Maxwellian. Later work by Kallfelz (Kallfelz and Reichardt 1965, 1967; Kallfelz and Kladnik 1967) has shown that the trial function may be modified so that the resulting

expression for $\Psi(0,0,E)$ need no longer have the form of a Maxwellian; nevertheless the energy dependence of the trial function remains pre-assigned. By iterating the trial function (in which the parameters are estimated by the variational principle) twice through the defining transport equation Kallfelz is able to obtain substantial agreement with experimental results for the emergent neutron distribution from a water moderator and with the results of our own calculations performed at about the same time. All of these results are discussed in detail later in this chapter.

Conkie (1960) has adopted a purely P_1 approximation in terms of the neutron distribution $N(z,\mu,v)$ where v is the magnitude of the neutron velocity and $N(z,\mu,v)$ is related to the neutron flux by:

$$\Psi(z,\mu,E) = v N(z,\mu,v) \quad . \quad (4.3)$$

Firstly the neutron distribution is expanded in terms of Legendre polynomials as far as the second or P_1 term; thus in the usual notation:

$$N(z,\mu,v) = \frac{1}{2} \sum_{n=0}^1 (2n+1) P_n(\mu) N_n(z,v) \quad (4.4)$$

with the result that the transport equation is replaced by two coupled integro-differential equations in the unknowns $N_0(z,v)$ and $N_1(z,v)$.

These are decomposed by the substitution:

$$N_n(z, \nu) = \sum_j a_j e^{g_j z} f_{nj}(\nu) \quad (4.5)$$

leading to coupled integral equations with eigenvalues g_j and eigenfunctions $f_{nj}(\nu)$. The coefficients a_j are determined by the boundary conditions of the Milne problem. The resulting equations can be solved by the method of polynomial approximation, in this case with Tchebycheff polynomials $\phi_m(y)$. We write:

$$f_{oj}(\nu) = M(\nu) \sum_{m=0}^M a_{jm} \phi_m(y) \quad (4.6)$$

where y is a suitable function of ν determined by Conkie. A similar expression holds for $f_{1j}(\nu)$. Thus, finally, we obtain a set of linear equations which can be solved by straightforward matrix manipulation, leading eventually to an expression for the total flux at the surface.

In contrast to the work of Kladnik and Kuscer, Conkie's treatment is dominated by the thermalisation aspects of the problem in that the P_1 approximation neglects transient solutions having the form $\exp\{-z/\ell_{\max}\}$. Mark's boundary conditions (Davison 1957, p129) are imposed so that an accurate estimate of the extrapolation length cannot be expected. The first recorded result for the proton gas ($z_0 = 0.76 \ell_{\max}$) is about 20% too low. Later work with the spherical harmonics method and a self-consistent iterative procedure (Conkie 1964) shows some improvement but even these results do not compare favourably with variational estimates of the extrapolation length. A paper by

Kiefhaber (1964) is also based on Conkie's earlier work, replacing the Tchebycheff polynomials by Laguerre polynomials but he compares only the integrated flux $\Psi_0(z,E)$ at the interface $z=0$ with experiment. His method of solution predicts only the total flux and no estimation of the angular variation is possible.

The present method is sensitive both to variations in the mean free path and to the details of the scattering model; this is more likely to be important for a coherently scattering crystalline moderator such as Beryllium or Graphite where the mean free path may vary considerably with energy. Furthermore it has the advantage that it reduces to the correct limits in the cases of "constant (transport) mean free path" and "no energy exchange".

In the remainder of this chapter we shall develop a theory for the thermal neutron Milne problem with anisotropic scattering and compare the results of calculations based on this theory with experimental measurements and other theoretical predictions. The particular case of linearly anisotropic scattering is considered in detail but we shall show that the method may be extended, in principle at least, to higher order anisotropy.

The basis of the method is to write the flux in the energy dependent problem in terms of the solution to the corresponding Milne problem and the associated half-space Green's functions. Both of these are discussed in Chapter 3 where we present approximate expressions for the one-speed Milne solutions and show that the Green's functions are expressible in terms of known functions (see §3.3 to §3.5). Starting

from the usual integro-differential form of the transport equation this is achieved in §4.2. In §4.3 we begin by deriving simple expressions for z_0 as appropriate averages over the corresponding one-speed extrapolation length for the two special cases of "constant transport mean free path" and "no energy exchange". This leads to a more useful expression for z_0 , for a quite general P_1 scattering kernel, based on the Green's function equations derived in §4.2 which reduces to the correct limits in the special cases outlined above. Still using the equations obtained in §4.2 one can then write down a functional for a variational principle (§4.4) which provides an estimate of the extrapolation length while the emergent angular distribution of neutrons may be determined by iterating the trial function. The choice of functional is discussed in the first part of this section. In §4.5 we present an alternative formulation of the variational principle which is especially useful if one represents linearly anisotropic scattering by the transport approximation while §4.6 deals with the extension of the method to higher order anisotropy. A simple trial function for the transient flux is introduced in §4.7 and in §4.8 numerical results obtained by inserting this trial function into the variational principle are discussed. The description of the numerical methods is deferred to an appendix.

§4.2 The Transport Equation

In plane geometry the transport equation for the neutron flux $\Psi(z, \mu, E)$ in the absence of capture is given by (1.6) and for linearly anisotropic scattering only the first two terms on the right hand side of (1.6) are non-zero: thus the transport equation becomes:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \Psi(z, \mu, E) = \frac{1}{2} \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi_0(z, E') + \frac{3}{2} \mu \int_0^{\infty} dE' \Sigma_1(E' \rightarrow E) \Psi_1(z, E') \quad (4.7)$$

with the boundary condition at the interface:

$$\Psi(0, \mu, E) = 0 \quad 0 < \mu \leq 1. \quad (4.8)$$

At large z , the neutron flux has the asymptotic form:

$$\Psi(z, \mu, E) \sim \Psi_{\text{asy}}(z, \mu, E) = \frac{1}{2} \left[z + z_0(E) - \mu \ell_T(E) \right] M(E) \quad (4.9)$$

where $\ell_T(E)$ is the transport mean free path determined by the condition that (4.9) be a solution of (4.7), that is:

$$\ell(E) - \ell_T(E) = - \ell(E) \int_0^{\infty} dE' \Sigma_1(E \rightarrow E') \ell_T(E') \quad (4.10)$$

where we have also used the detailed balance condition (1.8) in the form:

$$M(E) \Sigma_n(E \rightarrow E') = M(E') \Sigma_n(E' \rightarrow E). \quad (4.11)$$

For a real moderator $z_0(E)$ is independent of energy and is the linear extrapolation length appropriate to the energy dependent Milne problem. It represents the distance from the boundary, outside the medium, at which the asymptotic scalar flux $\Psi_{o,asy}(z,E)$ falls to zero.

Two conservation conditions may be obtained by integrating the transport equation which are valid for all z including the boundary region. Integrating (4.7) over angle and energy it may be shown that the total current:

$$J(z) = \int_0^{\infty} dE \int_{-1}^{+1} d\mu \mu \Psi(z,\mu,E) \quad (4.12)$$

is a constant, as we might expect with no capture. Adopting the normalisation implied by (4.9):

$$J = \bar{\ell}_T/3 \quad (4.13)$$

where the bar signifies a Maxwellian average:

$$\bar{X} = \int_0^{\infty} dE M(E) X(E) \quad (4.14)$$

Another conservation condition is obtained by multiplying (4.7) by $\mu \ell_T(E)$ and integrating over angle and energy. Defining:

$$K(z) = \int_0^{\infty} dE \ell_T(E) \int_{-1}^{+1} d\mu \mu^2 \Psi(z,\mu,E) \quad (4.15)$$

we find that:

$$K(z) = \frac{\bar{\ell}_T}{3} (z + z_0) \quad . \quad (4.16)$$

Substitution of (4.9) into (4.15) gives:

$$z_0 \bar{\ell}_T = \int_0^{\infty} dE M(E) \ell_T(E) z_0(E) \quad . \quad (4.17)$$

The method we propose depends on the observation that (4.7) may be rearranged to resemble a one-speed equation. Dividing (4.7) by the Maxwellian distribution and separating the right hand side:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \psi(z, \mu, E) = \frac{1}{2\ell(E)} \psi_0(z, E) + \frac{1}{2} S_0(z, E) + \frac{3}{2} \mu \int_0^{\infty} dE' \Sigma_1(E \rightarrow E') \psi_1(z, E) \quad (4.18)$$

where

$$\Psi(z, \mu, E) = M(E) \psi(z, \mu, E) \quad (4.19)$$

and

$$S_n(z, E) = \int_0^{\infty} dE' \Sigma_n(E \rightarrow E') \left[\psi_n(z, E') - \psi_n(z, E) \right] \quad . \quad (4.20)$$

Equation (4.18) has the appearance of a one-speed Milne equation at energy E with isotropic scattering and having two sources; (a) an isotropic source $S_0(z, E)$ and (b) a $P_1(\mu)$ source

$3\mu \int_0^{\infty} dE' \Sigma_1(E \rightarrow E') \psi_1(z, E')$. Thus we may immediately write:

$$\begin{aligned} \psi(z, \mu, E) = N(E) \rho(z, \mu, \ell(E)) + \int_0^{\infty} dz' S_0(z', E) \rho_0(z' \rightarrow z, \mu; \ell(E)) \\ + 3 \int_0^{\infty} dz' \rho_1(z' \rightarrow z, \mu; \ell(E)) \int_0^{\infty} dE' \Sigma_1(E \rightarrow E') \psi_1(z', E') \end{aligned} \quad (4.21)$$

where $\rho(z, \mu, \ell(E))$ is the solution of the one-speed Milne problem with isotropic scattering and the half-space Green's function

$\rho_n(z' \rightarrow z, \mu; \ell(E))$ for $n=0,1$ represents the angular flux from a $P_n(\mu')$ source at z' in a medium which scatters neutrons isotropically and has mean free path $\ell(E)$ - all of which have been defined in Chapter 3.

$N(E)$ is a normalising factor which will be determined by the asymptotic form of $\psi(z, \mu, E)$.

§4.3 An Expression for the Extrapolation Length

In this section we shall show that a general expression for the extrapolation length may be written down as a sum of three terms of which the first may be evaluated exactly. Then in §4.4 we shall derive a variational principle to provide an estimate of the last two terms.

It is revealing to write (4.7) in the form:

$$\begin{aligned} \left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \psi(z, \mu, E) = \frac{1}{2\ell(E)} \psi_0(z, E) + \frac{3}{2} \mu \Sigma_1(E) \psi_1(z, E) \\ + \frac{1}{2} S_0(z, E) + \frac{3}{2} \mu S_1(z, E) \end{aligned} \quad (4.22)$$

where $S_0(z, E)$ and $S_1(z, E)$ are defined by (4.20). There are two special cases when the solution of (4.22) may be written down:

(a) if $\Sigma_0(E)$ and $\Sigma_1(E)$ are both independent of energy then the equation is separable in space and energy. The solution which satisfies the boundary conditions is:

$$\Psi(z, \mu, E) = M(E) \rho^A(z, \mu, l_t) \quad (4.23)$$

since, under these conditions, both source terms are zero and we find:

$$z_0 = c l_t \quad (4.24)$$

(b) if there is no coupling between different energies, i.e. $\Sigma_n(E \rightarrow E') = \Sigma_n(E) \delta(E - E')$ then $S_n(z, E) = 0$ and

$$\Psi(z, \mu, E) = M(E) \rho^A(z, \mu, l_t(E)) \quad (4.25)$$

$$z_0(E) = c l_t(E) \quad (4.26)$$

where

$$l_t(E) = \frac{l(E)}{1 - \Sigma_1(E) l(E)} \quad (4.27)$$

In each case, by equation (4.17)

$$z_0 = c \overline{l_t^2} / \overline{l_t} \quad (4.28)$$

More generally we may write:

$$z_0 = \frac{c \overline{l_T^2}}{\overline{l_T}} + \frac{3 z_0}{\overline{l_T}} \quad (4.29)$$

where Z_0 tends to zero as the rate of thermalisation tends to zero and as deviations from constant (transport) mean free path tend to zero.

It should be said that equation (4.23) may also be obtained from (4.18) by means of the simple relationship:

$$\frac{\partial}{\partial z} \psi_1(z, E) = S_0(z, E) \quad (4.30)$$

which results from integrating (4.18) over angle. Integrating (4.30) over z we find:

$$\psi_1(z \rightarrow \infty, E) - \psi_1(z, E) = -\frac{l_T(E)}{3} - \psi_1(z, E) = \int_z^\infty S_0(z', E) dz' \quad (4.31)$$

and therefore (4.18) may be written:

$$\begin{aligned} \left[\mu \frac{\partial}{\partial z} + \frac{1}{l(E)} \right] \psi(z, \mu, E) &= \frac{1}{2l(E)} \psi_0(z, E) - \frac{\mu}{2} \int_0^\infty dE' \Sigma_1(E \rightarrow E') l_T(E') + \frac{1}{2} S_0(z, E) \\ &- \frac{3}{2} \mu \int_0^\infty dE' \Sigma_1(E \rightarrow E') \int_z^\infty S_0(z', E') dz' \end{aligned} \quad (4.32)$$

Using the fact that $\rho_1^A(z, l_t) = -l_t/3$ we see that when the mean free path and transport mean free path are constant (4.23) is a solution of (4.18) because then $S_0(z, E) = 0$ and $l_T(E)$ reduces to $l_t(E)$. The reduction for case (b) may also be carried through very simply starting with equation (4.18).

Thus although the solutions in these two limiting cases arise most naturally from a consideration of (4.22) it is also possible by means of the useful relationship (4.30) to obtain the same solutions from (4.18): and it is the latter form of the transport equation (4.18) which will concern us in this and the next section.

The problem now is to find an expression for Z_0 in (4.29). The first step is to determine the normalising factor $N(E)$ which appears in (4.21). We consider the first Legendre moment of (4.21):

$$\begin{aligned} \psi_1(z, E) = N(E) \rho_1(z, \ell(E)) + \int_0^{\infty} dz' S_0(z', E) \rho_{01}(z' \rightarrow z; \ell(E)) \\ + 3 \int_0^{\infty} dz' \rho_{11}(z' \rightarrow z; \ell(E)) \int_0^{\infty} dE' \Sigma_1(E \rightarrow E') \psi_1(z', E') \end{aligned} \quad (4.33)$$

and replace $\rho_{01}(z' \rightarrow z; \ell(E))$ and $\rho_{11}(z' \rightarrow z; \ell(E))$ by (3.30) and (3.36) respectively to obtain:

$$\psi_1(z, E) = N(E) \rho_1(z, \ell(E)) - \int_z^{\infty} dz' S_0(z', E) \quad (4.34)$$

Introducing the notation

$$\psi(z, \mu, E) = \psi_{asy}(z, \mu, E) - \phi(z, \mu, E) \quad (4.35)$$

into (4.31) we have:

$$\phi_1(z, E) = \int_z^{\infty} S_0(z', E) dz' \quad (4.36)$$

Substituting (4.36) into (4.34), imposing (4.9) and the fact that $\rho_1(z, l(E)) = -l(E)/3$ we find that:

$$N(E) = l_T(E)/l(E) . \quad (4.37)$$

Taking the zero'th Legendre moment of (4.21) it may then easily be shown that:

$$\begin{aligned} \psi_0(z, E) = & \frac{l_T(E)}{l(E)} \rho_0(z, l(E)) + \int_0^\infty dz' S_0(z', E) \rho_{00}(z' \rightarrow z; l(E)) \\ & - 3 \int_0^\infty dz' \rho_{10}(z' \rightarrow z; l(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z', E') + z \left(1 - \frac{l_T(E)}{l(E)} \right) \end{aligned} \quad (4.38)$$

For large z , remembering that in this limit $S_0(z, E)$ tends to zero, (4.38) becomes:

$$\begin{aligned} z_0 = & c l_T(E) + \frac{3}{l(E)} \int_0^\infty dz' S_0(z', E) \rho_0(z', l(E)) \\ & + \frac{9}{l(E)} \int_0^\infty dz' \rho_1(z', l(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z', E') \end{aligned} \quad (4.39)$$

which is a result that may also be obtained by multiplying (4.18) by the adjoint flux $\rho(z, -\mu, l(E))$ of the isotropic, one-speed Milne problem and integrating over space and angle.

Equation (4.39) is an exact relationship which for the correct choice of $\psi_0(z,E)$ and $\psi_1(z,E)$ predicts a constant z_0 , independent of energy. In the subsequent theory, however, we shall only be able to approximate the flux by a fairly simple analytic function of (z,E) : in that case it is necessary to eliminate the energy dependence in (4.39) by some form of averaging procedure. Such a device is provided by (4.17). Substituting (4.39) into (4.17) or alternatively multiplying (4.39) by $M(E) \ell_T(E)$ and integrating over energy we find:

$$z_0 = \frac{\overline{c\ell_T^2}}{\ell_T} + \frac{3}{\ell_T} \int_0^\infty dE M(E) \frac{\ell_T(E)}{\ell(E)} \int_0^\infty dz S_0(z,E) \rho_0(z,\ell(E))$$

$$+ \frac{9}{\ell_T} \int_0^\infty dE M(E) \frac{\ell_T(E)}{\ell(E)} \int_0^\infty dz \rho_1(z,\ell(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z,E')$$

(4.40)

where we also note that

$$S_0(z,E) = \int_0^\infty dE' \Sigma_0(E \rightarrow E') \left[\phi_0(z,E) - \phi_0(z,E') \right]$$

(4.41)

and we shall henceforth refer to this source term as $s_0(z,E)$ to remind us that it is independent of the asymptotic part of $\psi_0(z,E)$. Having acquired an expression for the extrapolation length (4.40) in which we can calculate the first term we now require a means of estimating the remaining terms: this is achieved through a variational principle.

§4.4 The Variational Principle

Davison (1957,p202) and Rowlands (1961), amongst others, have described in some detail the application of variational principles to inhomogeneous integral equations in order to obtain an estimate of some weighted average of the (unknown) solution. In a previous paper (Schofield 1963; see also Tait 1964) these methods were applied to the Milne problem with isotropic scattering where it was shown that for the equation:

$$\psi_0(z,E) = \rho_0(z,\ell(E)) + \int_0^{\infty} dz' s_0(z',E) \rho_{00}(z' \rightarrow z; \ell(E)) \quad (4.42)$$

the functional

$$\begin{aligned} Z_0[\phi_0(z,E)] = & \\ & \int_0^{\infty} dE M(E) \int_0^{\infty} dz s_0(z,E) \left[2 \rho_0(z,\ell(E)) - \psi_0(z,E) \right. \\ & \left. + \int_0^{\infty} dz' s_0(z',E) \rho_{00}(z' \rightarrow z; \ell(E)) \right] \end{aligned} \quad (4.43)$$

is stationary when $\psi_0(z,E)$ satisfies (4.42) and, in that case:

$$Z_0[\phi_0(z,E)] = \int_0^{\infty} dE M(E) \int_0^{\infty} dz s_0(z,E) \rho_0(z,\ell(E)) \quad (4.44)$$

It should be noted that the functional is finite only because $s_0(z,E)$ decays exponentially [$\sim \exp\{-z/\ell_{\max}\}$] away from the boundary: also the functional is independent of the asymptotic part of the flux so that we may, if we wish, replace $-\psi_0(z,E)$ by $\phi_0(z,E)$. The only way in which

this differs from the variational principle described by Davison is that instead of the adjoint flux $\psi_0(z,E)$ we have used the adjoint to $s_0(z,E)$ where:

$$s_0^+(z,E) = M(E) s_0(z,E) \quad . \quad (4.45)$$

An additional difficulty arises for the same problem with linearly anisotropic scattering. In this case (4.42) is replaced by two coupled inhomogeneous integral equations given by the zeroth and first Legendre moments of (4.21):

$$\begin{aligned} \psi_0(z,E) &= \frac{\ell_T(E)}{\ell(E)} \rho_0(z,\ell(E)) + \int_0^\infty dz' S_0(z',E) \rho_{00}(z' \rightarrow z; \ell(E)) \\ &\quad + 3 \int_0^\infty dz' \rho_{10}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \psi_1(z',E'), \\ \psi_1(z,E) &= \frac{\ell_T(E)}{\ell(E)} \rho_1(z,\ell(E)) + \int_0^\infty dz' S_0(z',E) \rho_{01}(z' \rightarrow z; \ell(E)) \\ &\quad + 3 \int_0^\infty dz' \rho_{11}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \psi_1(z',E'). \end{aligned} \quad (4.46)$$

However the functional (4.43) may not be generalised immediately for, while $S_0(z,E)$ decays exponentially away from the boundary, the term $\int_0^\infty dE' \Sigma_1(E \rightarrow E') \psi_1(z,E')$ is finite for large z and hence would cause the functional to diverge. Instead we express (4.46) in terms of the zeroth and first moments of the transient flux, $\phi_0(z,E)$ and $\phi_1(z,E)$; that is

$$\begin{aligned}
-\phi_0(z, E) &= \left[\frac{\ell_T(E)}{\ell(E)} \rho_0(z, \ell(E)) - \psi_{0_{\text{asy}}}(z, E) + z \left(1 - \frac{\ell_T(E)}{\ell(E)} \right) \right] \\
&+ \int_0^\infty dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E)) - 3 \int_0^\infty dz' \rho_{10}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z', E') \\
-\phi_1(z, E) &= \left[\frac{\ell_T(E)}{\ell(E)} \rho_1(z, \ell(E)) - \psi_{1_{\text{asy}}}(z, E) \right] \\
&+ \int_0^\infty dz' s_0(z', E) \rho_{01}(z' \rightarrow z; \ell(E)) - 3 \int_0^\infty dz' \rho_{11}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z', E')
\end{aligned}$$

(4.47)

and we see that the only significant difference is to alter the "source term" in each equation. This leads to the choice of the following functional as the natural extension of (4.43) for the two coupled equations (4.47):

$$\begin{aligned}
& \mathcal{Z}_0 \left[\phi_0(z, E); \phi_1(z, E) \right] \\
&= \int_0^\infty dE M(E) \int_0^\infty dz s_0(z, E) \left\{ 2 \left[\frac{\ell_T(E)}{\ell(E)} \rho_0(z, \ell(E)) \rightarrow \psi_{0 \text{asy}}(z, E) + z \left(1 - \frac{\ell_T(E)}{\ell(E)} \right) \right] + \phi_0(z, E) \right. \\
&+ \left. \int_0^\infty dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E)) - 3 \int_0^\infty dz' \rho_{10}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z', E') \right\} \\
&+ 3 \int_0^\infty dE M(E) \int_0^\infty dz \int_0^\infty dE'' \Sigma_1(E \rightarrow E'') \phi_1(z, E'') \left\{ 2 \left[\frac{\ell_T(E)}{\ell(E)} \rho_1(z, \ell(E)) \rightarrow \psi_{1 \text{asy}}(z, E) \right] + \phi_1(z, E) \right. \\
&+ \left. \int_0^\infty dz' s_0(z', E) \rho_{01}(z' \rightarrow z; \ell(E)) - 3 \int_0^\infty dz' \rho_{11}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z', E') \right\}.
\end{aligned} \tag{4.48}$$

It is easily found that (4.48) is stationary when $\phi_0(z, E)$ and $\phi_1(z, E)$ satisfy (4.47) and that then $\mathcal{Z}_0[\phi_0(z, E); \phi_1(z, E)]$ is given by:

$$\begin{aligned}
\mathcal{Z}_0 \left[\phi_0(z, E); \phi_1(z, E) \right] &= \int_0^\infty dE M(E) \left[\frac{\ell_T(E)}{\ell(E)} \int_0^\infty dz s_0(z, E) \rho_0(z, \ell(E)) \right. \\
&+ \left. \left(1 - \frac{\ell_T(E)}{\ell(E)} \right) \int_0^\infty dz \cdot z s_0(z, E) \right].
\end{aligned} \tag{4.49}$$

Using the fact that

$$\int_0^{\infty} dz \cdot z s_0(z, E) = \int_0^{\infty} dz \int_z^{\infty} dz' s_0(z', E) = \int_0^{\infty} dz \phi_1(z, E) \quad (4.50)$$

together with the detailed balance condition and equation (4.10) we find that the functional given by (4.49) reduces to Z_0 as expressed by (4.29) and (4.40). While it is evident that the replacement of some of the Green's functions and of $\rho_1(z, \ell(E))$ and $\psi_{1asy}(z, E)$ by their actual values would greatly simplify the form of many of the preceding equations they have all been retained explicitly in order that the relationship of the various terms and the eventual extension to higher order anisotropy will be more readily apparent.

The functional is independent of the addition to $\phi_0(z, E)$ of any energy independent function of z which is not surprising since Z_0 itself is unchanged by such a function. In particular it is unaffected by the addition of the asymptotic part of $\psi_0(z, E)$. This means that in calculating the flux and emergent angular distribution by means of any restricted trial function one should use a first iteration of the following equation which may be derived from (4.38) by subtracting out the asymptotic part:

$$\begin{aligned} \phi_0(z, E) = & \frac{\ell_T(E)}{\ell(E)} \rho_{0tr}(z, \ell(E)) - \int_0^{\infty} dz' s_0(z', E) \left[\rho_{00}(z' \rightarrow z; \ell(E)) - \frac{3}{\ell(E)} \rho_0(z', \ell(E)) \right] \\ & - 3 \int_z^{\infty} dz' \int_0^{\infty} dE' \Sigma_1(E \rightarrow E') \phi_1(z', E') \quad (4.51) \end{aligned}$$

where

$$\rho(z, \mu, \ell(E)) = \rho_{\text{asy}}(z, \mu, \ell(E)) - \rho_{\text{tr}}(z, \mu, \ell(E)) \quad (4.52)$$

In particular, from (3.23)

$$\begin{aligned} \phi_0(0, E) &= \frac{\ell_T(E)}{\ell(E)} \rho_{0_{\text{tr}}}(0, \ell(E)) - \int_0^\infty dz s_0(z, E) \left[\sqrt{3} \rho_0^t(z, \ell(E)) - \frac{3}{\ell(E)} \rho_0(z, \ell(E)) \right] \\ &- 3 \int_0^\infty dz \int_0^\infty dE^t \Sigma_1(E \rightarrow E^t) \phi_1(z, E^t) \quad (4.53) \end{aligned}$$

Naturally the right hand sides of (4.51) and (4.53) are also independent of the addition to the uniterated $\phi_0(z, E)$ of energy independent functions of z . An expression for $\Psi(0, -\mu, E)$ in terms of $\phi_0(z, E)$ and $\phi_1(z, E)$ which may be obtained by integrating (4.7) over z will be given in §4.8.

Before discussing an appropriate trial function for $\phi(z, \mu, E)$ we should like to consider the problem from a different viewpoint, commenting briefly on the transport equation and also to demonstrate the application of this method to higher order anisotropy.

§4.5 An Alternative Variational Principle

An alternative variational principle may also be derived which bears a closer resemblance to the approach adopted by Schofield (1963) for isotropic scattering. In this section we shall give only a brief outline of the procedure. In this case the fundamental transport equation is not written in the form (4.18): instead we start with equation (4.22) which resembles a one-speed equation with linearly anisotropic scattering having two sources, (a) an isotropic source $s_0(z, E)$ and (b) a linearly anisotropic source $3\mu S_1(z, E)$ both of which vanish when there is no energy exchange. Therefore in terms of the Green's functions:

$$\begin{aligned} \psi(z, \mu, E) = q(E) \rho^A(z, \mu, l_t(E)) + \int_0^\infty dz' \rho_0^A(z' \rightarrow z, \mu; l_t(E)) s_0(z', E) \\ + 3 \int_0^\infty dz' \rho_1^A(z' \rightarrow z, \mu; l_t(E)) s_1(z', E) \end{aligned} \quad (4.54)$$

where $q(E)$ is a normalising factor. Following the procedure from (4.33) onwards it is easily shown that:

$$q(E) = l_T(E) / l_t(E) \quad (4.55)$$

and

$$\begin{aligned} z_0 = cl_T(E) + \frac{3}{l_t(E)} \int_0^\infty dz' s_0(z', E) \rho_0^A(z', l_t(E)) \\ - \frac{9}{l_t(E)} \int_0^\infty dz' s_1(z', E) \rho_1^A(z', l_t(E)) \end{aligned} \quad (4.56)$$

with

$$s_n(z, E) = \int_0^\infty dE' \Sigma_n(E \rightarrow E') \left[\phi_n(z, E) - \phi_n(z, E') \right]. \quad (4.57)$$

Consequently

$$\begin{aligned} z_0 = \frac{c \overline{l_T^2}}{\overline{l_T}} + \frac{3}{\overline{l_T}} \int_0^\infty dE M(E) \frac{l_T(E)}{l_t(E)} \int_0^\infty dz' s_0(z', E) \rho_0^A(z', l_t(E)) \\ - \frac{9}{\overline{l_T}} \int_0^\infty dE M(E) \frac{l_T(E)}{l_t(E)} \int_0^\infty dz' s_1(z', E) \rho_1^A(z', l_t(E)) \end{aligned} \quad (4.58)$$

and the functional becomes:

$$\begin{aligned}
\mathbf{z}_0 \left[\phi_0(z, E); \phi_1(z, E) \right] = & \\
\int_0^\infty dE M(E) \int_0^\infty dz s_0(z, E) \left\{ 2 \left[\frac{\ell_T(E)}{\ell_t(E)} \rho_0^A(z, \ell_t(E)) - \psi_{0, \text{asy}}(z, E) + z \left(1 - \frac{\ell_T(E)}{\ell_t(E)} \right) \right] + \phi_0(z, E) \right. & \\
+ \int_0^\infty dz' \rho_{00}^A(z' \rightarrow z; \ell_t(E)) s_0(z', E) - 3 \int_0^\infty dz' \rho_{10}^A(z' \rightarrow z; \ell_t(E)) s_1(z', E) \left. \right\} & \\
+ 3 \int_0^\infty dE M(E) \int_0^\infty dz s_1(z, E) \left\{ 2 \left[\frac{\ell_T(E)}{\ell_t(E)} \rho_1^A(z, \ell_t(E)) - \psi_{1, \text{asy}}(z, E) \right] + \phi_1(z, E) \right. & \\
+ \int_0^\infty dz' \rho_{01}^A(z' \rightarrow z; \ell_t(E)) s_0(z', E) - 3 \int_0^\infty dz' \rho_{11}^A(z' \rightarrow z; \ell_t(E)) s_1(z', E) \left. \right\} & \quad (4.59)
\end{aligned}$$

the motivation for this choice having been explained in the previous section. It is a simple exercise to show that (4.58) is equivalent to (4.40) by means of the relationship which exists between the solutions of the one-speed Milne problem for isotropic and linearly anisotropic scattering and the same goes for the other equations mentioned above. Although this approach would appear to be the more natural extension of the variational principle proposed by Schofield (1963) for isotropic scattering it does have one drawback. If we consider the more general problem when n terms are retained in the expansion of the scattering kernel the variational principle described in §4.4 would require us to determine the Green's functions, in an isotropically scattering medium, for angular dependent sources $P_j(\mu)$ where j runs from 0 to n . But

the latter variational principle requires the determination of the Green's functions for the same sources in a medium with anisotropic scattering of order n . For $n > 1$ it is unlikely that these will be easily calculated except through Case's method and this approach rarely leads to simple, useful expressions for the unknown quantity, in this case the Green's functions.

Nevertheless the theory described in this section does lend itself to a discussion of the "transport approximation". In this approximation which is often used to represent linearly anisotropic scattering (sometimes without much justification) there is assumed to be no energy exchange in the anisotropic scattering. That is:

$$\Sigma_1(E \rightarrow E') = \Sigma_1(E) \delta(E - E') . \quad (4.60)$$

It should be emphasised that this approximation is not as restrictive as some other definitions of the transport approximation in which it is assumed that P_1 scattering can be adequately represented by a suitably adjusted isotropic scattering kernel (see Chapter 6).

With $\Sigma_1(E \rightarrow E')$ given by (4.60), $s_1(z, E)$ is zero and $q(E) = 1$ so that the zero'th moment of (4.54) is:

$$\psi_0(z, E) = \rho_0^A(z, l_t(E)) + \int_0^\infty dz' s_0(z', E) \rho_{00}(z' \rightarrow z; l_t(E)) \quad (4.61)$$

while the functional becomes:

$$Z_0[\phi_0(z,E)] = \int_0^\infty dE M(E) \int_0^\infty dz s_0(z,E) \left\{ 2 \rho_0^A(z, l_t(E)) + \phi_0(z,E) + \int_0^\infty dz' s_0(z',E) \rho_{00}^A(z' \rightarrow z; l_t(E)) \right\}. \quad (4.62)$$

Both (4.61) and (4.62) can be likened to the corresponding equations in Schofield's paper. Of course these equations may also be derived from the former variational principle but the simplification which arises for the transport approximation is not so immediately obvious in that case. Hence the transport approximation provides one example of a situation in which the use of Green's functions with anisotropic scattering results in, at least, a considerable simplification in the formal theory.

§4.6 Higher Order Anisotropic Scattering

In principle higher order anisotropic scattering presents no extra problems other than the determination of the appropriate Green's functions. In view of the remarks made in the previous section we shall confine our attention to the variational principle given in §4.4 and present here the procedure for treating n'th order anisotropic scattering: finally, as an example, we shall quote the results for second order or P_2 anisotropy.

For n'th order scattering the transport equation may be written:

$$\begin{aligned}
\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \psi(z, \mu, E) &= \frac{1}{2\ell(E)} \psi_0(z, E) + \frac{1}{2} S_0(z, E) + \frac{3}{2} \mu \int_0^\infty dE' \Sigma_1(E \rightarrow E') \psi_1(z, E') \\
&+ \sum_{m=2}^n \frac{(2m+1)}{2} P_m(\mu) \int_0^\infty dE' \Sigma_m(E \rightarrow E') \psi_m(z, E') . \quad (4.63)
\end{aligned}$$

It is easily verified that the asymptotic flux is the same as for linearly anisotropic scattering, equation (4.9), with the result that

$\psi_{m_{asy}}(z, E)$ is zero for $m \geq 2$. Thus the transport equation may be rewritten in terms of the Green's function as:

$$\begin{aligned}
\psi_m(z, E) &= \frac{\ell_T(E)}{\ell(E)} \rho_m(z, \ell(E)) + \int_0^\infty dz' s_0(z', E) \rho_{0m}(z' \rightarrow z; \ell(E)) \\
&+ 3 \int_0^\infty dz' \rho_{1m}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \psi_1(z', E') \\
&- \sum_{p=2}^n (2p+1) \int_0^\infty dz' \rho_{pm}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_p(E \rightarrow E') \phi_p(z', E') \\
&\quad m=0, 1 \dots n \quad (4.64)
\end{aligned}$$

Considering the form of this equation for $m=0$ and large z we find:

$$\begin{aligned}
z_0 &= c l_T(E) + \frac{3}{l(E)} \int_0^\infty dz s_0(z, E) \rho_0(z, l(E)) \\
&+ \frac{9}{l(E)} \int_0^\infty dz \rho_1(z, l(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z, E') \\
&+ \frac{3}{l(E)} \sum_{p=2}^n (-1)^{p+1} (2p+1) \int_0^\infty dz \rho_p(z, l(E)) \int_0^\infty dE' \Sigma_p(E \rightarrow E') \phi_p(z, E')
\end{aligned} \tag{4.65}$$

where we have made use of (3.34) and (3.32). Hence

$$\begin{aligned}
z_0 &= \frac{c l_T}{l_T} + \frac{3}{l_T} \int_0^\infty dE M(E) \frac{l_T(E)}{l(E)} \int_0^\infty dz s_0(z, E) \rho_0(z, l(E)) \\
&+ \frac{9}{l_T} \int_0^\infty dE M(E) \frac{l_T(E)}{l(E)} \int_0^\infty dz \rho_1(z, l(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z, E') \\
&+ \frac{3}{l_T} \sum_{p=2}^n (-1)^{p+1} (2p+1) \int_0^\infty dE M(E) \frac{l_T(E)}{l(E)} \int_0^\infty dz \rho_p(z, l(E)) \int_0^\infty dE' \Sigma_p(E \rightarrow E') \phi_p(z, E')
\end{aligned} \tag{4.66}$$

The first term on the right hand side of (4.66) may be determined exactly; when $\psi_m(z, E)$ satisfies (4.64) a stationary value is obtained for the general functional:

$$\begin{aligned}
& \mathcal{Z}_0 \left[\phi_0(z, E); \phi_1(z, E) \dots \phi_n(z, E) \right] = \\
& \int_0^\infty dE M(E) \int_0^\infty dz s_0(z, E) \left\{ 2 \left[\frac{\ell_T(E)}{\ell(E)} \rho_0(z, \ell(E)) - \psi_{0 \text{asy}}(z, E) + z \left(1 - \frac{\ell_T(E)}{\ell(E)} \right) \right] \right. \\
& \quad + \phi_0(z, E) + \int_0^\infty dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E)) \\
& \quad \left. - \sum_{p=1}^n (2p+1) \int_0^\infty dz' \rho_{p0}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_p(E \rightarrow E') \phi_p(z', E') \right\} \\
& + \sum_{m=1}^n (-1)^{m+1} (2m+1) \int_0^\infty dE M(E) \int_0^\infty dz \int_0^\infty dE'' \Sigma_m(E \rightarrow E'') \phi_m(z, E'') \\
& \quad \times \left\{ 2 \left[\frac{\ell_T(E)}{\ell(E)} \rho_m(z, \ell(E)) - \psi_{m \text{asy}}(z, E) \right] \right. \\
& \quad + \phi_m(z, E) + \int_0^\infty dz' s_0(z', E) \rho_{0m}(z' \rightarrow z; \ell(E)) \\
& \quad \left. - \sum_{p=1}^n (2p+1) \int_0^\infty dz' \rho_{pm}(z' \rightarrow z; \ell(E)) \int_0^\infty dE' \Sigma_p(E \rightarrow E') \phi_p(z', E') \right\} \\
& \hspace{20em} (4.67)
\end{aligned}$$

which is then equal to the remaining terms in (4.66).

With P_2 scattering, for example, the functional may be greatly simplified. In Chapter 3 the Green's functions have been written down and it was found that:

$$\rho_{11}(z' \rightarrow z; l(E)) = \rho_{12}(z' \rightarrow z; l(E)) = \rho_{21}(z' \rightarrow z; l(E)) = 0 \quad (4.68)$$

while other terms which occur in the functional may also be set equal to zero.

e.g.

$$\frac{l_T(E)}{l(E)} \rho_1(z, l(E)) - \psi_{1asy}(z, E) = 0 \quad (4.69)$$

$$\frac{l_T(E)}{l(E)} \rho_{2asy}(z, l(E)) - \psi_{2asy}(z, E) = 0 \quad (4.70)$$

Thus it may be verified that the functional becomes:

$$\begin{aligned} Z_0 \left[\phi_0(z, E) \dots \phi_2(z, E) \right] = & \int_0^\infty dE M(E) \int_0^\infty dz s_0(z, E) \left\{ 2 \left[\frac{l_T(E)}{l(E)} \rho_0(z, l(E)) + z \left(1 - \frac{l_T(E)}{l(E)} \right) \right] + \phi_0(z, E) \right. \\ & + \int_0^\infty dz' \rho_{00}(z' \rightarrow z; l(E)) s_0(z', E) - 3 \int_0^\infty dz' \rho_{10}(z' \rightarrow z; l(E)) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z', E') \\ & \left. + 5 \int_0^\infty dz' \rho_{20}(z' \rightarrow z; l(E)) \int_0^\infty dE' \Sigma_2(E \rightarrow E') \phi_2(z', E') \right\} \end{aligned}$$

$$\begin{aligned}
& +3 \int_0^\infty dE M(E) \int_0^\infty dz \int_0^\infty dE'' \Sigma_1(E \rightarrow E'') \phi_1(z, E'') \left\{ \phi_1(z, E) + \int_0^\infty dz' \rho_{01}(z' \rightarrow z; l(E)) s_0(z', E) \right\} \\
& -5 \int_0^\infty dE M(E) \int_0^\infty dz \int_0^\infty dE'' \Sigma_2(E \rightarrow E'') \phi_2(z, E'') \left\{ 2 \frac{l_T(E)}{l(E)} \rho_{2_{tr}}(z, l(E)) + \phi_2(z, l(E)) \right. \\
& \left. + \int_0^\infty dz' \rho_{02}(z' \rightarrow z; l(E)) s_0(z', E) - 5 \int_0^\infty dz' \rho_{22}(z' \rightarrow z; l(E)) \int_0^\infty dE' \Sigma_2(E \rightarrow E') \phi_2(z', E') \right\}.
\end{aligned}
\tag{4.71}$$

Furthermore $\rho_{01}(z' \rightarrow z; l(E))$ and $\rho_{10}(z' \rightarrow z; l(E))$ have a very simple form and the remaining Green's functions may be expressed in terms of $\rho_{00}(z' \rightarrow z; l(E))$. Although a considerable simplification has been possible, the fact remains that for higher than first order anisotropy the equations rapidly become unwieldy and this effectively sets a limit on the usefulness of the present procedure for highly anisotropic scattering.

§4.7 The Trial Function

We now return to the variational principle outlined in §4.4 and choose the simplest trial function to suggest itself; namely a separable function of the form:

$$\phi(z, \mu, E) = e^{-z/L_T} \phi(\mu, E) \tag{4.72}$$

where L_T and $\phi_0(E)$, $\phi_1(E)$ are to be determined. Inserting (4.72) into the functional (4.48) and making some obvious simplifications we find

$$Z_0[\phi_0(E); \phi_1(E)] =$$

$$\int_0^{\infty} dE M(E) s_0(E) \left\{ 2 \tilde{\rho}(\ell(E), L_T) + \frac{L_T}{2} \phi_0(E) + G_{00}(\ell(E), L_T) s_0(E) \right. \\ \left. + 3 G_{10}(\ell(E), L_T) \int_0^{\infty} dE' \Sigma_1(E \rightarrow E') \phi_1(E') \right\} \\ + 3 \int_0^{\infty} dE M(E) \int_0^{\infty} dE' \Sigma_1(E \rightarrow E') \phi_1(E') \left\{ \frac{L_T}{2} \phi_1(E) + G_{01}(\ell(E), L_T) s_0(E) \right\} \quad (4.73)$$

where

$$s_0(E) = \int_0^{\infty} dE' \Sigma_0(E \rightarrow E') \left[\phi_0(E) - \phi_0(E') \right] \quad (4.74)$$

$$\tilde{\rho}(\ell(E), L_T) = \int_0^{\infty} dz e^{-z/L_T} \left[\frac{\ell_T(E)}{\ell(E)} \rho_0(z, \ell(E)) - z \frac{\ell_T(E)}{\ell(E)} \right] \quad (4.75)$$

$$G_{mn}(\ell(E), L_T) = \int_0^{\infty} dz \int_0^{\infty} dz' \rho_{mn}(z' \rightarrow z; \ell(E)) e^{-(z+z')/L_T} \quad (4.76)$$

and therefore

$$G_{01}(\ell(E), L_T) = - G_{10}(\ell(E), L_T) \quad (4.77)$$

All these functions are either evaluated very simply or may be expressed in terms of similar functions occurring in the paper of Schofield (1963), which have already been determined. Demanding that the first order variation in $Z_0[\phi_0(E); \phi_1(E)]$ vanishes for arbitrary variations in $\phi_0(E)$ and $\phi_1(E)$ we obtain an equation for the optimum form of $\phi_0(E)$ for a given L_T :

$$\tilde{\rho}(\ell(E), L_T) + \frac{L_T}{2} \phi_0(E) + G_{00}(\ell(E), L_T) s_0(E) - \frac{3L_T^3}{2} \int_0^\infty dE' \Sigma_1(E \rightarrow E') s_0(E') = C \quad (4.78)$$

where C is an arbitrary constant whose value does not affect Z_0 and ϕ_1 is given by:

$$\phi_1(E) = L_T s_0(E) . \quad (4.79)$$

Equation (4.78) is solved for various values of L_T and the value of L_T which optimises the functional is obtained by interpolation.

We can now see that it is difficult in practice to extend the method to higher order anisotropy, at least for those trial functions which do not pre-assign the energy dependence. Equation (4.78) is solved by the "multipoint" approach described in Chapter 2 as a set of linear equations in the unknowns $\phi(E_i)$ where E_i are the energy mesh points (of which there are about 70 in our calculations). As the order of the anisotropy increases the number of equations to be solved soon becomes very large and a limit is set by the computer time and capacity available.

For isotropic scattering calculations were also performed with the trial function:

$$\phi(z, \mu, E) = e^{-z/\ell(E)} \phi(\mu, E) . \quad (4.80)$$

Then the equation corresponding to (4.78) is:

$$P(E) + Q(E) \phi_0(E) + \int_0^{\infty} dE' R(E \rightarrow E') \phi_0(E') = 0 \quad (4.81)$$

where

$$P(E) = \frac{\tilde{\rho}_0(\ell(E), \ell(E))}{\ell(E)} - \int_0^{\infty} dE' \Sigma_0(E \rightarrow E') \tilde{\rho}_0(\ell(E'), \ell(E)) \quad (4.82)$$

$$Q(E) = 1.5 \tilde{\rho}^2(\ell(E), \ell(E)) / \ell^4(E) \quad (4.83)$$

$$R(E \rightarrow E') = -\Sigma_0(E \rightarrow E') \left[\frac{\ell(E)\ell(E')}{\ell(E)+\ell(E')} + \frac{g(\ell(E), \ell(E'); \ell(E))}{\ell(E)} + \frac{g(\ell(E), \ell(E'); \ell(E'))}{\ell(E')} \right]$$

$$+ \int_0^{\infty} dE'' \Sigma_0(E \rightarrow E'') \Sigma_0(E'' \rightarrow E') g(\ell(E), \ell(E'); \ell(E'')) \quad (4.84)$$

and

$$\tilde{\rho}_0(\ell(E), \ell(E')) = \int_0^{\infty} dz \rho_0(z, \ell(E)) e^{-z/\ell(E')} \quad (4.85)$$

$$g(L_1, L_2; \ell(E)) = \int_0^{\infty} dz \int_0^{\infty} dz' \rho_{00}(z' \rightarrow z; \ell(E)) e^{-(z/L_1 + z'/L_2)} \quad (4.86)$$

The function $g(L_1, L_2; \ell(E))$ may be determined in a similar, but less straightforward fashion, to $G_{00}(\ell(E), L_T)$. Naturally the optimisation procedure is avoided in this case.

The numerical methods for solving (4.78) and (4.81) are described in an appendix (§4A.1): suffice it to say that the "z integrations" may be performed analytically leaving only the integrations over energy to be done numerically. The result of calculations with these trial functions will be reported in the next section.

§4.8 Results and Discussion

(i) Isotropic Scattering

While the theory for an isotropic scattering kernel has been described elsewhere (Schofield 1963; Tait 1964) no numerical results have so far been reported. There would have been little point in extending the theory to include anisotropic scattering if the results for isotropic scattering had not been reassuring. For this reason we have tabulated some results obtained for various simple isotropic scattering models which may be compared with results previously obtained by other methods. The scattering models chosen for consideration were the monatomic gas of atomic mass A ($A=1,3,12$), the proton gas represented by Corngold's separable kernel and the Nelkin model for water (at a temperature of 300°K) as embodied in the GAKER computer code (Honeck 1961) with oxygen included as a free gas of mass $A=16$.

In Table 4.I the exact value of the extrapolation length (in units of the maximum value of the mean free path ℓ_{\max}) for the separable kernel (Williams 1964a) is compared with that obtained with the two trial functions $\phi_0(E) e^{-z/L_T}$ and $\phi_0(E) e^{-z/\ell(E)}$ which are used in the present theory. Also included is the extrapolation length when there is no energy exchange. Williams (1964a) has also calculated the angular distribution of emergent neutrons $\psi(0, \mu, E)$. In Table 4.II his results are compared not only with the present theory with the trial function $\phi_0(E) e^{-z/L_T}$ but also with the results obtained by Eisenhauer (1964) and Kallfelz and Reichardt (1967). The latter use the variational principle of Kladnik and Kuscer (1961) with an improved

trial function and determine the spectra by performing two iterations on the flux. It is clear from Table 4.II that the results of Eisenhauer are least accurate at grazing incidence where the numerical approximations in the THERMOS computer code find it difficult to cope with the singularity at $\mu=0$. A similar comparison of the emergent spectra for the full proton gas kernel is shown in Table 4.III. Here Williams (1964b) has applied perturbation theory while some so-called "exact" results may be obtained from the THERMOS calculations of Eisenhauer by assuming that the same numerical errors occur in this computation as occur in the separable kernel computations. From Tables 4.II,III we may conclude that for the proton gas moderator it is the energy dependence of the mean free path and not the details of the scattering mechanism which essentially determines the emergent neutron distribution. From Table 4.IV we see that for the extrapolation length this is true not only of the proton gas but also of all the free gas moderators. These results tend to confirm Williams' suggestion (1964a) that the values of z_0 for the separable and δ -function kernels will bracket the true value of z_0 .

In Table 4.V the emergent neutron distribution $\Psi(0, -\mu, E)$ for the free gas of atomic mass $A=12$ at $\mu=0,1$ is presented in order that when calculations are made for the separable kernel we shall be able to see whether the energy exchange mechanism is equally unimportant in determining $\Psi(0, -\mu, E)$ for heavier moderators. Such calculations may be made with the present theory: however Arkuszewski (1967) has already evaluated $\Psi(0, -\mu, E)$ by the Wiener-Hopf technique for the separable

kernel but no numerical results have been published for atomic mass 12.

If the transient flux can be represented by a trial function of the form $\phi_0(E) e^{-z/L_T}$ with a fair degree of accuracy we might expect L_T to be, in some sense, an average of the discrete and continuum eigenvalues (with the exception of the diffusion length). If this is the case we would expect $L_T > \ell_{\max}$ only when a thermalisation length is well established. When the continuum eigenvalues dominate we expect the trial function $\phi_0(E) e^{-z/\ell(E)}$ to be more appropriate. Among the models considered here only the free gas of atomic mass 12 has a well established thermalisation length and we see in Table 4.VI that this is the only moderator for which the former trial function gives the more accurate extrapolation length. Corroboration is provided by equation (4.39) by which we can obtain some idea of the relative merits of the trial functions. For a water moderator with isotropic scattering, for example, the error in $z_0(E)$ given by (4.39) is never more than about 1% in the important range $10^{-2} \leq E \leq 10^{-1}$ eV with the trial function $\phi_0(E) e^{-z/\ell(E)}$ whereas for the trial function $\phi_0(E) e^{-z/L_T}$ the error rises to about 5% in the same energy range. Similar results are obtained for the other low mass moderators while for the free gas of mass $A=12$ there is no significant difference between the results obtained with the two trial functions.

In spite of the weight of evidence in favour of $\phi_0(E) e^{-z/l(E)}$ we shall confine our attention to the trial function $\phi_0(E) e^{-z/L_T}$ as the easier function to manipulate. Further discussion of the energy and spatial dependence of possible trial functions will be deferred to §4.8, (ii).

(ii) Linearly Anisotropic Scattering

One of the main purposes of extending the theory to include anisotropic scattering was to be able to predict the extrapolation length and emergent spectra for a real moderator in which the effect of neutron capture is likely to be negligible. In this section we make the comparison for a water moderator. The fact that our calculations were made for a temperature of 300°K while the various experiments were generally performed two or three degrees lower will not significantly affect the conclusions of any comparison between theory and experiment.

With the trial function $\phi_0(E) e^{-z/L_T}$, the extrapolation length was estimated to be 0.341 cms. which is within the bounds set by the experiments of Carroll and Stooksberry (1964) in a steady state experiment and Walker, Brown and Wood (1965) in a pulsed experiment. Their experiments suggest an extrapolation length of about 0.35 cms. Our result is in excellent agreement with that of Kladnik (1965) who, in applying a variational principle to the problem of the pulsed infinite slab found $z = 0.339$ cms. The energy distribution of neutrons emerging at various angles to the water surface has been determined by Sinclair (1966) and Kallfelz (1965-1967, see references in §4.1). Their results for $\mu=1.0, 0.2, 0.0$ are shown in Figures 4.I, II and III

together with the predictions of this variational principle - similar results are found at other angles.

The discrepancy between the results of Sinclair and Kallfelz for large E and $\mu > 0$ may be explained in terms of the sources used. While Sinclair uses a fast source Kallfelz also employs a cadmium chopper to ensure that all the neutrons in the medium are thermalised. Thus we should expect our results to compare more favourably with those of Kallfelz as, indeed, they do. However we are unable to explain why Sinclair's curve lies below that of Kallfelz for large E and $\mu = 0$. For neutrons emitted perpendicular to the surface ($\mu = 1$) our calculations are in excellent agreement with the results of Kallfelz over the whole energy range. For $\mu < 1$ the agreement is still most satisfactory except for $\mu = 0$. In that case, while our results compare very favourably for large energies the predicted spectrum is somewhat too hard for energies less than about 0.03 eV. Our calculations are therefore least accurate for small μ and E , but it has been pointed out by Williams (1964a) that this is the least important region for calculating quantities of most practical use such as the total emitted flux $\Psi_0(O, E)$ and the energy averaged angular moments. We may obtain some idea of the increasing error as μ approaches zero by considering the mean energy of the emergent distribution defined by:

$$\bar{E}(\mu) = \frac{\int_0^{\infty} dE E^{1/2} \Psi(O, \mu, E)}{\int_0^{\infty} dE E^{-1/2} \Psi(O, \mu, E)}. \quad (4.87)$$

We find that $\bar{E}(1)$ is 18.5% greater than the mean energy of a Maxwellian distribution at the moderator temperature compared with the experimental value of about 18%. For $\mu=0$ we find $\bar{E}(0)$ is 12.7% greater than the mean energy of a Maxwellian distribution compared with about 10% reckoned from the experimental points of Kallfelz (and 5% from Sinclair's results). These and other results are given in Table 4.VII. While it is apparent that our calculated values for $\bar{E}(\mu)$ are actually within the experimental bounds it is equally clear from Figures 4.I,II,III that there is still a small but definite discrepancy between theory and experiment for small μ .

Kallfelz and Reichardt (1967) have also done some calculations based on the variational principle of Kladnik and Kuscer (1961) but with an improved trial function for the transient flux having a spatial dependence $e^{-z/\ell_{\max}}$ and performing two iterations on the flux. In some more very recent calculations (Kallfelz and Kladnik 1967) the spatial dependence has been modified to $e^{-z/r \ell_{\max}}$ with $r=0.3$ following some work by Kladnik (1964) which showed this to be more appropriate for the one-speed problem. Their results are included in Table 4.VII from which it is clear that there is still room for improvement at least to the extent of mutual consistency between the two trial functions. One might instead consider r as a variational parameter, as in the present theory, and determine the value of r which optimises the functional. From our own computations it is found that, in general, $L_T \gtrsim 0.5 \ell_{\max}$ which suggests that although the trial function with

$r = 0.3$ may be the appropriate choice in the one-speed problem it may not be equally acceptable in the energy dependent case. This point has been discussed by Schofield (1963; see also Tait 1964) who emphasises that there is a significant difference between the one-speed and energy dependent problems. Since more than one collision may be necessary, in the energy dependent problem, to bring a neutron into thermal equilibrium, L_T will probably be greater than the corresponding one-speed value and for heavier moderators may even be far greater than l_{\max} .

It appears that after two iterations of the trial function Kallfelz obtains only slightly better agreement with the experimental results than we obtain from the present variational principle after one iteration.

While some of the discrepancy at $\mu=0$ may be attributed to the effects of higher order anisotropy, the inadequacy of LeCaine's approximate solution and the limitations of the numerical integration procedures the most likely cause of error lies in the choice of trial function. Integrating (4.7) over z in the fashion described after (3.50) and performing the integrations analytically wherever possible it may be shown that the angular distribution of emergent neutrons is given by:

$$\begin{aligned} \Psi(0, \mu, E) = & \frac{M(E)}{2} \left[z_0 + \mu l_T(E) - \frac{1}{\mu} \int_0^\infty dz e^{-z/\mu} l(E) \int_0^\infty dE' \Sigma_0(E \rightarrow E') \phi_0(z, E') \right. \\ & \left. + 3 \int_0^\infty dz e^{-z/\mu} l(E) \int_0^\infty dE' \Sigma_1(E \rightarrow E') \phi_1(z, E') \right] \end{aligned}$$

$$0 \leq \mu \leq 1 \qquad (4.88)$$

$$\Psi(0,0,E) = \frac{M(E)}{2} \left[z_0 - \ell(E) \int_0^{\infty} dE' \Sigma_0(E \rightarrow E') \phi_0(0,E') \right]. \quad (4.89)$$

Clearly as μ approaches zero the most important contribution to the integrals in (4.88) comes from z close to the origin. The trial function for the transient flux was chosen primarily for its simplicity and probably the most important of its shortcomings is that it does not have the correct behaviour at the origin: the derivative of the transient flux should have a logarithmic singularity at this point. Thus we expect $\phi_0(z,E)$ to be least accurate for small z and this is reflected in the increasing error in $\Psi(0,\mu,E)$ as μ approaches zero. Nevertheless it is remarkable that such a simple trial function should produce such accurate results for almost the whole range of μ and E .

Because of the singularity in the gradient of the transient flux one would expect that considerable improvement could be obtained with a trial function of the form:

$$\phi_0(z,E) = \phi_0(E) \left[E_2(z/L_T) - A E_3(z/L_T) \right] \quad (4.90)$$

where L_T may be replaced by $\ell(E)$. Such a trial function is the obvious extension of LeCaine's one-speed solution and retains the important singularity in the spatial derivative. It has been proposed already by Williams (1964b) and the calculations of Eisenhauer (1964) suggest that a good first guess would be to replace $\phi(E)$ by $\Sigma(E)$. Unfortunately this would then add considerable complexity to the calculations.

With the Nelkin model for water the transport approximation is seen to be a very good representation of linearly anisotropic scattering. For example the extrapolation length is found to be 0.341 ± 0.001 cms. in each case. Likewise the predicted emergent spectra are almost identical. A comparison of the emergent spectra for $\mu=0$ with (a) isotropic scattering (b) the transport approximation and (c) linearly anisotropic scattering is shown in Figure 4. IV where all the curves are normalised so that the current is given by:

$$J = \bar{l}_T / 3 . \quad (4.91)$$

A similar set of curves is obtained for all other angles.

In calculating the diffusion length and associated parameters, Honeck (1962) too was able to show that for "Nelkin water" the assumption of purely elastic P_1 scattering was a very good approximation.

Calculations were also performed for the proton gas moderator: it was found that in this case the extrapolation length was $0.969 l_{\max}$ in the transport approximation and $0.938 l_{\max}$ for the full kernel. Once again the latter value is in excellent agreement with Kladnik's (1965) result of $0.934 l_{\max}$. A difference in the spectra was also more easily distinguished. Both of these effects are undoubtedly due to the stronger energy exchange exhibited by the proton gas kernel. Independently Kallfelz and Reichardt (1967) arrived at similar conclusions.

Finally in Table 4. VIII we have presented $\bar{E}^f(\mu)$ for the proton gas where:

$$\bar{E}^f(\mu) = \frac{\int_0^{\infty} dE E \Psi(0, \mu, E)}{\int_0^{\infty} dE \Psi(0, \mu, E)}. \quad (4.92)$$

This table demonstrates very plainly the effect of anisotropic scattering in each of the approximations and further illustrates the point, already made, that the stronger energy exchange effects inherent in the proton gas lead to significant differences in the emergent spectra for the transport approximation and the full P_1 scattering kernel.

APPENDIX

§4A.1 Numerical Computations

The computations involved in the determination of the extrapolation length and emergent flux are similar in many respects to those described in §2A.1. For example the same scattering kernels are used and are read from tape in the same way: the energy integrations are performed with the same numerical integration methods and evaluated for similar energy meshes. Nevertheless some indication of the important stages in the calculation is required and the description to be given is valid with only trivial modifications for both anisotropic and isotropic scattering.

Firstly we should emphasise that, wherever possible, a system of checks on the accuracy and consistency of the calculations was maintained throughout but these will not be described here. Equation (4.78) is solved by considering it as a set of coupled linear equations in the unknowns $\phi_0(E_i)$ where E_i are the N energy mesh points. After some rearrangement (4.78) may be written in the general form:

$$\sum_{j=1}^N A(E_j, E_i) \phi_0(E_j) = B(E_i) \quad i=1, 2, \dots, N \quad (4A.1)$$

where we have made an initial guess for the variational parameter L_T . This set of equations is again solved by pivotal condensation using double length arithmetic to evaluate $\phi_0(E_i)$. Calculations were also performed based on the iterative procedure suggested by MacMillan in Nelkin (1957). Knowing $\phi(E_i)$ we obtain $\phi_1(E_i)$ from (4.79) and hence we

can evaluate Z_0 without difficulty.

Further guesses are made for L_T and the whole process is repeated until we find, to some predetermined accuracy, the value of L_T which optimises the functional. This is achieved by fitting quadratic algebraic equations to the inverse of the functional Z_0 evaluated at three successive values of L_T and finding the minimum of this quadratic equation. The value of L_T corresponding to this minimum is chosen as a fourth point and the best three (determined by the smallest estimates of $1/Z_0$) are fitted by another quadratic equation. This procedure is repeated until the required accuracy is attained. Having determined Z_0 and hence z_0 for the optimum L_T and $\phi_0(E_i)$ it is straightforward to evaluate the emergent flux by simple numerical integration over the energy variable in (4.88) and (4.89).

For comparison with the results of Williams (1964b) at energies $E=0.09kT, kT$ and $1.96kT$ we interpolate between energy mesh points using a Lagrange formula based on an even order polynomial of order $(2n-2)$ which passes through n points - the particular advantage of this method is that equal intervals are not required.

	Exact Value by Wiener-Hopf Method	Green's Function Approach; Trial Functions		Exact Value for δ -function kernel
		$\phi_0(E)e^{-z/L_T}$	$\phi_0(E)e^{-z/l(E)}$	
z_0	0.53775	0.53825	0.53813	0.54517

TABLE 4.1 The extrapolation length for the proton gas as represented by the separable kernel (in units of l_{\max}): also included is the value when there is no energy exchange.

μ	E = 0.09kT				E = 1.0kT				E = 1.96kT			
	Williams	Present Theory	Kallfelz	Eisenhauer	Williams	Present Theory	Kallfelz	Eisenhauer	Williams	Present Theory	Kallfelz	Eisenhauer
0.0	0.845	0.851	0.852		0.845	0.851	0.852		0.845	0.851	0.852	
0.1	0.936	0.940	0.944	0.950	1.052	1.054	1.057	1.057	1.082	1.084	1.087	1.087
0.2	1.009	1.013		1.016	1.218	1.221		1.221	1.274	1.276		1.277
0.3	1.076	1.081		1.081	1.375	1.377		1.377	1.455	1.456		1.457
0.4	1.140	1.146		1.144	1.526	1.529		1.529	1.630	1.631		1.633
0.5	1.202	1.209	1.205	1.205	1.674	1.677	1.672	1.677	1.802	1.802	1.800	1.805
0.6	1.263	1.270		1.266	1.820	1.822		1.823	1.972	1.972		1.975
0.7	1.322	1.330		1.325	1.965	1.967		1.967	2.140	2.140		2.143
0.8	1.381	1.390		1.383	2.108	2.110		2.110	2.307	2.306		2.310
0.9	1.439	1.448		1.441	2.250	2.252		2.253	2.474	2.472		2.476
1.0	1.496	1.503	1.494	1.498	2.392	2.394	2.392	2.395	2.639	2.637	2.640	2.642

TABLE 4.II The angular distribution of emergent neutrons $\psi(0, \mu, E)$ for the proton gas as represented by the separable kernel: the distribution is normalised to unit current.

μ	E = 0.09kT				E = 1.0kT				E = 1.96kT			
	Eisenhauer	Present Theory	Kallfelz	Williams	Eisenhauer	Present Theory	Kallfelz	Williams	Eisenhauer	Present Theory	Kallfelz	Williams
0.0			0.782	0.771			0.833	0.836			0.866	0.860
0.1	0.876	0.879	0.883	0.873	1.034	1.033	1.040	1.045	1.091	1.093	1.095	1.092
0.2	0.952			0.952	1.202			1.213	1.281			1.282
0.3	1.022			1.023	1.359			1.370	1.461			1.461
0.4	1.089	1.097		1.091	1.512	1.511		1.521	1.635	1.636		1.636
0.5	1.155			1.156	1.661			1.670	1.807			1.807
0.6	1.217			1.219	1.807			1.816	1.976			1.976
0.7	1.278	1.288		1.281	1.953	1.953		1.960	2.144	2.143		2.144
0.8	1.340			1.342	2.101			2.104	2.311			2.310
0.9	1.399			1.401	2.239			2.246	2.477			2.476
1.0	1.458	1.469	1.456	1.460	2.382	2.383	2.382	2.388	2.642	2.641	2.643	2.641

TABLE 4. III The angular distribution of emergent neutrons $\psi(0, \mu, E)$ for the full proton gas kernel; the distribution normalised to unit current.

		Separable kernel (Williams 1964a)	Full kernel (present theory)	δ -function kernel (Williams 1964a)
Monatomic ↑ Gases ↓	A=1	0.5378	0.5387	0.5454
	A=3		0.6282	(0.6308)
	A=12	0.6851	0.6854	0.6857
"Nelkin water"		0.3695	0.3719	0.3773

TABLE 4. IV The extrapolation length (in units of l_{\max}) for various moderators with isotropic scattering. The figure in the last column for A=3 is from our own calculations.

← Energy →				
μ	0.088kT	1.020kT	2.114kT	3.865kT
0.0	0.8099	3.9765	2.7851	0.8807
1.0	2.1161	11.4450	8.0495	2.5548

TABLE 4.V The emergent distribution $\Psi(0, \mu, E)$ at various values of μ, E for the free gas moderator having atomic mass $A=12$; the normalisation is such that $J = \bar{l}/3$.

	Trial Function	Monatomic gases				"Nelkin Water"
		A = 1	A = 3	A = 12	A=1: Separable kernel	
z_0	$\phi_0(E)e^{-z/l}(E)$	-0.1592 E-2 ⁺	-0.7025 E-3	-0.8865 E-4	-0.1744 E-2	-0.4476 E-3
	$\phi_0(E)e^{-z/L_T}$	-0.1552 E-2	-0.6908 E-3	-0.8991 E-4	-0.1714 E-2	-0.4450 E-3
L_T		0.542	0.702	1.052	0.428	0.389

TABLE 4.VI The quantity z_0 given by $z_0 = \frac{cl^2}{l} + \frac{3z_0}{l}$ and the variational parameter L_T measured in cms. for Nelkin water and in units of l_{max} for the monatomic gases.

⁺ denotes the power of ten by which the numbers should be multiplied.

μ	Experiment (Kallfelz 1967)	Theory of Kladrnik and Kušcer (1961) Spatial dependence of trial function $\phi(z, \mu, E) = \phi(\mu, E)e^{-z/l}$ max	$\phi(z, \mu, E) = \phi(\mu, E)e^{-z/0.3l}$ max	Present Theory
1.0	19 ± 2	17.9	17.6	18.5
0.2	13 ± 2	12.6		14.4
0.0	10 ± 3	10.6	11.4	12.7

TABLE 4.VII

The percentage increase in the mean energy of the neutron distribution emerging at various angles from a water surface compared with the mean energy (\bar{E}_M) of a Maxwellian energy distribution at the moderator temperature.

$$\text{Percentage increase} = \frac{\bar{E}(\mu) - \bar{E}_M}{\bar{E}_M} \quad [\text{see (4.87)}]$$

μ	Isotropic Scattering		Transport Approximation	Linearly Anisotropic Scattering
	Separable kernel	Full kernel		
0.0	0.0	2.45	6.22	3.72
1.0	6.35	6.64	11.35	9.66

TABLE 4.VIII

The percentage increase in the mean energy of the emergent angular flux for a proton gas moderator compared with the mean energy of a Maxwellian flux distribution at the moderator temperature (\bar{E}_M^f).

$$\text{Percentage increase} = \frac{\bar{E}^f(\mu) - \bar{E}_M^f}{\bar{E}_M^f}$$

[see (4.92)]

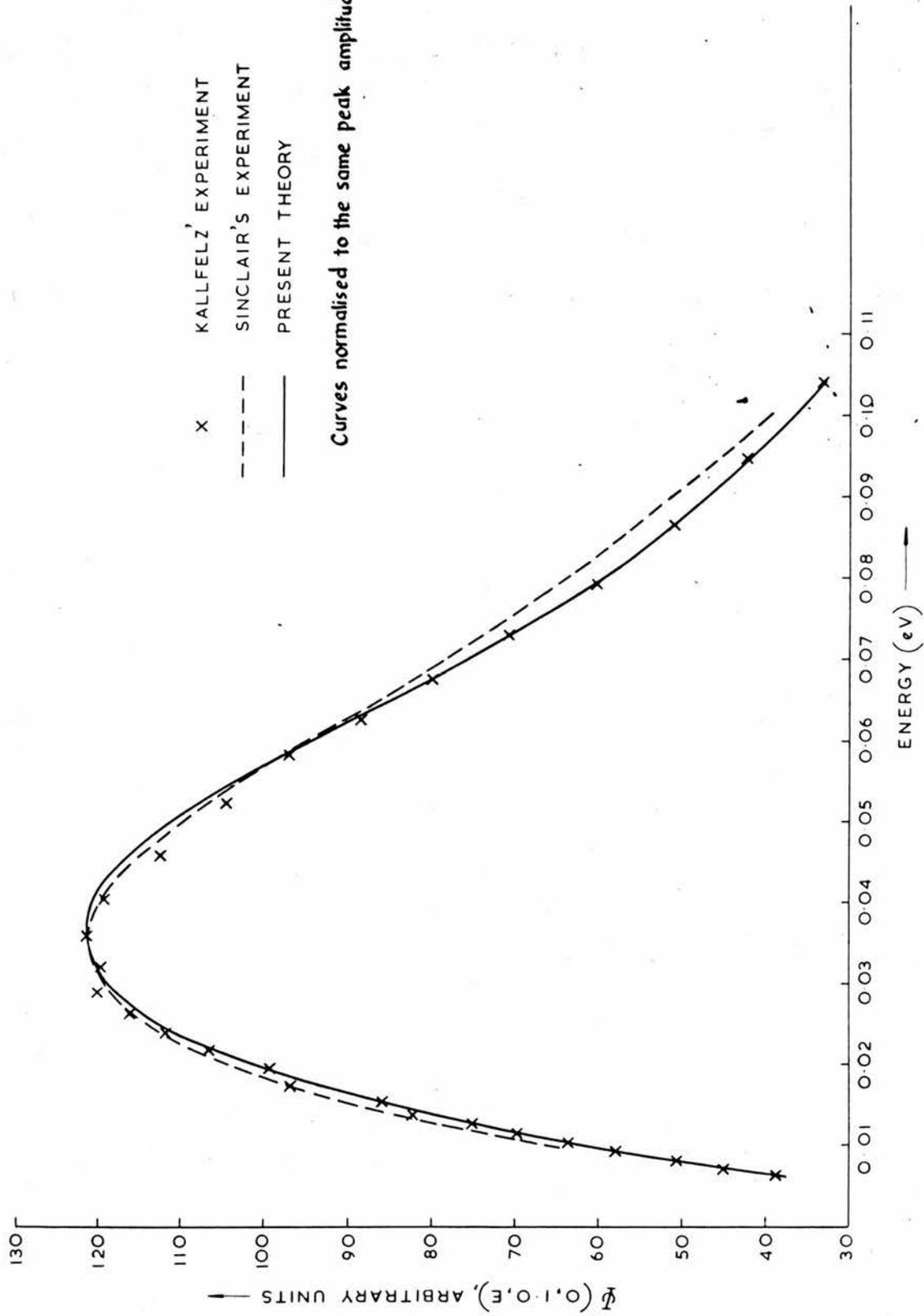


FIG 4 I

Energy spectrum of neutrons emerging from a plane water surface, $\mu = 1.0$

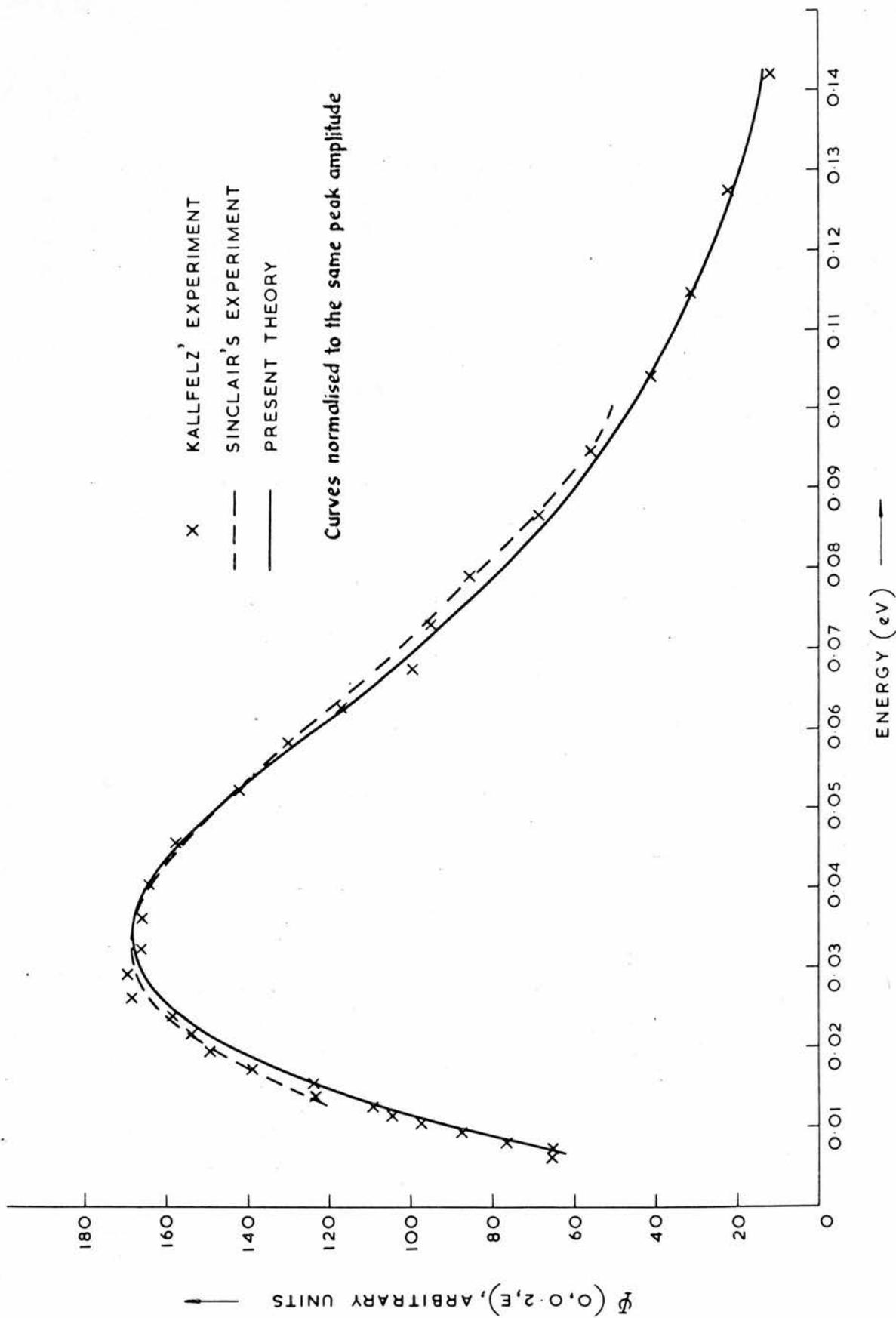


FIG. 4-II

Energy spectrum of neutrons emerging from a plane water surface, $\mu=0.2$
 (Sinclair's results are for $\mu=0.191$)

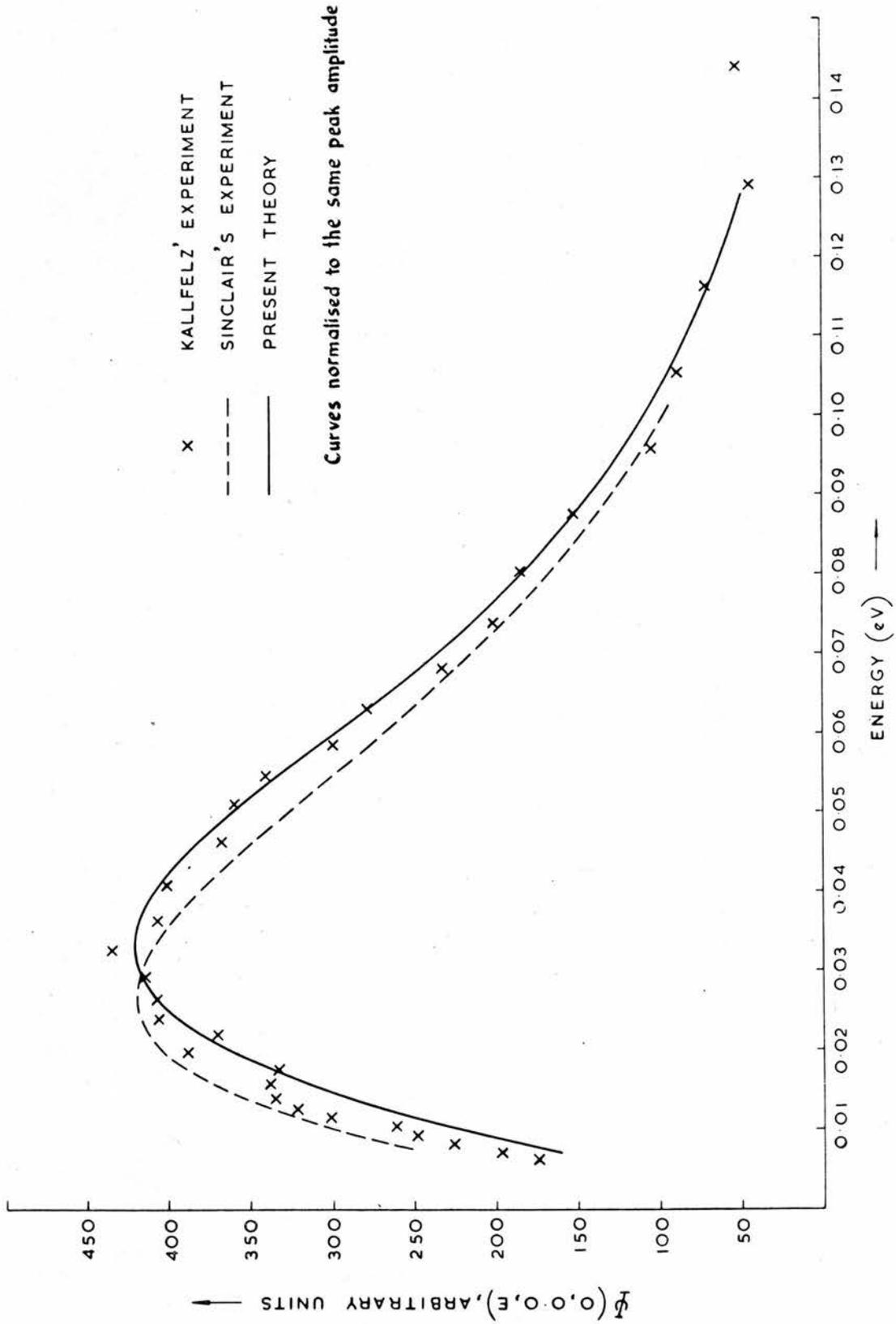


FIG 4·III

Energy spectrum of neutrons emerging from a plane water surface, $\mu=0\cdot0$

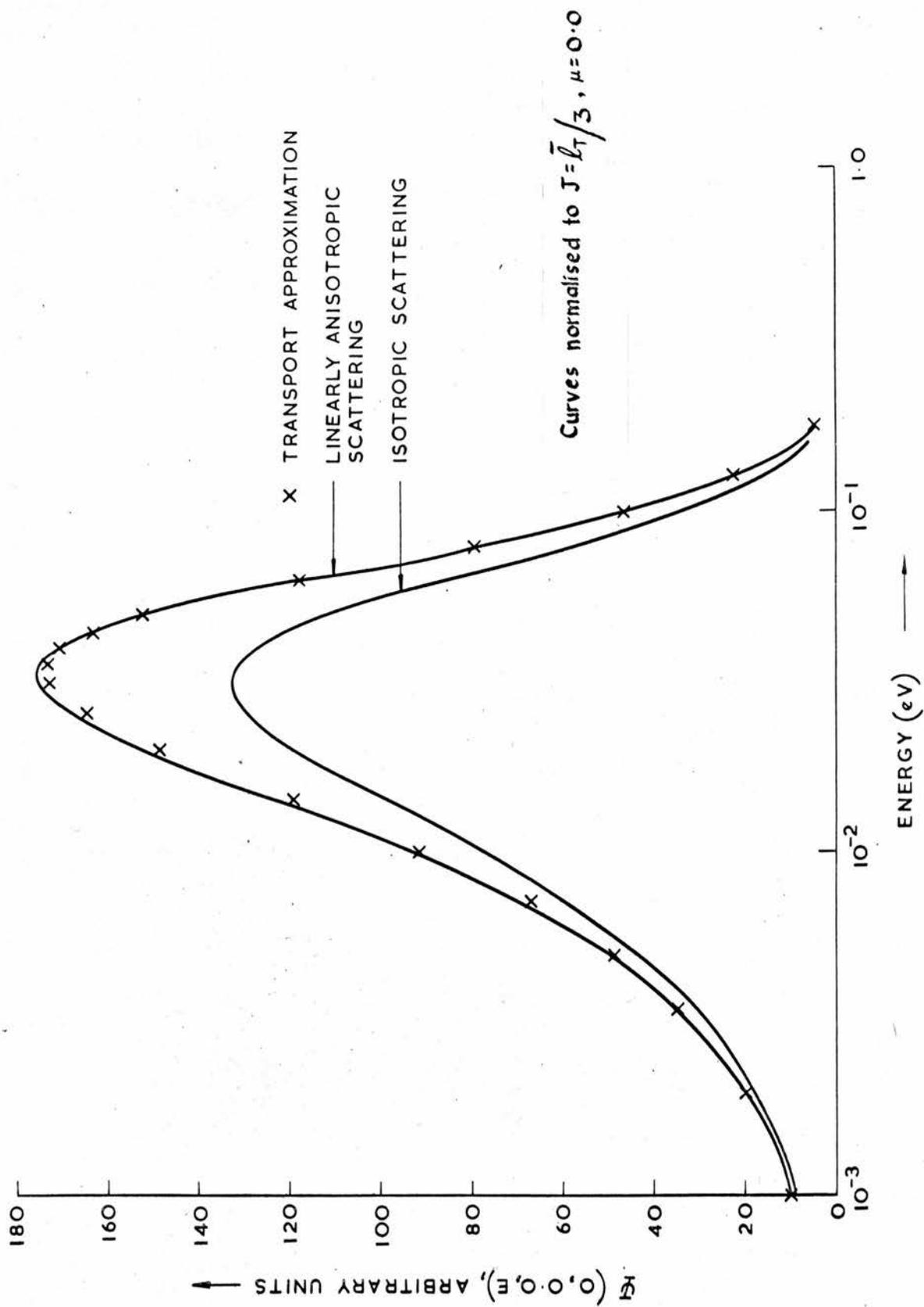


FIG. 4. IV

Energy spectrum of neutrons emerging from a plane water surface for various scattering models

CHAPTER 5

THE THERMAL NEUTRON MILNE PROBLEM WITH CAPTURE

§5.1 Introduction

In this chapter we shall show how the theory developed in Chapter 4 has to be modified to account for neutron capture. So far the theory has only been worked out in detail for isotropic scattering but the possibility of including anisotropic scattering will be discussed in the next chapter.

If neutrons are captured as well as scattered, the form of the asymptotic flux is displaced from a Maxwellian distribution and this has a direct effect on those neutrons, emitted perpendicularly from the surface, which have come predominantly from the inner regions of the moderator. Thus the mean energy of the neutron distribution emitted at angles close to the perpendicular may be significantly affected by the presence of absorption. On the other hand the neutron distribution emitted at grazing angles to the surface is influenced mainly by the transient region close to the surface and it has been shown that the distribution at these angles is not affected by absorption to the same extent (Arkuszewski 1967).

While there have been other treatments of the energy dependent Milne problem with capture, few have reported any numerical results. With the separable kernel, for example, Mika (1965) has obtained an exact solution by an extension of Case's method but even for this simple kernel the approach does not lend itself to the performance of calculations and no results are reported. However it has been shown by Arkuszewski (1967) that for

half-space problems Case's method is entirely equivalent to the Wiener-Hopf approach and this latter technique leads to more easily evaluated expressions for the extrapolation length and emergent angular distribution. Arkuszewski quotes results for the free gas moderator with various absorption laws. For a quite general P_1 scattering kernel Kladnik and Kušcer (1962) have extended their variational method to include capture but once again their treatment fails to produce the correct answers in the two special cases mentioned in §4.3.

The basis of the method is similar to that given in the previous chapter. In §5.2 a complete description of the form of the asymptotic flux is presented followed by a definition of the extrapolation length and related parameters for capturing media. The transport equation is then rewritten in terms of the corresponding one-speed solution and the associated Green's function for an isotropic source. An additional difficulty which arises when there is capture lies in the choice of one-velocity solutions. It is shown that the appropriate one-speed solutions are those in which the "capture" is such as to give an asymptotic solution having the same form as that for the energy dependent problem, namely that determined by the thermal neutron diffusion length. The correct choice of these solutions will be clarified and defined more precisely in §5.2.

From the transformed equations obtained in §5.2 it is possible to write down a variational principle to provide an estimate of a quantity a which is closely related to the extrapolation length - this is done in §5.3. The expressions obtained are similar in form to those

obtained in Chapter 4 for z_0 [see (4.40)]. That is to say, we obtain an expression for a which is the sum of two terms, the first being a weighted energy average of the one-speed counterpart of a while the second is estimated by the variational principle. In §5.4 an alternative derivation of this expression for a is given which makes use of two integral conditions. The same simple trial function is introduced in §5.5 permitting the analytical evaluation of some of the integrals involved in the calculation. However the details of the subsequent numerical computations are relegated to an appendix. In §5.6 some results are presented and compared with other predictions whenever they are available while in the latter half of the section we summarize some of the more important conclusions which can be drawn from this treatment.

It is assumed throughout that the capture is sufficiently weak that the diffusion length exists (see Chapter 2).

§5.2 The Transport Equation

In the usual notation the transport equation with isotropic scattering is:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \Psi(z, \mu, E) = \frac{1}{2} \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi_0(z, E') \quad z > 0 \quad (5.1)$$

where $\ell(E)$ now represents the total mean free path given by:

$$\ell^{-1}(E) = \Sigma_0(E) + \Sigma_a(E) \quad (5.2)$$

with $\Sigma_0(E)$, $\Sigma_a(E)$ the total scattering and absorption cross-sections respectively. The boundary condition at the interface is, as before,

$$\Psi(0, \mu, E) = 0 \quad 0 < \mu \leq 1 \quad (5.3)$$

while the boundary condition at infinity corresponds to a source of neutrons at a large distance from the boundary. Attention is restricted to those cases in which the capture is sufficiently weak that there exists a thermal neutron diffusion length L (we have dropped the subscript 0 from L_0 for convenience). That is we assume that there is a solution of (5.1) which goes to zero for $E \rightarrow 0, \infty$ having the form $M(E) g(E, \mu) \exp\{z/L\}$ with L greater than the maximum value of the mean free path ℓ_{\max} . As we saw in some detail in Chapter 2 such solutions exist provided that the capture does not exceed some limiting value depending on the scattering properties of the moderator and the particular energy dependence of the absorption law. If, on the other hand, there is no diffusion length the emergent flux will not be uniquely determined without further specification of the source.

If there is a diffusion length then $g(E, \mu)$ satisfies:

$$\left[\frac{\mu}{L} + \frac{1}{\ell(E)} \right] g(E, \mu) = \frac{1}{2} \int_0^{\infty} dE' \Sigma_0(E \rightarrow E') g_0(E') \quad (5.4)$$

The diffusion length is the largest value of L for which (5.4) has a solution.

The boundary condition at infinity is then replaced by the condition that for large z the flux has the asymptotic form given by this exponentially increasing solution. This then corresponds to a source of neutrons in thermal equilibrium with the medium. Corresponding to this exponentially increasing solution there is a decreasing solution $M(E) \approx g(E, \mu) \exp\{-z/L\}$. The solution of the problem is therefore a linear combination of these two solutions plus solutions of (5.1) which decay faster than $\exp\{-z/L\}$ as z increases. Such solutions may be of two types (Case 1960; Zelazny 1966 - see also Chapter 2). There may be other solutions of (5.4) satisfying the boundary conditions on E for discrete values of $L > l_{\max}$. In addition there are always singular solutions behaving as $\exp\{-z/L\}$ for $l \leq l_{\max}$: these singular solutions contain δ -functions in energy where $l(E) = L/\mu$.

One could, of course, define a whole class of Milne problems simply by imposing different boundary conditions. One might, for instance, insist that at large distances the flux should have the form $\exp\{z/L_i\}$ where L_i is one of the other discrete eigenvalues (e.g. L_1 , the thermalisation length) or $\exp\{z/l\}$ where $l \leq l_{\max}$. However it follows from the orthogonality of the solutions that only one pair of eigenfunctions $g(E, \pm\mu)$ exists which are everywhere positive namely those associated with the diffusion length ($\pm L$). In any case if the source is at a distance $z \gg L_1$ from the boundary these modes will have decayed before the interface makes itself felt. We may therefore disregard all other solutions on physical grounds.

The solution may then be written down as the sum of an asymptotic part $\Psi_{\text{asy}}(z, \mu, E)$ and a transient part $\Psi_{\text{tr}}(z, \mu, E)$ where:

$$\Psi_{\text{asy}}(z, \mu, E) = \left[g(E, -\mu) e^{z/L} + a g(E, \mu) e^{-z/L} \right] M(E) \quad (5.5)$$

and $\Psi_{\text{tr}}(z, \mu, E)$ vanishes faster than $\exp\{-z/L\}$.

The important parameter a defines the effective boundary condition for the asymptotic flux. It is related to the extrapolation length z_0 defined by:

$$z_0 = \chi_{\text{asy}}(0) / \chi'_{\text{asy}}(0) \quad (5.6)$$

$$\chi_{\text{asy}}(z) = \int_0^{\infty} dE \int_{-1}^{+1} d\mu \Psi_{\text{asy}}(z, \mu, E); \quad (5.7)$$

that is

$$z_0 = (1+a)L / (1-a) \quad (5.8)$$

Often used instead of z_0 is the extrapolated end-point z_0^i defined by:

$$\chi_{\text{asy}}(-z_0^i) = 0 \quad (5.9)$$

and when there is no capture $z_0 = z_0^i$. The terminology adopted here is that given by Davison (1957, p73). As the capture tends to zero L becomes infinite while z_0 remains finite having a limiting value z_0^0 which is given by (4.40) with $\Sigma_1(E \rightarrow E')$ set equal to zero. Thus we expect:

$$a \sim -1 + \frac{2z_0^0}{L} \quad \text{as } L \rightarrow \infty . \quad (5.10)$$

As in Chapter 4 we wish to write the solution of (5.1) in terms of the solution to the one-speed Milne problem and the corresponding half-space Green's functions. Dividing (5.1) by $M(E)$ it may be rewritten in the form:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \psi(z, \mu, E) = \frac{c(E)}{2\ell(E)} \psi_0(z, E) + \frac{1}{2} S_0(z, E) \quad (5.11)$$

where $\psi(z, \mu, E)$ is defined by (4.19) and:

$$S_0(z, E) = \int_0^{\infty} dE' \Sigma_0(E \rightarrow E') \psi_0(z, E') - \frac{c(E)}{\ell(E)} \psi_0(z, E) . \quad (5.12)$$

Thus the flux can be written down immediately in terms of the one-speed Milne solutions for multiplication $c(E)$ and the corresponding Green's function acting on the 'source' $S_0(z, E)$. By choosing $c(E)$ so that the one-speed solutions have an asymptotic spatial dependence appropriate to the diffusion length L , that is taking (Davison 1957, p52; see also (2.5)):

$$c^{-1}(E) = \frac{L}{2\ell(E)} \ln \left[\frac{L + \ell(E)}{L - \ell(E)} \right] \quad (5.13)$$

the equation becomes

$$\psi_0(z, E) = \rho_0(z, \ell(E), L) + \int_0^{\infty} dz' S_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E), L) . \quad (5.14)$$

The normalisation of $\rho_0(z, \ell(E), L)$ is such that it has the same asymptotic energy dependence as $\psi_0(z, E)$ which means that it has the form:

$$\rho_{o\text{asy}}(z, \ell(E), L) = g_o(E) \left[e^{z/L} + a \left(\frac{\ell(E)}{L} \right) e^{-z/L} \right] \quad (5.15)$$

where $a \left(\frac{\ell(E)}{L} \right)$ is a known function of $\ell(E)/L$ only (Davison 1967, Chap.6). A further important consequence of this choice of $c(E)$ is that $S_o(z, E)$ then vanishes more rapidly than $\exp\{-z/L\}$ and therefore the term involving $S_o(z, E)$ in (5.14) does not contribute to the exponentially increasing part of the flux. It follows from (5.4) that:

$$\frac{c(E)}{\ell(E)} g_o(E) = \int_0^\infty dE' \Sigma_o(E \rightarrow E') g_o(E') \quad (5.16)$$

so that writing

$$\psi_o(z, E) = g_o(E) \left[e^{z/L} + a e^{-z/L} \right] + \phi_o(z, E) \quad (5.17)$$

we find

$$S_o(z, E) = \int_0^\infty dE' \Sigma_o(E \rightarrow E') \phi_o(z, E') - \frac{c(E)}{\ell(E)} \phi_o(z, E) \quad (5.18)$$

and we shall refer to this 'source' as $s_o(z, E)$ to indicate that it is independent of the asymptotic part of $\psi_o(z, E)$. It should be noticed that for convenience we have changed the sign of $\phi_o(z, E)$ in (5.17) as compared with equation (4.35) in the no-capture problem.

§5.3 The Variational Principle

By the analysis of §5.2 the original homogeneous equation for the angular dependent neutron distribution has been reduced to an inhomogeneous integral equation for the neutron flux $\psi_0(z, E)$. Following the method of Chapter 4 for the no-capture case a variational principle can be written down for the transient flux $\phi_0(z, E)$. Consider the functional:

$$\mathcal{Z}_0[\phi_0(z, E)] =$$

$$\int_0^\infty dE M(E) \int_0^\infty dz s_0(z, E) \left[2\rho_0(z, \ell(E), L) - \phi_0(z, E) + \int_0^\infty dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E), L) \right]$$

(5.19)

Note that for the functional to exist $\phi_0(z, E)$ must be restricted to decay faster than $\exp\{-z/L\}$. It is easily verified that the condition for the first order variation of \mathcal{Z}_0 to vanish for arbitrary changes in $\phi_0(z, E)$ is:

$$\int_0^\infty dE' \left[\Sigma_0(E \rightarrow E') - \frac{c(E)}{\ell(E)} \delta(E - E') \right] \left\{ \rho_0(z, \ell(E'), L) - \phi_0(z, E') + \int_0^\infty dz' s_0(z', E') \rho_{00}(z' \rightarrow z; \ell(E'), L) \right\} = 0 \quad (5.20)$$

Comparing (5.20) with (5.16) we see that, provided (5.16) gives a

unique relationship between $c(E)$ and $g_0(E)^+$, (5.20) is equivalent to:

$$\phi_0(z,E) - \rho_0(z,\ell(E),L) - \int_0^\infty dz' s_0(z',E) \rho_{00}(z' \rightarrow z; \ell(E),L) = f(z) g_0(E) \quad (5.21)$$

where $f(z)$ is an arbitrary function of z . With

$$f(z) = - \left[e^{z/L} + a e^{-z/L} \right] \quad (5.22)$$

equation (5.21) reduces to (5.14). The derivation of (5.20) from (5.19) depends on (a) the symmetry of the Green's function in z and z' as implied by the optical reciprocity theorem and (b) the detailed balance condition. The latter also implies that the addition to $\phi_0(z,E)$ of any function of z multiplied by $g_0(E)$ leaves the value of Z_0 unchanged.

When $\phi_0(z,E)$ satisfies (5.21):

$$Z_0[\phi_0(z,E)] = \int_0^\infty dE M(E) \int_0^\infty dz s_0(z,E) \rho_0(z,\ell(E),L). \quad (5.23)$$

It will now be shown how this is related to the parameter a and hence to the extrapolation length. To see this we multiply both sides of (5.1) by the adjoint to the one-speed angular flux $\rho(z,-\mu,\ell(E),L)$ and integrate over angle and over z from 0 to Z_0 . The left hand side gives:

⁺ If (5.16) does not give a unique relationship between $c(E)$ and $g_0(E)$ this implies that there is more than one $g(E,-\mu)$ associated with the diffusion length. Thus we require an additional specification of the choice of $g(E,-\mu)$ corresponding to a diffusion length L .

$$\begin{aligned}
& \int_0^Z dz \int_{-1}^{+1} d\mu \rho(z, -\mu, \ell(E), L) \left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \Psi(z, \mu, E) \\
&= \left[\int_{-1}^{+1} d\mu \mu \rho(z, -\mu, \ell(E), L) \Psi(z, \mu, E) \right]_0^Z \\
&\quad + \int_0^Z dz \int_{-1}^{+1} d\mu \Psi(z, \mu, E) \left[-\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \rho(z, -\mu, \ell(E), L) \\
&= \int_{-1}^{+1} d\mu \mu \rho(Z, -\mu, \ell(E), L) \Psi(Z, \mu, E) \\
&\quad + \frac{1}{2} \int_0^\infty dz \Psi_0(z, E) \frac{c(E)}{\ell(E)} \rho_0(z, \ell(E), L) \tag{5.24}
\end{aligned}$$

since for $z=0$ either $\rho(z, -\mu, \ell(E), L)$ or $\Psi(z, \mu, E)$ vanishes. Combining with the right hand side and taking the limit $Z \rightarrow \infty$ yields:

$$\begin{aligned}
a M(E) \int_{-1}^{+1} \mu g^2(E, \mu) d\mu &= a \left(\frac{\ell(E)}{L} \right) M(E) \int_{-1}^{+1} \mu g^2(E, \mu) d\mu \\
&\quad + \frac{1}{2} M(E) \int_0^\infty dz s_0(z, E) \rho_0(z, \ell(E), L) \tag{5.25}
\end{aligned}$$

where we have used the asymptotic forms (5.5) and (5.15) and the condition:

$$\int_{-1}^{+1} \mu g(E, \mu) g(E, -\mu) d\mu = 0 . \tag{5.26}$$

Now integrating (5.25) over energy and substituting for (5.23) we obtain finally:

$$a \int_0^{\infty} dE M(E) F(E) = \int_0^{\infty} dE M(E) a \left(\frac{\ell(E)}{L} \right) F(E) + Z_0 [\phi_0(z, E)] \quad (5.27)$$

where

$$F(E) = 2 \int_{-1}^{+1} \mu g^2(E, \mu) d\mu = -2 \int_{-1}^{+1} \mu g^2(E, -\mu) d\mu. \quad (5.28)$$

A useful expression for $g(E, -\mu)$ is obtained by dividing (5.4) by $\left(\frac{\mu}{L} + \frac{1}{\ell(E)} \right)$ and simplifying the numerator through (5.16): substitution into (5.28) and integration over μ finally yields:

$$F(E) = \frac{L}{\ell(E)} c(E) \left[\frac{\ell^2(E) - L^2(1-c(E))}{L^2 - \ell^2(E)} \right] g_0^2(E). \quad (5.29)$$

Connection with the no-capture case (Schofield 1963) is made by noting that as the capture tends to zero:

$$a \left(\frac{\ell(E)}{L} \right) \sim -1 + \frac{2c \ell(E)}{L} \quad (5.30)$$

where $c \doteq 0.7104$ and

$$1 - c(E) \sim \frac{1}{2} \frac{\ell^2(E)}{L^2} \quad (5.31)$$

so that

$$a \sim -1 + \frac{2c\bar{\ell}^2}{L\bar{\ell}} + \text{a term depending on } s_0(z,E) \quad (5.32)$$

with

$$\bar{x} = \int_0^{\infty} dE M(E) x(E) g^2(E). \quad (5.33)$$

Thus one can express the parameter a , and hence the extrapolation length, as the sum of a term representing an appropriate average over the one-speed parameters and a term which depends on the distortion of the transient flux near the boundary due to energy exchange and capture. The second term can be estimated with the variational principle and optimising $Z_0[\phi_0(z,E)]$ for a restricted set of trial functions $\phi_0(z,E)$. In the no-capture problem the extrapolation length itself was given by an analogous sum.

Although a good value of a may be obtained from such a restricted set $\phi_0(z,E)$ care must be exercised in estimating the flux and angular distribution with the optimised $\phi_0(z,E)$. As pointed out previously a is unchanged by the addition to $\phi_0(z,E)$ of an arbitrary function of z times $g_0(E)$. Thus in order to obtain $\psi(z,\mu,E)$ we must iterate the flux through an equation which is also independent of added multiples of $g_0(E)$ to the original trial function. The required equation may be found in the following way: equation (5.14) is rewritten as:

$$g_0(E) \left[e^{z/L} + a e^{-z/L} \right] + \phi_0(z, E) =$$

$$g_0(E) \left[e^{z/L} + a \left(\frac{\ell(E)}{L} \right) e^{-z/L} \right] + \rho_{0_{tr}}(z, \ell(E), L) + \int_0^{\infty} dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E), L)$$

where

$$\rho(z, \mu, \ell(E), L) = \rho_{asy}(z, \mu, \ell(E), L) + \rho_{tr}(z, \mu, \ell(E), L). \quad (5.35)$$

Multiplying throughout by $F(E)/2g_0(E)$ we obtain

$$\begin{aligned} \frac{aF(E)}{2} + e^{z/L} \frac{F(E)}{2g_0(E)} \phi_0(z, E) &= a \left(\frac{\ell(E)}{L} \right) \frac{F(E)}{2} + e^{z/L} \frac{F(E)}{2g_0(E)} \rho_{0_{tr}}(z, \ell(E), L) \\ &+ e^{z/L} \frac{F(E)}{2g_0(E)} \int_0^{\infty} dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E), L). \end{aligned} \quad (5.36)$$

Comparing (5.36) with (5.25) we see that:

$$\begin{aligned} \phi_0(z, E) &= \rho_{0_{tr}}(z, \ell(E), L) + \int_0^{\infty} dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E), L) \\ &\rightarrow e^{-z/L} \frac{g_0(E)}{F(E)} \int_0^{\infty} dz' s_0(z', E) \rho_0(z', \ell(E), L). \end{aligned} \quad (5.37)$$

An expression for the emergent angular flux $\Psi(0, -\mu, E)$ in terms of the iterated total flux given by (5.37) may be obtained by integrating (5.1) over z :

$$\Psi(0, \mu, E) = \frac{M(E)}{2} \left\{ \left[\frac{1}{1 - \frac{\mu \ell(E)}{L}} + \frac{a}{1 + \frac{\mu \ell(E)}{L}} \right] c(E) g_0(E) + \frac{1}{\mu} \int_0^\infty dz e^{-z/\mu \ell(E)} \int_0^\infty dE' \Sigma_0(E \rightarrow E') \phi_0(z, E') \right\} .$$

$$0 \leq \mu \leq 1 \quad (5.38)$$

A measure of the accuracy of the trial function itself is provided by (5.25) which, whilst being an identity for the exact choice of $\phi_0(z, E)$, is only approximately true for any restricted trial function. It was for this reason that we integrated over (5.25) in the manner indicated to obtain (5.27) for the parameter a_0 .

§5.4 K-Integrals of the Transport Equation

Before adopting a trial function for the transient flux we consider two integral conditions, analogous to the conservation conditions of the no-capture case (see §4.2), which permit an alternative derivation of (5.27).

Defining $K_n(z)$ by:

$$K_n(z) = \int_0^\infty dE \int_{-1}^{+1} d\mu \mu g_n(E, \mu) \Psi(z, \mu, E) \quad n=1,2 \quad (5.39)$$

where $g_n(E, \mu)$ are the odd and even parts of $g(E, \mu)$

$$2g_1(E, \mu) = g(E, \mu) + g(E, -\mu)$$

$$\frac{2g_2(E, \mu)}{L} = g(E, \mu) - g(E, -\mu) \quad (5.40)$$

it may be shown (Kladnik and Kušcer 1962) that the integrals $K_n(z)$ satisfy the coupled differential equations:

$$\begin{aligned} \frac{d}{dz} K_1(z) &= -K_2(z)/L^2 \\ \frac{d}{dz} K_2(z) &= -K_1(z) \end{aligned} \quad (5.41)$$

for which the asymptotic part of $\Psi(z, \mu, E)$ is a particular solution. The angular flux may be written, in terms of the Green's function, in the form:

$$\Psi(z, \mu, E) = \rho(z, \mu, \ell(E), L) + \int_0^{\infty} dz' s_0(z', E) \rho_0(z' \rightarrow z, \mu; \ell(E), L) \quad (5.42)$$

so that asymptotically

$$\begin{aligned} \Psi_{\text{asy}}(z, \mu, E) &= g(E, -\mu) e^{z/L} + a e^{-z/L} g(E, \mu) \\ &= g(E, -\mu) e^{z/L} + a \left(\frac{\ell(E)}{L} \right) e^{-z/L} g(E, \mu) \\ &\quad + \lim_{z \rightarrow \infty} \int_0^{\infty} dz' s_0(z', E) \rho_0(z' \rightarrow z, \mu; \ell(E), L). \end{aligned} \quad (5.43)$$

Substituting into $K_1(z) - K_2(z)$ would do equally well - cancelling the terms involving $g(E, -\mu) e^{z/L}$ from each side and using (5.26) we find:

$$\begin{aligned}
\frac{ae^{-z/L}}{2} \int_0^{\infty} dE M(E) F(E) &= \frac{e^{-z/L}}{2} \int_0^{\infty} dE M(E) a \left(\frac{\ell(E)}{L} \right) F(E) \\
+ \lim_{z \rightarrow \infty} \int_0^{\infty} dE M(E) \int_{-1}^{+1} d\mu \mu [g(E, \mu) + g(E, -\mu)] &\int_0^{\infty} dz' s_0(z', E) \rho_0(z' \rightarrow z, \mu; \ell(E), L)
\end{aligned} \tag{5.44}$$

The last term in (5.44) may be simplified by consideration of the transport equation for the Green's function:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \rho_0(z' \rightarrow z, \mu; \ell(E), L) = \frac{c(E)}{2\ell(E)} \rho_{00}(z' \rightarrow z; \ell(E), L) + \frac{1}{2} \delta(z - z'). \tag{5.45}$$

Multiplying (5.45) by $\rho(z, -\mu, \ell(E), L)$ and integrating, as in §5.3, over z and μ we find:

$$\begin{aligned}
\lim_{z \rightarrow \infty} \int_{-1}^{+1} \mu \rho(z, -\mu, \ell(E), L) \rho_0(z' \rightarrow z, \mu; \ell(E), L) d\mu \\
= \frac{1}{2} \int_0^{\infty} \rho_0(z', \ell(E), L) \delta(z^+ - z') dz^+ = \frac{1}{2} \rho_0(z', \ell(E), L)
\end{aligned} \tag{5.46}$$

that is

$$\begin{aligned}
\lim_{z \rightarrow \infty} \int_{-1}^{+1} \mu \rho_0(z' \rightarrow z, \mu; \ell(E), L) \left[g(E, \mu) e^{z/L} + a \left(\frac{\ell(E)}{L} \right) g(E, -\mu) e^{-z/L} \right] d\mu \\
= \frac{1}{2} \rho_0(z', \ell(E), L) .
\end{aligned} \tag{5.47}$$

Multiplying (5.44) by $\mu g(E, -\mu)$, integrating over angle and using (5.26) we obtain:

$$\lim_{z \rightarrow \infty} \int_{-1}^{+1} d\mu \mu g(E, -\mu) \int_0^{\infty} dz' s_0(z', E) \rho_0(z' \rightarrow z, \mu; \ell(E), L) = 0 \quad (5.48)$$

Then inserting (5.48) into (5.47) and both of these into (5.44) finally yields the desired result, namely (5.27).

§5.5 The Trial Function

As in the no-capture case we assume a simple trial function of the form:

$$\phi_0(z, E) = e^{-z/L_T} \phi_0(E) \quad (5.49)$$

where both L_T and $\phi_0(E)$ are to be determined. Inserting (5.49) into the functional (5.19) we obtain:

$$\mathcal{Z}_0[\phi_0(E)] = \int_0^{\infty} dE M(E) s_0(E) \left\{ 2\tilde{\rho}_0(\ell(E), L, L_T) - \frac{L_T}{2} \phi_0(E) + G(\ell(E), L, L_T) s_0(E) \right\} \quad (5.50)$$

with

$$s_0(E) = \int_0^{\infty} dE' \Sigma_0(E \rightarrow E') \phi_0(E') - \frac{c(E)}{\ell(E)} \phi_0(E) \quad (5.51)$$

and $\tilde{\rho}_0(\ell(E), L, L_T)$ and $G(\ell(E), L, L_T)$ are defined similarly to the no-capture case:

$$\tilde{\rho}_0(\ell(E), L, L_T) = \int_0^{\infty} dz e^{-z/L_T} \rho_0(z, \ell(E), L) \quad (5.52)$$

$$G(\ell(E), L, L_T) = \int_0^{\infty} dz \int_0^{\infty} dz' \rho_{00}(z' \rightarrow z; \ell(E), L) e^{-(z+z')/L_T}. \quad (5.53)$$

Demanding that the first order variation in $\mathcal{Z}_0[\phi_0(E)]$ vanishes for arbitrary variations in $\phi_0(E)$ we obtain an equation for the optimum form of $\phi_0(E)$ for a given L_T :

$$\tilde{\rho}_0(\ell(E), L, L_T) - \frac{L_T}{2} \phi_0(E) + G(\ell(E), L, L_T) s_0(E) = C g_0(E) \quad (5.54)$$

where C is an arbitrary constant. Equation (5.54) is solved for various values of L_T and the value of L_T which optimises the functional is obtained by interpolation.

In order to continue we require useful expressions for $\rho_0(z, \ell(E), L)$ and $\rho_{00}(z' \rightarrow z; \ell(E), L)$ which will enable us to determine $\tilde{\rho}_0(\ell(E), L, L_T)$ and $G(\ell(E), L, L_T)$. In the remainder of this section we shall show that $\rho_{00}(z' \rightarrow z; \ell(E), L)$ may ultimately be written in terms of $\rho_0(z, \ell(E), L)$ and then briefly mention an approximate expression for $\rho_0(z, \ell(E), L)$ which is sufficiently accurate for our purposes and yet retains a fairly simple form

$$\rho_{00}(z' \rightarrow z; \ell, L) \text{ is given in terms of } \rho_{q_0}(z, \ell, L) \text{ by (3.20).}$$

Making use of the fact that (Davison 1957, eqn.6.60)

$$\rho_{q_0}(0, \ell, L) = \frac{\ell}{c} \left[\frac{1}{(1-c)^{1/2}} - 1 \right] \quad (5.55)$$

it is straightforward to show that

$$G(\ell(E), L, L_T) = \frac{c(E)}{\ell(E)} [1-c(E)] \frac{\tilde{\rho}_{q_0}^2(\ell(E), L, L_T)}{2L_T} + [1-c(E)] \tilde{\rho}_{q_0}(\ell(E), L, L_T) - \frac{L_T \ell(E)}{2} \quad (5.56)$$

where

$$\tilde{\rho}_{q_0}(\ell(E), L, L_T) = \int_0^{\infty} dz e^{-z/L_T} \rho_{q_0}(z, \ell(E), L) \quad (5.57)$$

Furthermore Davison (1957, eqn. 6.61) has shown that $\rho_{q_0}(z, \ell, L)$ is related to $\rho_0(z, \ell, L)$:

$$\rho_{q_0}(z, \ell, L) = \frac{1}{c|j(O, \ell, L)|} \left[L \rho_0(z, \ell, L) - \int_0^z \rho_0(u, \ell, L) du - \ell |j(O, \ell, L)| \right] \quad (5.58)$$

where $j(O, \ell, L)$ is the emergent current in the source-free case.

Thus:

$$\begin{aligned} & \tilde{\rho}_{q_0}(\ell(E), L, L_T) \\ &= \frac{1}{c|j(O, \ell(E), L)|} \left[L \tilde{\rho}_0(\ell(E), L, L_T) - \int_0^{\infty} dz e^{-z/L_T} \int_0^z \rho_0(u, \ell(E), L) du \right] - \frac{L_T \ell(E)}{c(E)} \\ &= \frac{1}{c|j(O, \ell(E), L)|} \left[L \tilde{\rho}_0(\ell(E), L, L_T) - L_T \tilde{\rho}_0(\ell(E), L, L_T) \right] - \frac{L_T \ell(E)}{c(E)} \end{aligned} \quad (5.59)$$

Again by reference to Davison (1957, eqns. 6.21 and 6.46) we find that, with the normalisation adopted in (5.15), the emergent current is given by:

$$|j(O, \ell(E), L)| = \frac{2g_0(E)L}{\ell(E)} \left| a \left(\frac{\ell(E)}{L} \right) \right|^{\frac{1}{2}} \left[\frac{(1-c(E))(L^2c(E)-L^2+\ell^2(E))}{2(L^2-\ell^2(E))} \right]^{\frac{1}{2}} \quad (5.60)$$

Once again rather unwieldy exact expressions for $\rho_0(z, \ell(E), L)$ may be found by the Wiener-Hopf method (Davison 1957, p.67) but a more useful approximate expression has been found by LeCaine (1950) with a variational principle: allowing for the different normalisation she obtained:

$$\rho_0(z, \ell(E), L) = g_0(E) \left[e^{z/L} + a \left(\frac{\ell(E)}{L} \right) e^{-z/L} + 2 \left| a \left(\frac{\ell(E)}{L} \right) \right|^{\frac{1}{2}} \left\{ A \left(\frac{\ell(E)}{L} \right) G_3(z, \ell(E), L) + B \left(\frac{\ell(E)}{L} \right) G_2(z, \ell(E), L) \right\} \right] \quad (5.61)$$

where

$$G_3(z, \ell(E), L) = c(E) \ell(E) L \int_1^{\infty} \frac{e^{-zt/\ell(E)}}{t(L^2t^2 - \ell^2(E))} dt \quad (5.62)$$

$$G_2(z, \ell(E), L) = -c(E) L^2 \int_1^{\infty} \frac{e^{-zt/\ell(E)}}{(L^2t^2 - \ell^2(E))} dt \quad (5.63)$$

The coefficients $A \left(\frac{\ell(E)}{L} \right)$, $B \left(\frac{\ell(E)}{L} \right)$ and $a \left(\frac{\ell(E)}{L} \right)$ are given by the variational principle. With this form of $\rho_0(z, \ell(E), L)$ LeCaine reports a maximum error in the extrapolated end-point $z'_0 \left(\frac{\ell(E)}{L} \right)$ where:

$$a\left(\frac{\ell(E)}{L}\right) = - \exp \left\{ - 2z'_0 \left(\frac{\ell(E)}{L}\right) \middle/ L \right\} \quad (5.64)$$

of about 0.3% which occurs when there is no capture and an expected error of about 0.05% in the emergent angular distribution.

After evaluation of several integrals the insertion of (5.61) into (5.52) leads to:

$$\begin{aligned} \tilde{\rho}_0(\ell(E), L, L_T) = & g_0(E) \left[\frac{L_T L}{L - L_T} + a\left(\frac{\ell(E)}{L}\right) \frac{L_T L}{L + L_T} \right. \\ & + \frac{2 \left| a\left(\frac{\ell(E)}{L}\right) \right|^{\frac{1}{2}} c(E) L_T L^3}{(L^2 - L_T^2) \ell(E)} \left\{ A \left(\frac{\ell(E)}{L}\right) \left(\frac{L_T^2}{L^2} \ln \left| 1 + \frac{\ell(E)}{L_T} \right| - \frac{1}{2} \ln \left| 1 - \frac{\ell^2(E)}{L^2} \right| - \frac{L_T \ell(E)}{c(E) L^2} \right) \right. \\ & \left. \left. + B \left(\frac{\ell(E)}{L}\right) \left(\frac{L_T}{L} \ln \left| 1 + \frac{\ell(E)}{L_T} \right| - \frac{L_T}{2L} \ln \left| 1 - \frac{\ell^2(E)}{L^2} \right| - \frac{\ell(E)}{c(E) L} \right) \right\} \right] \end{aligned} \quad (5.65)$$

with the restriction, already mentioned, that $L_T < L$.

We have estimated the extrapolated end-point with the trial function (5.49) in a number of cases: these are discussed in the next section.

§5.6 Results and Discussion

There have been other treatments of the energy dependent Milne problem with capture but few have reported the results of any numerical computations. Recently, however, Arkuszewski (1967) has obtained an exact solution using the Wiener-Hopf technique for the separable kernel with $1/\sqrt{v}$ type absorption. We may therefore get some idea of the accuracy of the present method by comparing our results for the separable kernel with those of Arkuszewski: in particular we shall deal mainly with the free gas moderator of atomic mass A with $1/v$ type absorption and include a comparison of the results obtained by using the separable and true kernels to represent this moderator. No real comparison with the experimental results for water can be made without introducing anisotropic scattering.

The first step in the calculation is the determination of the diffusion length L_0 . In some previous direct numerical computations in the B_0 approximation (see Chapter 2) the critical value of the absorption parameter β above which the diffusion length ceases to exist has been determined for various scattering models where β is defined by:

$$\Sigma_a(E) = \beta \left(\frac{kT}{E} \right)^{\frac{1}{2}} ; \quad \ell_{\max} = 1. \quad (5.66)$$

Thus the limits within which this theory is applicable are already determined.

In Tables 5.I to 5.IV we have tabulated the diffusion length, the extrapolated end-point and the corresponding value of a for a free gas moderator with a concentration of $1/v$ absorber given by the parameter

β , equation (5.66). Generally speaking the boundary condition implied by z_0^i is easier to apply than the extrapolation length but mathematically z_0 is to be preferred because it imposes conditions on the asymptotic flux at the boundary itself instead of at a point "in vacuo" at some distance from the medium. However the extrapolated end-point is tabulated here for the sake of direct comparison with the results of Arkuszewski who assumes a spatial dependence for the asymptotic flux of the form $\text{Sinh}\left(\frac{z-z_0^i}{L}\right)$ so that a is related to z_0^i by:

$$a = - \exp \left\{ -2z_0^i/L \right\} . \quad (5.67)$$

In the limit of no-capture ($\beta=0.0$ and $L=\infty$) the results were obtained with the theory mentioned briefly in Chapter 1 and described in greater detail by Schofield (1963) for the same trial function. In that case the extrapolated end-point ($z_0^i=z_0$) is given directly as an appropriate average over the one-speed value ($cl(E)$; $c \doteq 0.7104$) with a correction term ε estimated by the variational principle, that is:

$$z_0^i = \frac{c\bar{l}}{2} - \varepsilon \quad \bar{x} = \int_0^\infty dE M(E) x(E) . \quad (5.68)$$

For the problem with capture we have seen that the analogous result is:

$$a = \frac{\int_0^\infty dE M(E) a \left(\frac{l(E)}{L} \right) F(E)}{\int_0^\infty dE M(E) F(E)} - a_1 \quad (5.69)$$

Both ε and a_1 are included in the tables.

The computed diffusion lengths which have been discussed in Chapter 2 are seen to be in very good agreement with Arkuszewski's throughout: we expect the results for the full kernel to be equally accurate since the computations were consistent. This suggests that Wood's results for the proton gas (Wood 1965) are fractionally too low.

While the extrapolated end-point also shows good agreement to within about 1% the results for $\beta > 0$ are generally somewhat too low. The one-speed values of $z_0^1(\nu)$ determined from LeCaine's variational principle are themselves slightly low in the range $\nu \gtrsim 0.95$ but this region does not contribute significantly to the result even for high β . The difference is caused predominantly by the inadequacy of the integration procedure in calculating the leading term in (5.27) and could be improved at the expense of computer time and capacity. This was particularly noticeable in the calculations performed in the no-capture problem where it was fairly easy to calculate $\overline{l^N}$ from analytic formulae for $l(E)$ to any required accuracy. It was found that when cl^2/\overline{l} was calculated in the course of the computation by the simple trapezium rule integration procedure the results were generally about 0.1% too low, caused mainly by the inability of the trapezium rule to integrate accurately over the discontinuity in the gradient of $\Sigma_0(E \rightarrow E')$ at $E=E'$.

The simplicity of the trial function will also introduce errors which have been discussed in detail in the previous chapter.

In the present calculations we expect the error in the leading term on the right of (5.27) to be of the same order of magnitude as the correction term: nevertheless the smallness of the correction term itself is certainly significant.

A few calculations were done with other inverse power absorption laws ($\Sigma_a \propto 1/V^N$) without producing any significantly new results.

In conclusion we should like to make the following remarks:

(i) the expression

$$\frac{\int_0^{\infty} dE M(E) a \left(\frac{\ell(E)}{L} \right) \int_{-1}^{+1} d\mu \mu g^2(E, \mu)}{\int_0^{\infty} dE M(E) \int_{-1}^{+1} d\mu \mu g^2(E, \mu)} \quad (5.70)$$

is found always to be a lower bound on the magnitude of a ; a plausibility argument to demonstrate this has already been presented by Schofield (1963) for the capture-free case. Furthermore we expect it to give a fairly close approximation to the true a and hence to the extrapolation length.

(ii) in the capture-free Milne problem with isotropic scattering it is easily seen from §4.3 or from Schofield (1963) that in the special cases of "no energy exchange" and "constant mean free path" the extrapolation length is given by:

$$z_0 = c \ell^2 / \bar{\ell} \quad c \doteq 0.7104 \quad (5.71)$$

While we would agree with Arkuszewski (1967) that no such simple relationship exists for these limiting cases in the same problem with capture we should like to suggest that a simple definition similar to (A-12) for \bar{z}_0 in Williams paper (Williams 1964a; Schofield 1963 or equation (4.17)) does indeed exist and is expressed implicitly by equation (5.27).

The fact remains, as pointed out by Arkuszewski, that no direct comparison between the extrapolation length obtained with the separable kernel (strong energy exchange) and the δ -function kernel (no energy exchange) is possible when there is neutron capture. This comparison was most useful in the no-capture problem for it had been suggested that these limits set lower and upper bounds on the extrapolation length (Williams 1964a).

The difficulty is associated with the fact that it becomes impossible to define a unique diffusion length in the limit of no energy exchange - for each energy there is a different L and yet when we admit even a small amount of energy exchange it is assumed that a unique diffusion length exists. This is so far unexplained.

(iii) it has often been suggested in recent years that the extrapolation length, diffusion length and emergent angular distribution are determined to a large extent by the energy dependence of the mean free path of the moderator rather than the details of the transfer cross-section $\Sigma_0(E \rightarrow E')$. (Williams 1964a,b; Eisenhauer 1964; Arkuszewski 1967;).

It is certainly true that the extrapolation length is rather insensitive to, although not entirely independent of $\Sigma_0(E \rightarrow E')$ (Williams 1964a; see also Chapter 4). Even though the scattering matrix plays a greater part in determining z_0 for finite absorption when the asymptotic spectrum is no longer Maxwellian the effect here is still small. For example z_0 varies by no more than about 3% between the separable and true kernels for the moderators and absorber concentrations considered here.

On the other hand the diffusion length does appear to be influenced to a significant extent by the energy exchange properties, at least for the heavier moderators. From Tables 5.I and 5.II we see that for $A=1,2$ the agreement between the separable and true kernels is extremely good, the difference in the values of L being not more than about 2%. However for mass $A=12$ (Table 5.IV) the difference has increased to more than 10%. This effect is even more noticeable if we consider the critical absorption parameter β_c given in Chapter 2. It is clear therefore that we cannot disregard the details of the scattering mechanism for heavier moderators.†

As for the emergent angular distribution it is again clear that the spectra will differ little for low mass numbers and without capture (see Chapter 4). For mass $A=12$ but still without capture we have tabulated our results for the true kernel (see Table 4.V in the previous

† The comparison made by Arkuszewski (1967) between the diffusion lengths for the free gas moderators as represented by the separable and full kernels is invalid. In the first place the result ascribed to Wood for $A=4$ is misquoted. Secondly the results for $A=1$ were obtained in the B_0 approximation while those for $A=2,4$ were made with diffusion theory. The difference in the results for these two approximations will be of the same magnitude as the difference we are looking for between the (consistent) results for the separable and true kernels.

chapter) in order that they might be compared with future calculations on the separable kernel to determine whether higher mass numbers will separate the spectra for these two kernels. Such calculations may be performed based on the theory in the preceding chapter or numerical values obtained for the graphs shown in Arkuszewski (1967).

In any case it has been suggested that this insensitivity may be restricted to non-absorbing media (Eisenhauer 1964). It would therefore be interesting to extend the present calculations to predict the emergent spectra in order to test this hypothesis.

APPENDIX

§5A.1 Numerical Procedures

In this appendix we describe very briefly the numerical methods employed in finding the extrapolation length for which results are quoted in Tables 5.I to 5.IV. The methods for finding the diffusion length and associated eigenfunction have already been outlined in Appendix §2A.1 while the methods for determining the extrapolation length for an optimum value of L_T through the solution of (5.54) have been given in Appendix §4A.1. There remains but one additional feature of these calculations which deserves mention namely the approximate solution of the one-speed Milne problem.

In the no-capture problem described in Chapter 4 the determination of the variational parameters of the one-speed solution was a straightforward procedure worked out by LeCaine (1947) and the only energy dependence lay in the scaling factor of the mean free path. But in the present problem, for a fixed diffusion length, there is also besides the scaling factor $\ell(E)$ the energy dependence of $c(E)$ given by equation (5.13). This means that for each energy the variational parameters have to be redetermined.

LeCaine (1950) has given a prescription for determining the quantities $A(\nu)$, $B(\nu)$ and $z_0'(\nu)$ with $\nu = \ell(E)/L$ in (5.61) and (5.64) through the equations:

$$\frac{B(\nu)}{A(\nu)} = \frac{2 L_2 K_1 - L_1 K_2}{2 L_1 K_3 - L_2 K_2} \quad (5A.1)$$

$$\frac{4 K_1 K_3 - K_2^2}{4 \left[L_1^2 K_3 + L_2^2 K_1 - L_1 L_2 K_2 \right]} = \frac{-1}{\left[\left(\text{Cosh } 2\nu z'_0 + 1 \right) \ln(1-\nu^2) + \frac{2\nu^2}{1-\nu^2} \right] \frac{c(\nu)}{8\nu^2}} \quad (5A.2)$$

$$A(\nu) = \frac{\sqrt{\frac{\nu^2 - (1-c(\nu))}{2(1-\nu^2)}} - \text{Sinh } \nu z'_0}{-\frac{c(\nu)}{2\nu} \ln(1-\nu^2) - \frac{B}{A}} \quad (5A.3)$$

with

$$c(\nu) = \frac{L}{2\ell(E)} \ln \left| \frac{L + \ell(E)}{L - \ell(E)} \right| = \frac{1}{2\nu} \ln \left| \frac{1 + \nu}{1 - \nu} \right| \quad (5A.4)$$

while L_1, L_2, K_1, K_2 and K_3 are complicated expressions, which may be evaluated analytically, involving integrals of the general form:

$$\int_0^\infty dz G_n(z, \nu) G_m(z, \nu) \quad m, n=2, 3 \quad (5A.5)$$

$$\int_0^\infty dz G_n(z, \nu) \int_0^\infty dz' G_m(z', \nu) E_1(|z-z'|) \quad m, n=2, 3$$

and $G_n(z, \nu)$ is defined by (5.62), (5.63). It should be noticed that the factor 4 in the denominator of (5A.2) has been omitted from both the references listed. (There is also a factor $\frac{1}{2}$ missing from the equation for K_3 given by LeCaine).

For $0.5 \leq \nu \leq 1.0$ the computer programme to evaluate these parameters was checked against results tabulated by LeCaine although here again there are misprints. There is no doubt however that our calculations lead to accurate results in this range of ν .

In the calculations the region $0.0 \leq \nu \leq 0.5$ will assume equal importance but a detailed investigation into the quantities appearing in (5A.1) to (5A.3) and the integrals K_n, L_n reveals the possibility that, because of the finite word length of the computer unacceptable cancellation may occur. Much of this cancellation may be avoided by expanding the various functions in terms of the parameter ν . The general term of the non-trivial expansion of each of the integrals L_n ($n=1,2$) and K_n ($n=1,2,3$) may be written down in terms of the integrals J_{mn} and P_{mn} defined in Appendix II of Kourganoff (1952). These can be generated by recurrence relations also given by Kourganoff.

Comparison of results obtained in this way with those obtained directly shows that while a great deal of cancellation does occur the analytic expressions produce results correct to at least six figures in $A(\nu)$, $B(\nu)$ and $z_0^1(\nu)$ which is sufficient for our purposes.

Sykes (1954) has adopted this expansion method for very small absorption retaining only terms up to ν^2 in the expansion of $\rho_0(z, l(E), L)$.

LeCaine also quotes a series expansion in $(1-\nu)$ for ν very close to unity.

A=1		Arkuszewski (1967) (S.K.)	Present Theory		Wood (1965)
			(S.K.)	(T.K.)	
$\beta=0.0$	z_0^t	0.5377	0.5382	0.5389	
	ε	0.0075	0.0070	0.0063	
$\beta=0.1$	L	1.6895	1.6921	1.7046	1.685
	z_0^t	0.5555	0.5543	0.5597	
	a	-0.5181	-0.5193	-0.5185	
	a_1		0.0028	0.0023	
$\beta=0.2$	L	1.2088	1.2101	1.2284	1.213
	z_0^t	0.5780	0.5761	0.5870	
	a	-0.3843	-0.3859	-0.3845	
	a_1		0.0028	0.0021	
$\beta=0.3$	L	1.0003	1.0007	1.0239	
	z_0^t	0.6086	0.6054	0.6233	
	a	-0.2961	-0.2982	-0.2960	
	a_1		0.0026	0.0018	

TABLE 5.I

The diffusion length and extrapolated end-point for the free gas moderator of mass A with $l_{\max} = 1$ and absorber concentration β calculated for the separable kernel (S.K.) and the true kernel (T.K.). The parameters a, a_1 and ε are defined by (5.5) and (5.67) to (5.69).

A=2		Arkuszewski (1967) (S.K.)	Present Theory	
			(S.K.)	(T.K.)
$\beta=0.1$	L	1.7908	1.7926	1.8095
	z_0^r	0.6167	0.6148	0.6201
	a	-0.5022	-0.5036	-0.5039
	a_1		0.0016	0.0013
$\beta=0.2$	L	1.2784	1.2789	1.3033
	z_0^r	0.6364	0.6336	0.6443
	a	-0.3695	-0.3713	-0.3721
	a_1		0.0017	0.0012
$\beta=0.3$	L	1.0551	1.0549	1.0851
	z_0^r	0.6627	0.6587	0.6752
	a	-0.2848	-0.2869	-0.2881
	a_1		0.0017	0.0010

TABLE 5. II The diffusion length and extrapolated end-point for the free gas moderator of mass A with $\ell_{\max} = 1$ and absorber concentration β calculated for the separable kernel (S.K.) and the true kernel (T.K.). The parameters a, a_1 and ε are defined by (5.5) and (5.67) to (5.69).

A=8		Arkuszewski (1967) (S.K.)	Present Theory	
			(S.K.)	(T.K.)
$\beta=0.1$	L	1.8975	1.8948	1.9486
	z'_0	0.6834	0.6782	0.6850
	a	-0.4866	-0.4888	-0.4951
	a_1		0.0004	0.0002
$\beta=0.2$	L	1.3502	1.3472	1.4213
	z'_0	0.6969	0.6905	0.7041
	a	-0.3562	-0.3588	-0.3713
	a_1		0.0005	0.0002
$\beta=0.3$	L	1.1106	1.1073	1.1952
	z'_0	0.7162	0.7082	0.7270
	a	-0.2753	-0.2783	-0.2962
	a_1		0.0006	0.0001

TABLE 5. III

The diffusion length and extrapolated end-point for the free gas moderator of mass A with $\ell_{\max} = 1$ and absorber concentration β calculated for the separable kernel (S.K.) and the true kernel (T.K.). The parameters a, a_1 and ϵ are defined by (5.5) and (5.67) to (5.69).

A=12		Arkuszewski (1967) (S.K.)		Present Theory (S.K.) (T.K.)	
		$\beta=0.0$	z_0^t ε	0.6851 0.0006	
$\beta=0.1$	L	1.9125	1.9071	1.9845	
	z_0^t	0.6928	0.6857	0.6927	
	a	-0.4845	-0.4872	-0.4975	
	a_1		0.0003	0.0001	
$\beta=0.2$	L	1.3601	1.3550	1.4591	
	z_0^t	0.7051	0.6965	0.7099	
	a	-0.3546	-0.3577	-0.3779	
	a_1		0.0004	0.0001	
$\beta=0.3$	L	1.1181	1.1131	1.2335	
	z_0^t	0.7232	0.7127	0.7296	
	a	-0.2743	-0.2779	-0.3064	
	a_1		0.0006	0.0001	

TABLE 5. IV

The diffusion length and extrapolated end-point for the free gas moderator of mass A with $\ell_{\max} = 1$ and absorber concentration β calculated for the separable kernel (S.K.) and the true kernel (T.K.). The parameters a, a_1 , and ε are defined by (5.5) and (5.67) to (5.69).

CHAPTER 6

FURTHER APPLICATIONS OF THE GREEN'S FUNCTION APPROACH

§6.1 Introduction

In this last chapter we consider two more problems which may be treated by a modified form of the variational principle based on the Green's function technique which has been discussed in the preceding chapters. We find that we may obtain a useful expression for the extrapolation length for the Milne problem which takes account not only of capture but fission too (although the theory is still restricted to isotropic scattering). Then we return to the theory outlined in Chapter 5 to discuss how one might introduce anisotropic scattering into the theory for the "Milne problem with capture".

Finally we indicate a possible line of future research with the Green's function method and the difficulties we expect to have to overcome - this concerns a problem in a more complicated but more realistic geometry, namely the infinite slab. While none of these problems is treated in any great detail we are able to obtain some physical insight into these systems and demonstrate the particular difficulties which are encountered with each of them.

§6.2 The Thermal Neutron Milne Problem with Capture and Fission

In the Milne problems analysed in the preceding chapters we considered a semi-infinite moderator in which a stationary distribution of neutrons is maintained by a source, at a large distance from the boundary, in thermal equilibrium with the moderator. However a stationary distribution may also be sustained by fission, that is by fuel in such a concentration as to make the system just critical. In that case the transport equation becomes:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \Psi(z, \mu, E) = \frac{1}{2} \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi_0(z, E') + \frac{1}{2} \chi^*(E) \int_0^{\infty} v_{\infty}(E') \Sigma_f(E') \Psi_0(z, E') dE' \quad (6.1)$$

where we have assumed isotropic scattering. $\ell(E)$ is the total mean free path for scattering and absorption, $\Sigma_f(E)$ is the cross-section for fission and $v_{\infty}(E)$ is the number of neutrons produced as the result of fission by an incident neutron of energy E . $\chi^*(E)$ is given by:

$$\chi^*(E) = \chi(E)[1-\beta] + \chi_1(E) \beta \quad (6.2)$$

where $\chi(E)$, $\chi_1(E)$ are the normalised fission spectra of the prompt and delayed neutrons respectively and β is the total fraction of delayed neutrons. We shall adopt the abbreviation:

$$\Sigma_0^*(E' \rightarrow E) = \Sigma_0(E' \rightarrow E) + \chi^*(E) v_{\infty}(E') \Sigma_f(E') \quad (6.3)$$

with the result that the transport equation may be rewritten

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \Psi(z, \mu, E) = \frac{1}{2} \int_0^{\infty} dE' \Sigma_0^*(E' \rightarrow E) \Psi_0(z, E') . \quad (6.4)$$

The same boundary condition applies:

$$\Psi(0, \mu, E) = 0 \quad 0 < \mu \leq 1 \quad (6.5)$$

while asymptotically the flux has the form:

$$\Psi(z, \mu, E) \sim \Psi_{\text{asy}}(z, \mu, E) = \frac{1}{2} \left[z + z_0(E) - \mu \ell(E) \right] \Phi(E) \quad (6.6)$$

but now $\Phi(E)$ must satisfy the equation

$$\frac{\Phi(E)}{\ell(E)} = \int_0^{\infty} dE' \Sigma_0^*(E' \rightarrow E) \Phi(E') . \quad (6.7)$$

Equation (6.7) is in a sense an eigenvalue equation in which the fuel concentration replaces the criticality factor as the eigenvalue in question. Only if (6.7) has a solution for a particular fuel concentration will the system be critical and the asymptotic flux take the form (6.6). For real moderators $z_0(E)$ will again be independent of energy and represent the extrapolation length appropriate to this problem. Boffi et al (1962) have extended Nelkin's variational principle (Nelkin 1960b) to provide an estimate of z_0 through a trial function for the flux which does not take account of the transient flux close to the boundary. Naturally this method still suffers from the fact that when there is no capture (and consequently no fission) it does not give the correct values of z_0 in the two limiting cases of §4.3.

Following the procedure adopted by Boffi et al we define a quantity $L(z)$:

$$L(z) = \int_0^{\infty} dE \Phi^+(E) \int_{-1}^{+1} d\mu \mu \Psi(z, \mu, E) \quad (6.8)$$

and similarly

$$K(z) = \int_0^{\infty} dE \Phi^+(E) \ell(E) \int_{-1}^{+1} d\mu \mu^2 \Psi(z, \mu, E) \quad (6.9)$$

where $\Phi^+(E)$ must be a solution of:

$$\frac{\Phi^+(E)}{\ell(E)} = \int_0^{\infty} dE' \Sigma_0^*(E \rightarrow E') \Phi^+(E') \quad (6.10)$$

Following the usual well-established procedures we find that:

$$L(z) = L = \bar{\ell}/3 \quad (6.11)$$

and

$$K(z) = \frac{\bar{\ell}}{3} (z + z_0) \quad (6.12)$$

where now

$$\bar{x} = \int_0^{\infty} dE \Phi(E) \Phi^+(E) x(E) \quad (6.13)$$

We write the transport equation in the form:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \Psi(z, \mu, E) = \frac{1}{2\ell(E)} \Psi_0(z, E) + \frac{1}{2} S_0(z, E) \quad (6.14)$$

$$S_0(z, E) = \int_0^{\infty} dE' \Sigma_0^*(E' \rightarrow E) \Psi_0(z, E') - \frac{\Psi_0(z, E)}{\ell(E)} \quad (6.15)$$

and notice that asymptotically $S_0(z, E)$ tends to zero. The "source term" is therefore denoted by $s_0(z, E)$ to indicate that it depends only on the transient part of the flux $\phi_0(z, E)$ defined by:

$$\Psi_0(z, E) = \Psi_{0, \text{asy}}(z, E) + \phi_0(z, E) \quad (6.16)$$

Thus the transport equation may be written in the usual way in terms of the one-speed Green's function for an isotropic source in a non-capturing medium:

$$\Psi_0(z, E) = \Phi(E) \rho(z, \ell(E)) + \int_0^{\infty} dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E)) \quad (6.17)$$

where, now

$$s_0(z, E) = \frac{\phi_0(z, E)}{\ell(E)} - \int_0^{\infty} dE' \Sigma_0^*(E' \rightarrow E) \phi_0(z, E') \quad (6.18)$$

Asymptotically (6.17) becomes:

$$\Phi(E) \left[z + z_0 \right] = \Phi(E) \left[z + c\ell(E) \right] + \frac{3}{\ell(E)} \int_0^{\infty} dz' s_0(z', E) \rho_0(z', \ell(E)) \quad (6.19)$$

Inserting (6.19) into (6.9) for $K(z)$ we obtain an expression for the extrapolation length:

$$z_0 = \frac{\overline{c\ell^2}}{\ell} + \frac{3}{\ell} \int_0^\infty dE \Phi^+(E) \int_0^\infty dz s_0(z,E) \rho_0(z,\ell(E)). \quad (6.20)$$

Before writing down a functional for a variational principle which will provide us with an estimate for the last term in (6.20) we should introduce the adjoint flux $\Psi_0^+(z,E)$. This satisfies the transport equation:

$$\left[-\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \Psi^+(z,\mu,E) = \frac{1}{2} \int_0^\infty dE' \Sigma_0^*(E \rightarrow E') \Psi_0^+(z,E') \quad (6.21)$$

with the boundary condition:

$$\Psi^+(0,-\mu,E) = 0 \quad 0 < \mu \leq 1. \quad (6.22)$$

Defining the adjoint transient flux $\phi^+(z,E)$ similarly to (6.16) we see that the adjoint flux may also be written in terms of the Green's function:

$$\Psi_0^+(z,E) = \Phi^+(E) \rho_0(z,\ell(E)) + \int_0^\infty dz' s_0^+(z',E) \rho_{00}(z' \rightarrow z; \ell(E)) \quad (6.23)$$

with

$$s_0^+(z,E) = \frac{\phi_0^+(z,E)}{\ell(E)} = \int_0^\infty dE' \Sigma_0^*(E \rightarrow E') \phi_0^+(z,E'). \quad (6.24)$$

One can now write down a functional (Rowlands 1961)

$$\begin{aligned} \mathbf{z}_0 \left[\phi_0(z, E); \phi^+(z, E) \right] = & \int_0^\infty dE \int_0^\infty dz \left\{ s_0(z, E) \Phi^+(E) \rho_0(z, \ell(E)) + s_0^+(z, E) \Phi(E) \rho_0(z, \ell(E)) \right. \\ & \left. + s_0^+(z, E) \phi_0(z, E) + s_0^+(z, E) \int_0^\infty dz' s_0(z', E) \rho_{00}(z' \rightarrow z; \ell(E)) \right\} \quad (6.25) \end{aligned}$$

which is stationary when $\phi_0(z, E)$ and $\phi^+(z, E)$ satisfy (6.17) and (6.22) respectively and which then reduces to the last term in (6.20).

In the capture-free case without fission a great deal of simplification is possible since the adjoint is simply related to the flux itself; i.e.

$$\Psi_0(z, E) = M(E) \Psi_0^+(z, E) \quad (6.26)$$

but no simple relationship exists here. We therefore require trial functions for $\phi_0(z, E)$ and $\phi^+(z, E)$.

This is not the only drawback. In order to determine $\Phi(E)$ and $\Phi^+(E)$, for example, we have to solve (6.7) and (6.10). Previously, in solving equations of this type we have been able to neglect energies greater than a few electron-volts and adopt a 'multipoint' approach for a restricted energy range (say from 10^{-3} to 3 eV). In this case the energy range considered must be far greater, extending from fission to thermal energies: consequently the overall effort expended on purely numerical calculations would be far greater. While there has been little or no work done on the analytic solution of these equations it has been suggested (Williams 1966, p.510) that polynomial expansion methods could only be applied in a restricted energy range and the most useful approach might be through synthetic kernels.

The fact remains that while it is possible to write down a solution to this problem in principle the difficulties in obtaining numerical results will be greater than we have previously encountered.

§6.3 The Milne Problem with Anisotropic Scattering and Capture

In this section we extend the considerations of Chapter 5 to suggest a number of ways in which one might incorporate anisotropic scattering effects into the thermal neutron Milne problem with capture. The theory is not described in detail because the algebra soon becomes unwieldy. In any case it is unlikely that the spectra which we have determined for water moderators will be significantly altered by the relatively small neutron capture cross-sections of pure water.

For the present, in order to retain some degree of simplicity, we consider only the transport approximation in which we set $\Sigma_1(E \rightarrow E') = \Sigma_1(E) \delta(E - E')$: then the transport equation with capture becomes:

$$\left[\mu \frac{\partial}{\partial z} + \frac{1}{\ell(E)} \right] \psi(z, \mu, E) = \frac{c(E)}{2\ell(E)} \psi_0(z, E) + \frac{3}{2} \mu \Sigma_1(E) \psi_1(z, E) + \frac{1}{2} S_0(z, E) \quad (6.27)$$

where

$$S_0(z, E) = \int_0^{\infty} dE' \Sigma_0(E \rightarrow E') \psi_0(z, E') - \frac{c(E)}{\ell(E)} \psi_0(z, E) \quad (6.28)$$

and $c(E)$ is determined, in the usual way, by the fact that the appropriate one-speed solution should have the same asymptotic spatial dependence as $\psi(z, \mu, E)$, namely $e^{z/L}$ where L is the diffusion length.

Equation (6.27) may be treated as a one-speed equation with capture and linearly anisotropic scattering and an isotropic source $S_0(z,E)$. The choice of $c(E)$ prescribed above implies also that the asymptotic part of $S_0(z,E)$ is zero so that we may write:

$$\psi(z,\mu,E) = N(E) \rho^A(z,\mu,\ell_t(E),L) + \int_0^\infty dz' S_0(z',E) \rho_{00}^A(z' \rightarrow z, \mu; \ell_t(E), L) \quad (6.29)$$

and $N(E)$ will be equal to unity.

We still have to find useful expressions for the Green's function in (6.29). It may be possible to extend the derivation of $\rho_{00}(z' \rightarrow z; \ell, L)$ in terms of $\rho_{q_0}(z, \ell, L)$ to include anisotropic scattering: following the alternative derivation of Elliott (1955) it is certainly possible to write $\rho_{00}^A(z' \rightarrow z, \ell_t, L)$ in terms of $\rho_{00}^A(0 \rightarrow z; \ell_t, L)$ but we have not been able to establish a relationship between $\rho_{00}^A(0 \rightarrow z; \ell_t, L)$ and $\frac{\partial}{\partial z} \rho_{q_0}^A(z, \ell_t, L)$ corresponding to (3.21) or, indeed, any other simple relationship of this sort.

A closed expression for the Green's function has been outlined by Mika (1961) by means of a modified version of Case's method but, as we have come to expect of this approach, the result is fairly involved and is not easily incorporated into a practical numerical treatment of the variational principle. But at least we shall be able to obtain a very good approximation to the parameter a through a prescription similar to (5.70): we require only the one-speed equivalent $a \left(\ell(E)/L \right)$ which has been determined by a number of authors (e.g. Davison 1946) and the infinite medium solutions of the transport equation.

As we have seen before the alternative is to consider (6.27) as a one-speed equation with isotropic scattering and two sources. In that case the appropriate isotropic Green's functions and their angular moments may be determined by a recurrence relationship similar to that given in §3.3 but, unfortunately, they no longer possess a simple analytical form. For example we might compare:

$$\rho_{01}(z' \rightarrow z; \ell, L) = \frac{(1-c)}{\ell} \int_z^{\infty} \rho_{00}(z' \rightarrow z^+, \ell, L) dz^+ \quad (6.30)$$

with the simple expression (3.30) for the capture-free case.

Once again $c(E)$ is chosen to give the correct asymptotic spatial dependence but now there will be contributions from the asymptotic parts of $S_0(z, E)$ and $\psi_1(z, E)$ so that the normalisation factor $N(E)$ will no longer be equal to unity. In principle, however, as long as we can evaluate terms of the form:

$$\int_0^{\infty} dz' S_{0 \text{ asy}}(z', E) \rho_0(z', \ell(E), L) \quad \text{and} \quad \int_0^{\infty} dz' \psi_{1 \text{ asy}}(z', E) \rho_1(z', \ell(E), L)$$

which determine $N(E)$ and which occur if we follow the procedure described in §5.3 or §5.4, we expect to obtain an expression for the parameter a which may be estimated by a variational principle. Such integrals will not be trivial: moreover the complicated form of the Green's functions such as (6.30) soon makes the algebra intractable. Therefore we shall not consider the details of this approach further. The fact remains that the method could, in principle, be extended to account for a general $\Sigma_1(E \rightarrow E')$ kernel also.

If, instead, we look for approximate methods of tackling this problem we might decide to take account of the neutron capture exactly and approximate the anisotropy in the scattering. That being the case we are faced with two possibilities: either to approximate $\Sigma_n(E \rightarrow E')$ for $n \geq 1$ or to retain the correct anisotropy in the energy dependent equations and approximate the anisotropic one-speed Milne solutions and Green's functions.

Very little systematic work has been done in the first category besides the work of Pomraning (1966) who suggests approximations for all orders of anisotropy. We expect linearly anisotropy to be sufficient for most moderators and since our theory (including neutron capture) has only been worked out in detail for isotropic scattering we are wanting approximations which account for P_1 scattering in terms of an isotropic scattering kernel. Two ways have been suggested by Honeck (1964): in the first he assumed that:

$$\Sigma_{tr}(E' \rightarrow E) = \Sigma_0(E' \rightarrow E) - \Sigma_1(E' \rightarrow E) \quad (6.31)$$

where $\Sigma_{tr}(E' \rightarrow E)$ is the suitably adjusted isotropic kernel but this was shown to introduce significant errors due to the alteration of the off-diagonal elements. In another he suggested:

$$\Sigma_{tr}(E' \rightarrow E) = \Sigma_0(E' \rightarrow E) - \Sigma_1(E) \delta(E - E') \quad (6.32)$$

and found that for situations in which there are no strong spatial gradients this is generally satisfactory.

This approximation forms the basis of what is commonly known as the transport approximation which, for the present, we distinguish from that of §4.5. This approximation assumes a strong forward scattering and is only defined within the context of P_1 theory which takes no account of transient effects close to boundaries. Even in P_1 theory the approximation is only valid under certain conditions on the current or the kernel $\Sigma_1(E' \rightarrow E)$: if, for example, $\Sigma_1(E' \rightarrow E) = \Sigma_1(E) \delta(E - E')$ the transport approximation is justified within the limitations of P_1 theory and it is for this reason that, for want of a better name, we refer to the simplification of §4.5 by the same name.

In the present problem boundary effects are important causing strong spatial gradients and this treatment may lead to serious errors in some cases. However our experience in the no-capture case suggests otherwise and some recent work by Dorning (1967) in calculating decay constants and the integrated flux in small systems which are dominated by leakage tends to support this contention.

Another approximation which has been suggested (Michael 1966) is to simply replace $\Sigma_s(E)$ by the transport cross-section $\Sigma_s(E) \rightarrow \Sigma_1(E)$ and assume isotropic scattering. This approximation has enjoyed widespread use in one-speed theory where it predicts the diffusion length correctly for small absorption. Thus we might account for anisotropy in the one-speed solutions through this approximation. However, in general, it leads to rather poor results (Davison 1957, p241) due to the over-emphasis attached to the forward scattering.

§6.4 The Time Dependent Slab Problem

Lastly we mention a problem which has occupied our attention more recently, namely the possible application of the 'Green's function method' to the theory of pulsed neutron experiments in which we investigate the behaviour in time of a burst of neutrons injected into a finite assembly. Thus instead of the ideal infinite half-space geometry we consider now the more realistic but more complex infinite slab. We are especially interested in finding the asymptotic form of the flux, existing in the medium long after the original pulse, which is assumed to have the form:

$$\Psi(z, \mu, E, t) = \Psi(z, \mu, E) e^{-\lambda t} \quad (6.33)$$

where λ is the asymptotic time decay constant.

We confine our attention to a source-free infinite slab of finite thickness $2d$ (along the z axis) with the origin of the co-ordinate system at the centre of the slab. Assuming isotropic scattering, the transport equation for the time-asymptotic flux becomes:

$$\left[\mu \frac{\partial}{\partial z} + \Sigma(E) - \frac{\lambda}{v} \right] \Psi(z, \mu, E) = \frac{1}{2} \int_0^{\infty} dE' \Sigma_0(E' \rightarrow E) \Psi_0(z, E') \quad (6.34)$$

with

$$\Sigma(E) = \Sigma_s(E) + \Sigma_a(E) . \quad (6.35)$$

The time dependence is contained in the term $-\lambda/v$ which arises if we consider the first term on the left hand side of the general transport equation (1.1). We are interested mainly in the lowest eigenvalue λ although this does not preclude the possibility of a solution of (6.34) for higher eigenvalues λ_n .

Since the slab is surrounded by a vacuum no neutrons enter the surface from outside and the boundary conditions are therefore:

$$\begin{aligned}\Psi(-d, \mu, E) &= 0 & 0 < \mu \leq 1 \\ \Psi(d, \mu, E) &= 0 & -1 \leq \mu < 0.\end{aligned}\tag{6.36}$$

Our aim is to find the form of the emergent flux $\Psi(\pm d, \mu, E)$ and the corresponding time constant λ . We note that we may assume the medium to be purely scattering since if the absorption follows the $1/v$ law it will not affect the neutron distribution: the effect of capture will simply be to change the time constant λ by an amount $v \Sigma_a(E) = \text{constant}$. Furthermore we might formally treat (6.34) as the transport equation for a stationary system in which the total cross-section has been reduced by the fictitious capture λ/v . A much fuller description of the basic theory has been given by a number of authors (e.g. Williams 1966, p158): here we do no more than briefly mention the essential steps for a meaningful discussion of the possible application of the Green's function approach.

It is customary to start by seeking a solution of (6.34) corresponding to an infinite medium with an ansatz:

$$\Psi_{\text{asy}}(z, \mu, E) = M(E) g(E, \mu) e^{-iBz}\tag{6.37}$$

where B^2 is commonly referred to as the buckling of the system.

Inserting (6.37) into (6.34) we obtain an eigenvalue equation between B and $g(E, \mu)$:

$$\left[\Sigma^*(E) - iB\mu \right] g(E, \mu) = \frac{1}{2} \int_0^\infty dE' \Sigma_0(E \rightarrow E') g_0(E') \quad (6.38)$$

where

$$\Sigma^*(E) = \Sigma(E) - \lambda/v. \quad (6.39)$$

Such solutions exist in pairs, the other being $M(E) g(E, -\mu) e^{iBz}$.

Thus the first problem is to find the relationship between B and the slab thickness $2d$.

Once again one may define the extrapolated end-point. It is assumed that the slab is sufficiently thick for there to be a central region where the asymptotic solution is dominant; in that case because of the symmetry of the problem:

$$\chi_{asy}(z) = \int_0^\infty dE \int_{-1}^{+1} d\mu \Psi_{asy}(z, \mu, E) \quad (6.40)$$

will have the spatial dependence $\text{Cos } Bz$. Then the extrapolated end-point z'_0 is defined as the distance beyond the boundary of the slab at which the asymptotic integrated flux, if extrapolated across the boundary, would fall to zero: i.e.

$$B = \frac{\pi}{2(a+z'_0)} \quad (6.41)$$

A more rigorous definition which does not depend on the dominance of the asymptotic flux within the slab has been given by Kladnik (1965) in terms of an integral condition analogous to those described in §5.4. There may well be some interesting effects to be accounted for in this

context: for example it is expected that the extrapolated end-point will decrease with increasing B^2 (that is decreasing slab thickness) but then, in order to explain some experimentally observed effects, it must rapidly increase for high bucklings (Beckurts 1965).

Kladnik (1965) has developed a variational principle for this problem which provides an estimate of z_0^{\dagger} but unfortunately, for the trial function used, the leakage spectra at near grazing angles are not in agreement with experiment (Kallfelz and Reichardt 1965). The inclusion of more involved trial functions in Kladnik's variational method will not be easily achieved in this geometry and an extension of the variational principle described in the preceding chapters to cope with slab geometries becomes desirable.

We ought to mention first that the pulsed neutron problem is complementary to the diffusion length problem in the sense that if we plot a graph of λ versus B^2 this should be analytically continued for negative B^2 by the graph of β versus $1/L_0^2$. This is depicted in Figure 6.I. Until the work of Arai and Kuchle (1965) with a source decaying exponentially with time it was thought that the upper left quadrant was inaccessible to experiment. Now it is clear that the analytic continuation is complete. The analogue of the maximum absorption theorem described in Chapter 2 is that the time decay constant λ will disappear as the slab thickness is decreased (Albertoni and Montagnini 1965 -- see also other papers in this conference and the references cited therein). Thus for thin slabs there may not be an asymptotic exponential decay of the flux with time. Just as, in the

Milne problem, we had to restrict our attention to those situations in which the diffusion length exists so now we expect to be limited to situations in which λ exists.

In attempting to write the transport equation (6.34) in terms of the corresponding one-speed solutions and Green's functions and subsequently to write down a variational principle we meet a number of difficulties which we have been unable to resolve so far.

In retrospect it is clear that the appropriate choice of one-speed solutions was largely determined by the asymptotic spatial dependence of the energy dependent flux, that is by the boundary condition at infinity. For finite slab geometries we do not expect the asymptotic behaviour to attain such importance. After all the system does not extend to infinity except in the transverse directions and for small enough slabs the asymptotic behaviour may not dominate at any point in the slab, even in the centre. Furthermore the parameters z_0 and a appeared naturally in the half-space problems as the coefficients relating the two possible asymptotic solutions. When the boundary conditions at $z = \pm d$ are imposed for the slab problem the symmetry of the situation automatically determines the weightings to be attached to the two solutions $g(E, \mu) e^{-iBz}$ and $g(E, -\mu) e^{iBz}$ and it is difficult to see how a parameter analogous to z_0 or a might arise. In fact we do not know, at present, what parameter we might hope to be able to determine directly from the Green's function approach although ultimately we expect to estimate a quantity closely related to the extrapolated end-point.

We might therefore expect the one-speed solution to be determined by the boundary conditions at the surface of the slab. We are then faced with two equally unpleasant alternatives or so it appears. If we choose one-speed solutions appropriate to the same size of slab (always of thickness $2d$) this implies a different value of the buckling $B^2(E_i)$ for each energy point E_i in the range of interest and we should have to perform some averaging process to obtain the correct asymptotic spatial dependence e^{iBz} . On the other hand if we were to assume one-speed solutions with the asymptotic spatial dependence of the energy dependent flux this would imply that we were dealing with one-speed solutions appropriate to a range of slab thicknesses and, even more important, a range of time decay constants. Again some averaging process would be required to obtain the correct asymptotic dependence $e^{-\lambda t}$.

Of course we are also faced with the difficulty that there are no useful expressions for the Green's functions in slab geometry. However these might be obtained by means of a theorem described by Case et al (1953) and again by Hendry (1967) which states that a finite medium problem may be transformed to an infinite medium problem by imposing suitable sources in the positions of the original boundaries. These sources will involve the emergent flux at the boundaries which is, as yet, unknown but the work of Hendry suggests that one might still make use of this theorem by an iterative technique.

It must be admitted that the picture is confusing at present. The main difficulty lies in knowing the correct choice of one-speed solution.

But we have seen in previous chapters that the correct choice of one-speed solution will provide, by means of an appropriate average, a very accurate estimate of a parameter of great practical importance such as the extrapolation length without invoking the Green's functions explicitly or the variational principle. We are hopeful that a similar relationship exists here.

§6.5 Conclusion

In the bulk of this thesis we have been mainly concerned with the application of the Green's function approach to the thermal neutron Milne problem in its various forms and in the course of this work it has become apparent that we have in our hands a powerful method for tackling this problem. In this last chapter, we have also looked at a number of more complex situations with some degree of success.

We would like to conclude by saying that we believe that the potential of this method is not limited to situations having Milne problem characteristics. A great deal of work has already been done on a large number of one-speed problems and it is possible that if we could decide how to choose the appropriate one-speed solution in each case (this difficulty is discussed in §6.4 for the time dependent slab problem) a whole range of other energy dependent problems might be investigated by this method.

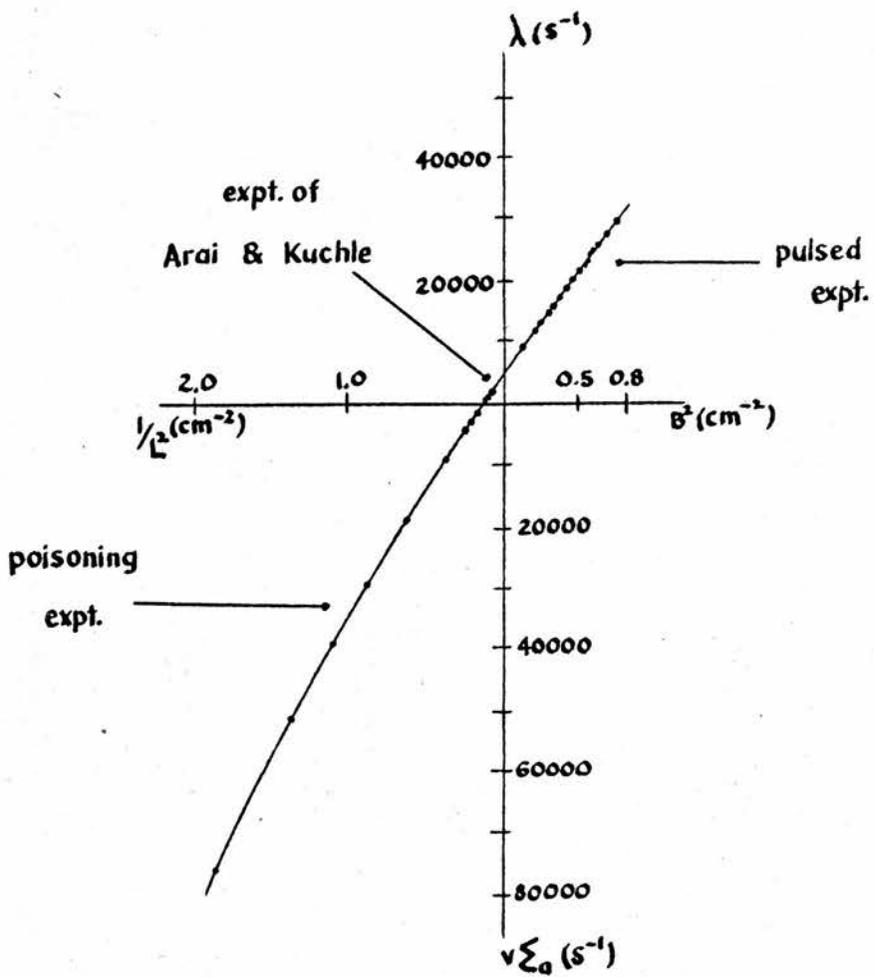


FIG. 6·I

The curve of λ versus B^2 analytically continued to negative B^2

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