THERMAL NEUTRON DISTRIBUTIONS NEAR MATERIAL DISCONTINUITIES

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ABSTRACT

A method is presented for the approximate calculation of the neutron flux near plane interfaces between different heavy monatomic gaseous media with absorption cross sections inversely proportional to the neutron velocity. Approximate analytic results are obtained for both the diffusion theory and transport theory models. It is found that the flux on each side of the interface can be approximated by the sum of two terms. One term has the same energy dependence that would exist in an infinite medium composed of the heavy monatomic gas that is on that side of the interface. The spatial dependence of this term is determined by diffusion theory. The other term, called a boundary layer correction, makes an appreciable contribution to the flux only near the interface. The procedure presented develops equations and boundary conditions which determine the different terms of the approximate flux. It is found that the approximate flux at the interface, for both diffusion and transport theory, is the average of the two infinite medium fluxes.

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I. INTRODUCTION

The primary task of reactor physics is to calculate the neutron density distribution within a given region of space containing specified materials. From a detailed description of the neutron density distribution all quantities (multiplication, reaction rates, etc.) necessary for the design of a reactor can be calculated. In general,the neutron density distribution depends on the neutron energy, the direction of neutron travel, the position in space, and time. In elementary energy-dependent problems the nucleus is assumed at rest before a collision, so that a neutron only loses energy in a collision with the nucleus. This is a valid approximation provided that the neutron energy is much greater than the average energy of the nucleii.

When the neutron energy is comparable to the average nuclear energy of motion, a different assumption must be made, because a neutron can either gain or lose energy in a collision with a moving nucleus. Neutron thermalization theory accounts for this nuclear motion. The effect of the nuclear motion is most important for neutrons with energies less than 1 ev (electron volt). The average energy of the nucleii is about 0.025 ev.

If neutrons of an arbitrary energy distribution are introduced into an infinite, homogeneous, non-absorbing medium, the resulting equilibrium distribution (after a sufficiently long time) would be a Maxwellian distribution characterized by the temperature of the medium. In a finite, inhomogeneous, or absorbing system the steady state neutron distribution will differ from a Maxwellian distribution. (For finite or absorbing systems there must be a source of neutrons to balance neutron losses if a steady state is to be maintained.) If the medium is finite or inhomogeneous the neutron distribution differs from a Maxwellian distribution because of the transport of neutrons out of the system or transport of neutrons between different regions of the system. Absorption further complicates the problem because of the finite time required for source neutrons to attain an equilibrium distribution.

Many authors consider the problem of an infinite homogeneous medium with a prescribed nuclear speed distribution. By using an elastic billiard ball model for a collision between a neutron and a nucleus and assuming isotropic scattering in the center of mass system, they are able to calculate the energy exchange cross sections needed to solve the neutron balance equation.

Wigner and Wilkins (1) considered the nucleii as a monatomic gas with a Maxwellian speed distribution. They numerically solved for the neutron density in an infinite medium composed of hydrogen with an absorption cross section inversely proportional to the neutron velocity. Wilkins (2) later reduced the balance equation to an approximate differential equation for a heavy monatomic gas.

Lathrop (3) considered two nuclear speed distributions using a harmonic oscillator model. One model used was a single energy oscillator, and the other assumed a distribution of oscillator energies. The neutron density was determined numerically in both cases.

More recent efforts have attempted to take into account spatial variations in nuclear properties. Kottwitz (4) solved for the neutron density in two semi-infinite half spaces consisting of non-absorbing heavy monatomic gases at different temperatures by using diffusion theory for the spatial transport of neutrons. Later papers (5-7) extended this application of diffusion theory to slab, cylindrical, and spherical geometries and to problems with absorption.

In these papers (4-7) the diffusion theory equation is solved by the separation of variables method which results in an eigenfunction expansion for the neutron density in each region. Then the coefficients of the eigenfunction expansions are determined by the interface conditions. This results in a recursion relation for the coefficients, in which the nth coefficient depends on the first n-1 coefficients. Hence,the coefficients may not be solved for explicitly. This yields rather cumbersome expressions for the neutron density although they are adaptable for machine calculations.

Ferziger and Leonard (8) used the one-dimensional transport equation, but they assumed constant cross section and isotropic scattering in the laboratory system. Bednarz and Mika (9) considered the one-dimensional transport problem and specialized to a fully degenerate scattering kernel. The assumption of constant cross section is unrealistic, particularly for the absorption cross section. It is better to assume isotropic scattering in the center of mass system than in the laboratory system. A fully degenerate scattering kernel is a very specialized case; none of the physical scattering models proposed up to the present time have this property.

Zelazny (10) uses the heavy gas scattering kernel and transport theory but assumes constant cross section. Again the assumption of constant cross section is unrealistic, even the scattering cross section is a function of energy for the heavy gas model (see equation 2). These papers (4-10) are restrictive because of the assumptions of a degenerate kernel, or constant cross section, or diffusion theory.

The analysis of this thesis is limited to steady state neutron distributions in plane geometry with step discontinuities in nuclear properties. The absorption cross section is taken to be inversely proportional to the neutron velocity which is a more realistic assumption than that of constant cross section (11). Such step discontinuities occur at the interface between the core and the reflector of a reactor where there is an abrupt change in the absorption and scattering cross sections. If, in addition, the reactor is gas cooled, the temperature changes very rapidly across the interface between the solid material and the gas coolant.

In this analysis the nucleii are assumed to be a monatomic gas in a Maxwellian energy distribution. Approximate analytic results are obtained for the case of heavy gases. Aamodt et al. (12) have shown that, regardless of the state of the material, the scattering kernel at high neutron energies approaches that of a heavy gas. Therefore, the assumption of a heavy monatomic gas implies that the results obtained in this thesis should be more accurate at high neutron energies, high energies being those greater than the temperature (measured in energy units) multiplied by the ratio of neutron to nuclear mass.

Throughout the thesis the neutron flux, which is the neutron density times the neutron velocity, shall be used as the dependent variable. For plane geometry, the neutron flux will be a solution of the time-independent, one-dimensional, linearized Boltzmann (or transport) equation:

$$\mu \frac{\partial\varphi(z, E, \mu)}{\partial z} + \left\{\sigma_s(E, z) + \sigma_a(E, z)\right\} \varphi(z, E, \mu)$$
$$= \int_0^{\infty} dE' \int_{-1}^{+1} d\mu' \; \sigma_s(E', \mu' \rightarrow E, \mu; z)\varphi(z, E', \mu') + S(z, E, \mu) \; , \quad (1)$$

together with appropriate boundary conditions. The symbols are:

z = spatial dimension

E = neutron energy

μ = cosine of the angle between the z axis and the direction of neutron travel

$\varphi(z, E, \mu)$ = angular neutron flux at z, E, and μ

$\sigma_a(E, z)$ = absorption cross section at E and z

$\sigma_s(E, z)$ = scattering cross section at E and z

$\sigma_s(E', \mu' \rightarrow E, \mu; z)$ = energy transfer cross section for neutrons going from E' and μ' to E and μ at z

$S(z, E, \mu)$ = independent source strength of neutrons at z, E, and μ.

The left-hand side of equation 1 represents the neutron loss from a volume element $dz\, dE\, d\mu$. The first term is the loss due to the spatial transport out of the volume element; and the second term, the loss due to collisions which remove a neutron from the volume element. The right-hand side represents the neutron gain into the volume element. The first term is the gain due to scattering collisions at z which result in neutrons with energy E going in direction μ. The second term represents the independent sources of neutrons. The source term may be omitted from the equation and instead imposed as a boundary condition.

The scattering cross section is related to the energy transfer cross section* by:

$$\sigma_s(E, z) = \int_0^{\infty} dE' \int_{-1}^{+1} d\mu' \; \sigma_s(E, \mu \rightarrow E', \mu'; z) \quad . \tag{2}$$

Thus $\sigma_s(E, \mu \rightarrow E', \mu'; z)\, dE'\, d\mu' / \sigma_s(E, z)$ is the probability that a neutron with energy E and direction μ will be scattered into the interval dE' about E' and $d\mu'$ about μ' at z.

For a monatomic gas in a Maxwellian distribution characterized by temperature T (measured in energy units), the energy transfer cross section is:

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*It is common to use σ_s for both cross sections, the difference being distinguished by the arguments. All cross sections are macroscopic cross sections measured in units cm^{-1}.

$$\sigma_s(E', \mu' \to E, \mu; z) = \frac{\sigma}{8\pi^2}\left(1+\frac{1}{m}\right)^2\left(\frac{E}{E'}\right)^{1/2}\int_{-\infty}^{\infty} dt \int_0^{2\pi} d\psi \, e^{it(E-E')}$$

$$\cdot \exp\left\{\frac{it-Tt^2}{m}\left(E+E'-2\mu_o(EE')^{1/2}\right)\right\}, \quad (3)$$

where

$$\mu_o = \mu\mu' + \left[(1-\mu^2)(1-\mu'^2)\right]^{1/2} \cos\psi \quad (4)$$

is the cosine of the angle between μ and μ'. The formula assumes elastic collisions between neutrons and nucleii and isotropic scattering in the center of mass of the neutron-nucleus system. (See reference 1 or 13 for a derivation of this formula.) The spatial dependence of the right-hand side of equation 3 is expressed in terms of m, σ, and T where m is the ratio of nuclear to neutron mass and σ is the free atomic scattering cross section. When equation 3 is substituted into equation 2 and the integrations performed, the result is

$$\sigma_s(E, z) = \sigma\left[(1 + T/2mE)\,\mathrm{erf}\,(mE/T)^{1/2} + \frac{e^{-mE/T}}{(\pi mE/T)^{1/2}}\right], \quad (5)$$

where

$$\mathrm{erf}\, x = \frac{2}{(\pi)^{1/2}}\int_0^x e^{-t^2}\, dt. \quad (5a)$$

The diffusion theory approximation may be developed from the transport equation 1 by expanding the angular flux, $\varphi(z, E, \mu)$, and the energy transfer cross section in Legendre polynomials. Using the orthogonality of the Legendre polynomials and retaining only the first two coefficients of the angular flux expansion,* the resulting equations are

$$\frac{\partial j(z,E)}{\partial z} + \left\{\sigma_s(E,z) + \sigma_a(E,z)\right\} \varphi(z,E)$$
$$= \int_0^{\infty} dE' \, \sigma_o(E' \rightarrow E;z) \, \varphi(z,E') \quad , \tag{6}$$

and

$$\frac{1}{3} \frac{\partial \varphi(z,E)}{\partial z} + \left\{\sigma_s(E,z) + \sigma_a(E,z)\right\} j(z,E)$$
$$= \int_0^{\infty} dE' \, \sigma_1(E' \rightarrow E;z) \, j(z,E') \quad , \tag{7}$$

where

$$\varphi(z,E) = \int_{-1}^{+1} \varphi(z,E,\mu) \, d\mu \tag{8}$$

is the flux (to be distinguished from the angular flux $\varphi(z,E,\mu)$ by its argument) and

$$j(z,E) = \int_{-1}^{+1} \mu\varphi(z,E,\mu) \, d\mu \tag{9}$$

is the current. From equation 3 the moments of the energy transfer cross section** are

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*This is equivalent to neglecting all moments of the angular flux higher than the first.

**The Jacobian of the transformation form $d\mu \, d\psi$ to $d\mu_o \, d\psi_o$ is one. The integration over ψ_o may then be done giving 2π.

$$\sigma_\ell(E'\to E;z) = \frac{\sigma}{4\pi}\left(1+\frac{1}{m}\right)^2\left(\frac{E}{E'}\right)^{1/2}\int_{-\infty}^{\infty}dt\int_{-1}^{+1}P_\ell(\mu_o)\,d\mu_o e^{it(E-E')}$$

$$\cdot\ \exp\left\{\frac{it - Tt^2}{m}\left(E + E' - 2\mu_o(EE')^{1/2}\right)\right\}. \quad (10)$$

The set of equations, 6 and 7, may be reduced to an approximate differential equation for the flux, $\varphi(z, E)$, by assuming m to be a large quantity. With this assumption the second exponential in equation 10 may be expanded in a power series of m^{-1}. The resulting terms in the series will be singular, but since the moments of the energy transfer cross section appear only in the integral terms of equations 6 and 7, the singular terms can be interpreted as the delta function and its derivatives. That is

$$\delta^n(E - E') = \frac{1}{2\pi}\int_{-\infty}^{\infty}dt\ (it)^n e^{it(E-E')}\ , \quad (11)$$

where

$$\int_{E-a}^{E+a}\delta^n(E-E')f(E')\,dE' = \left[\frac{d^n}{dE'^n}f(E')\right]_{E'=E}\ , \quad (12)$$

with $a > 0$. With this identification the moments of energy transfer cross section become

$$\frac{\sigma_o(E'\to E;z)}{\sigma} = \left(1+\frac{2}{m}\right)\delta(E-E') + \frac{E+E'}{m}\left(\frac{E}{E'}\right)^{1/2}\left\{\delta'(E-E')\right.$$

$$\left. + T\delta''(E - E')\right\} + O\left(\frac{1}{m^2}\right)\ , \quad (13)$$

for $\ell = 0$ and for $\ell = 1$

$$\frac{\sigma_1(E'\rightarrow E;z)}{\sigma} = \frac{2E}{3m}\left\{\delta'(E - E') + T\delta''(E - E')\right\} + O\left(\frac{1}{m^2}\right). \quad (14)$$

A similar expansion of the scattering cross section, equation 5, in powers of m^{-1} yields:

$$\frac{\sigma_s(E, z)}{\sigma} = 1 + \frac{T}{2mE} + O\left(\frac{e^{-mE/T}}{m^{5/2}}\right). \quad (15)$$

The substitution of equations 13, 14, and 15 into equations 6 and 7 and the elimination of the current, $j(z, E)$, between the two equations gives a single equation for the flux:

$$\left\{\frac{1}{3\sigma^2}\frac{\partial^2}{\partial z^2} + \frac{2}{m}\left(ET\frac{\partial^2}{\partial E^2} + E\frac{\partial}{\partial E} + 1 - \frac{m\sigma_a(E, z)}{2\sigma}\right)\right\}\varphi(z, E) = 0. \quad (16)$$

Equation 16 is the diffusion theory equation correct to terms of order m^{-1}. In this equation the diffusion term, $(1/3\sigma^2)(\partial^2\varphi(z, E)/\partial z^2)$, and the absorption term, $(2\sigma_a(E, z)/\sigma)(\varphi(z, E))$, are interpreted as being of order m^{-1}. Also it was assumed that $mE/T \gg 1$, so that the remainder term in the scattering cross section (equation 15) could be neglected.

The geometry considered in this thesis is that of a slab occupying the space from $z = 0$ to $z = -W$, imbedded in an infinite medium. The step discontinuities in nuclear properties are expressed by σ, T, and m each taking different constant values in the slab and in the surrounding medium. In the notation of this thesis the subscript "1" on a quantity will refer to the slab and the subscript "o" will refer to the infinite medium.

With this geometry the boundary condition for transport theory is that the angular flux, $\varphi(z, E, \mu)$, be continuous at the interfaces $(z = 0, -W)$. The boundary conditions for diffusion theory are derived from those of transport theory by taking moments of the interface continuity equation for the angular flux. This requires that the flux, $\varphi(z, E)$, and the current, $j(z, E)$, be continuous at the interfaces. Because the problem is symmetric about $z = -W/2$, the angular flux for transport theory or the flux for diffusion theory will only be determined in the region $z \geq -W/2$.

Specific approximate analytic results are obtained for the case of large m_i $(i = 0, 1)$. The equations for the slab $(i = 1)$ and the surrounding medium $(i = 0)$ are expanded and terms through order m_i^{-1} are kept. To be consistent a similar expansion should be performed on the interface conditions and the higher order terms should again be neglected. This is equivalent to expressing one of m_i's, say m_o, in terms of the other:

$$\frac{1}{m_o} = \frac{1}{m_1} + O\left(\frac{1}{m_1^2}\right) \quad . \tag{17}$$

Therefore, the assumption of large m_i and the approximation of keeping only the first order terms in m_i^{-1}, imply that $m_o = m_1 = m$. Thus, it is consistent with the m^{-1} approximation to assume that m is a constant throughout space. Then for $m \gg 1$ we can be sure that the equations and the interface conditions are satisfied to order m^{-1}.

In Part II the problem is solved using the diffusion theory, represented by equation 16. In Part III the transport equation 1 is solved to order m^{-1}. Part IV contains a discussion of the assumptions and the results.

II. DIFFUSION THEORY

A. Introduction

To illustrate the technique which will be utilized and for comparison reasons, the approximate model based on diffusion theory will be treated first. From part I the diffusion equation for slab geometry in the m^{-1} approximation is the following:

$$\frac{m}{6\sigma_i^2}\frac{\partial^2\varphi_i(z,E)}{\partial z^2} + ET_i\frac{\partial^2\varphi_i(z,E)}{\partial E^2} + E\frac{\partial\varphi_i(z,E)}{\partial E} + \left(1 - \frac{m\sigma_{ai}(E)}{2\sigma_i}\right)\varphi_i(z,E) = 0 \quad , \tag{18}$$

where if $i = 0$ the equation refers to $0 \leq z \leq \infty$ and if $i = 1$ the equation refers to that portion of the slab for which $-W/2 \leq z \leq 0$. The solution in the rest of space is obtained by symmetry about $z = -W/2$.

The equation is made dimensionless with the change of variables

$$\epsilon = \frac{E}{T_o} \quad , \qquad x = \frac{z}{W} \quad . \tag{19}$$

Then equation 18 becomes

$$\left\{\frac{1}{\lambda_o^2}\frac{\partial^2}{\partial x^2} + \epsilon\frac{\partial^2}{\partial\epsilon^2} + \epsilon\frac{\partial}{\partial\epsilon} + 1 - \frac{\Delta_o}{\sqrt{\epsilon}}\right\}\varphi_o(x,\epsilon) = 0 \quad , \tag{20}$$

for $0 \leq x \leq \infty$ and

$$\frac{1}{\lambda_1^2}\frac{\partial^2}{\partial x^2} + \epsilon a_1 \frac{\partial^2}{\partial \epsilon^2} + \epsilon \frac{\partial}{\partial \epsilon} + 1 - \Delta_1 \frac{a}{\epsilon} \quad \varphi_1(x, \epsilon) = 0 \quad , \tag{21}$$

for $-1/2 < x < 0$ where

$$a_i = \frac{T_i}{T_o} \quad , \quad i = 0, 1 \quad , \tag{22}$$

$$\lambda_i = \sigma_i W(6/m)^{1/2} \quad , \quad i = 0, 1 \quad , \tag{23}$$

and, for an absorption cross section inversely proportional to the neutron velocity, Δ_i is a constant given by

$$\Delta_i = \frac{m\sigma_{ai}(E)}{2\sigma_i} (\epsilon/a_i)^{1/2} \quad , \quad i = 0, 1 \quad . \tag{24}$$

For diffusion theory, the flux is to be continuous

$$\varphi_1(0, \epsilon) = \varphi_o(0, \epsilon) \quad , \tag{25}$$

and the current is to be continuous*

$$\frac{1}{\sigma_1}\frac{\partial\varphi_1(0, \epsilon)}{\partial x} = \frac{1}{\sigma_o}\frac{\partial\varphi_o(0, \epsilon)}{\partial x} \quad , \tag{26}$$

for all energies in the range of consideration.

Since the flux is equal to the neutron density multiplied by the neutron velocity, and since the neutron density must remain finite even for zero energy, the flux must be zero at zero energy. The large energy boundary condition will depend on whether or not absorption is present. For the pure scattering case $(\Delta_i = 0)$ there are no neutron losses from the system, consequently a neutron source is not needed and the energy range from zero to

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*For the large mass approximation $D_i = 1/3\sigma_i$ (cf. equation 144, page 57).

infinity is considered. For large energies the flux is to go to zero in such a way that the integral of the flux over all energies exists. If absorption is present, a source must also be present in order to balance the neutron losses and maintain a steady state. This is accomplished by limiting the energy range from zero to some high energy, say ϵ_o, and requiring the flux to equal some fixed distribution at ϵ_o.

In any equation in which a large parameter occurs, some of the terms of the equation may be small in different regions of the space of the independent variables. It may, therefore, be possible to obtain a good approximation to the exact solution to the equation by taking advantage of the fact that the parameter is large. For instance; in equations 20 and 21, λ_i is assumed large and in different regions of the x, ϵ plane some of the terms of the equation are small compared to the remaining terms.

The assumption that λ_i is large implies that the slab width W is much larger than $1/\sigma_i$, which is a measure of the mean free scattering length. Therefore it is expected that several mean free scattering lengths away from the interface, the energy dependence of the flux will be approximately the same as that of an infinite medium. Thus the approximate solution for the flux should be composed of two or more parts on each side of the interface. One will be the infinite medium solution, the rest will be what we might call "boundary layer corrections" near the interface which will blend one infinite medium solution into the other.

The equations and boundary conditions for the several parts of the solution are obtained from the original equations 20 and 21 and the original boundary conditions 25 and 26. This is accomplished by determining which terms of the original equations and boundary conditions are small and where they are small and then neglecting these small terms in the corresponding regions. For this purpose the following procedure is applied.

1. For investigation near the $x = \epsilon = 0$ corner of the x,ϵ plane, the change of variables

$$\xi_i = \lambda_i^{\alpha} x \quad ; \qquad \eta_i = \lambda_i^{\beta} \epsilon \quad , \qquad i = 0, 1 \quad , \tag{27}$$

   is introduced into the corresponding equation 20 (for $i = 0$) or 21 (for $i = 1$) and the boundary conditions 25 and 26. (The subscript i will, in the future, be omitted from ξ, η and λ since the subscript i on the flux, $\varphi_i(\xi, \eta)$, indicates which transformation ($i = 0$ or 1) is meant.)

2. The flux is expanded as

$$\varphi_i(\xi, \eta) = \sum_{n=0}^{\infty} \lambda_i^{-n} \varphi_i^{(n)}(\xi, \eta). \tag{28}$$

3. After the substitution of 27 and 28 into equations 20 and 21 and boundary conditions 25 and 26, coefficients of equal powers of λ are equated to zero. The equations thus obtained will clearly depend on the choice of α and β.

From the transformation 27 it is seen that for a fixed value of ξ and positive α that as λ goes to infinity x becomes smaller. For a fixed value of ξ and negative α, as λ goes to infinity x becomes larger. Therefore the equations derived for positive α should be approximately valid for small x; and the equations for negative α should be approximately valid for large x. (Note that these arguments are valid for the $x = 0$ interface only. To investigate the $x = -1$ interface the transformation $\xi = \lambda^{\alpha}(x+1)$ should be used instead of 27; and arguments similar to those above would be reapplied to this interface.) A similar physical interpretation can be given for the equations derived for positive and negative β.

Because of the above arguments, the equation obtained for $\alpha = \beta = 0$; (i.e., no change in the independent variables) is expected to be valid away from all boundaries of the region in which the original equation holds. For this reason the solution to the equation obtained for $\alpha = \beta = 0$ shall be called the "interior" approximation. The main characteristic of the interior approximation is that it fails to satisfy all of the boundary conditions; thus necessitating the use of boundary layer corrections near those boundaries where boundary conditions are violated.

There is no reason to expect that the series 28 is convergent to the exact solution to the equation, but at worst it is expected to be asymptotic to the exact solution. It is generally difficult to prove either property because the exact solution is not known and indirect arguments are difficult. Because of the suspected asymptotic behavior, only the $\varphi_i^o(\xi, \eta)$ terms will be evaluated, the remaining terms being of order λ^{-1}. The superscript "o" will be omitted from the following analysis; it being understood that the $\varphi_i(\xi, \eta)$ is only the first term of the series 28.

The equation for $\varphi_i(\xi, \eta)$ is obtained as outlined in step 3, page 16, or it can be equivalently obtained by making the change of variables 27 in equations 20 and 21 and allowing λ to go to infinity for different pairs of α and β. Equations 20 and 21 after the change of variables 27 may be written as

$$\left\{\lambda^{2\alpha-2} \frac{\partial^2}{\partial \xi^2} + \lambda^{\beta} \eta a_i \frac{\partial^2}{\partial \eta^2} + \eta \frac{\partial}{\partial \eta} + \left(1 - \lambda^{\beta/2} \Delta_i \left(\frac{a_i}{r_i}\right)^{1/2}\right)\right\} \varphi_i(\xi, \eta) = 0,$$

$$i = 0, 1 \quad . \qquad (29)$$

After division of equation 29 by the highest power of λ and passage to the limit of infinite λ, only the terms with coefficients of λ to the zeroth power remain. The resulting equations are best displayed in an α, β plane. It is shown in figure 1 that the result of this operation on equation 29 divides the α, β plane into three sections. For instance, if $\beta > \max\ (0,\ 2\alpha - 2)$ the resulting equation is always $\eta \varphi_{\eta\eta} = 0$.

The approximation method used for the analysis of this problem will consist of the following steps.*

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*A similar procedure is given in reference 14.

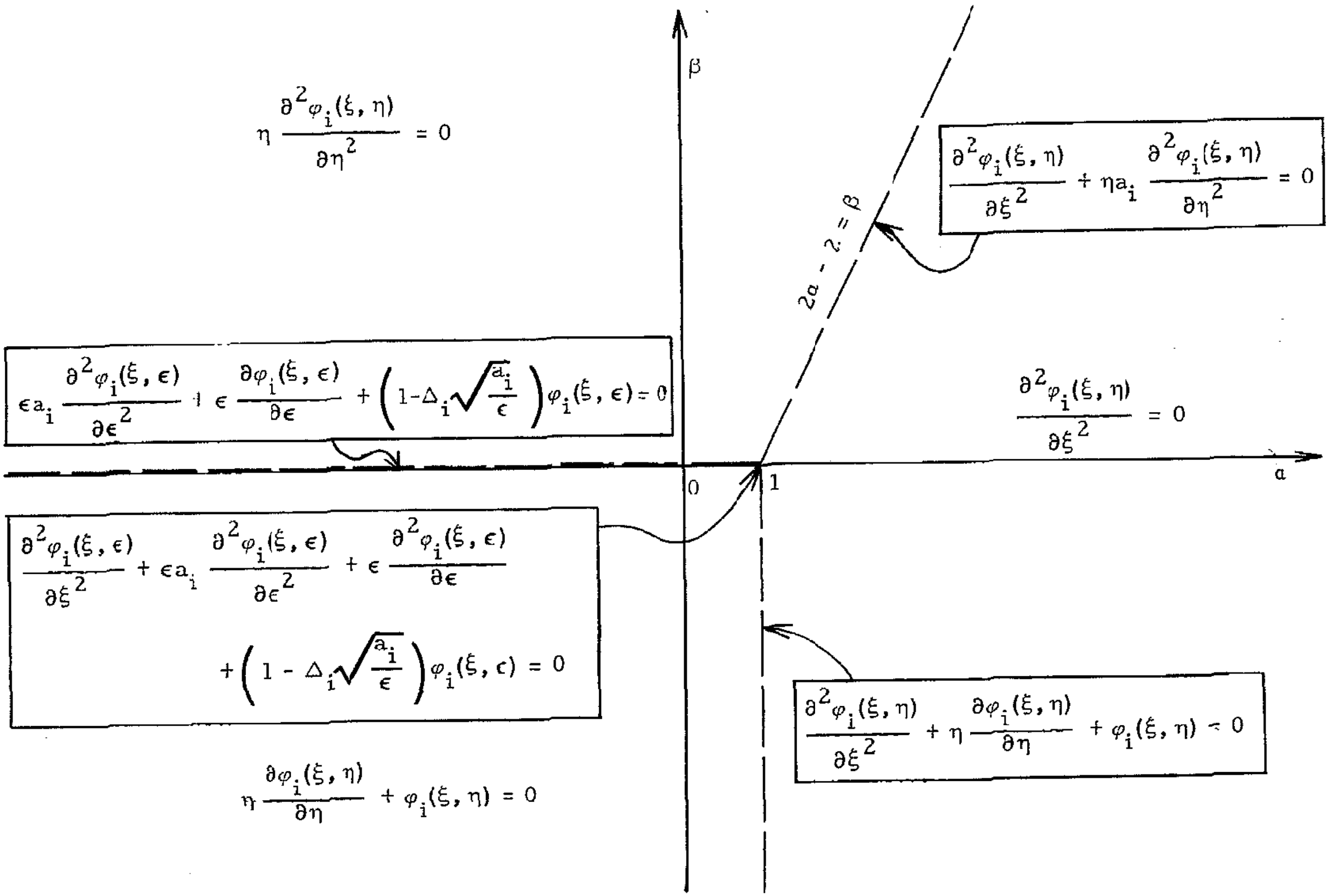

Figure 1. α, β plane for diffusion theory

1) The zeroth order interior equation is solved and as many boundary conditions as possible are satisfied.

2) It is ascertained which boundary conditions the interior solutions do not satisfy.

3) Appropriate zeroth order equations are selected by the α, β arguments, page 16, which are approximately valid near the boundaries determined in step 2. The solutions to these equations, called boundary layer corrections, are then added to the interior solutions so that the boundary conditions determined in step 2 are satisfied to order λ^{-1}.

4) The new approximate solution composed of the sum of the interior solution and boundary layer corrections, determined in step 3, is checked to see that all the boundary conditions and differential equations are satisfied to order λ^{-1}. This must be done because the new approximate solution may not satisfy all the boundary conditions that the interior solution did (see step 1). If the new approximation does not satisfy a certain boundary condition, steps 3 and 4 are performed again for this particular boundary. This procedure continues until all the boundary conditions are satisfied to order λ^{-1}.

The boundary conditions are satisfied to order λ^{-1} since only the zeroth term of the series 28 is calculated for each applicable α, β pair. The next term is the series 28 is of order λ^{-1}; hence, it is consistent to satisfy the boundary conditions only to order λ^{-1}. Higher order approximations may be obtained, at least in principle, by solving for more terms of the series 28.

There are two distinct problems of interest, absorbing media and pure scattering media. These must be investigated separately because different energy boundary conditions are involved in the statements of the corresponding boundary value problems. These two cases are considered successively in the remainder of Part II.

B. Scattering Case in Diffusion Theory

For pure scattering media an approximate solution to equations 20 and 21 with $\Delta_i = 0$ is desired. The equations for the boundary value problem then become

$$\frac{1}{\lambda_o^2}\frac{\partial^2\varphi_o(x,\epsilon)}{\partial x^2} + \epsilon\frac{\partial^2\varphi_o(x,\epsilon)}{\partial\epsilon^2} + \epsilon\frac{\partial\varphi_o(x,\epsilon)}{\partial\epsilon} + \varphi_o(x,\epsilon) = 0 \ , \qquad (30)$$

for $0 \le x < \infty$; $0 \le \epsilon < \infty$ and

$$\frac{1}{\lambda_1^2}\frac{\partial^2\varphi_1(x,\epsilon)}{\partial x^2} + \epsilon a_1\frac{\partial^2\varphi_1(x,\epsilon)}{\partial x^2} + \epsilon\frac{\partial\varphi_1(x,\epsilon)}{\partial\epsilon} + \varphi_1(x,\epsilon) = 0 \ , \qquad (31)$$

for $-1/2 \le x \le 0$; $0 \le \epsilon < \infty$. The boundary conditions for the problem are:

1) the flux is required to be a Maxwellian characterized by T_o at $x = \infty$

$$\varphi_o(\infty,\epsilon) = \frac{\epsilon}{T_o}e^{-\epsilon} \ , \qquad (32)$$

2) the flux and current must be continuous at the interface

$$\varphi_o(0, \epsilon) = \varphi_1(0, \epsilon) \quad , \tag{33}$$

$$\frac{1}{\sigma_o} \frac{\partial \varphi_o(0, \epsilon)}{\partial x} = \frac{1}{\sigma_1} \frac{\partial \varphi_1(0, \epsilon)}{\partial x} , \tag{34}$$

for all energies,

3) the flux must vanish at zero energy

$$\varphi_i(x, 0) = 0 \quad , \qquad i = 0, 1, \tag{35}$$

and

4) the flux goes to zero at large energies in such a way that the integral of the flux over all energies exist. That is, we require that

$$\int_0^\infty \varphi_i(x, \epsilon) \, d\epsilon \tag{36}$$

exists for all x.

The first step in obtaining an approximate solution to equations 30 and 31 is to solve the interior equation. From the α, β diagram, page 19, the interior equation $(\alpha = \beta = 0)$ is

$$\epsilon a_i \frac{\partial^2 \varphi_i(x, \epsilon)}{\partial \epsilon^2} + \epsilon \frac{\partial \varphi_i(x, \epsilon)}{\partial \epsilon} + \varphi_i(x, \epsilon) = 0, \qquad i = 0, 1. \tag{37}$$

The solution to this second order differential equation is

$$\varphi_i(x, \epsilon) = f_i(x) \frac{\epsilon}{a_i} e^{-\epsilon/a_i} + g_i(x) \frac{\epsilon}{a_i} e^{-\epsilon/a_i} \int_{-\infty}^{\epsilon/a_i} \frac{e^t}{t^2} dt \quad , \qquad i = 0, 1, \tag{38}$$

where $f_i(x)$ and $g_i(x)$ are arbitrary functions of x to be determined. The second term of the solution 38 is different from zero at $\epsilon = 0$ and behaves like $1/\epsilon$ for large ϵ (1,13,15,16). Thus to satisfy boundary conditions 35 and 36, $g_i(x)$ must be set equal to zero for $i = 0$ and $i = 1$.

The spatial dependence, $f_i(x)$, of the interior approximation is determined by considering the second order interior approximation $\varphi_i^{(2)}(x, \epsilon)$ (see equation 28). From the procedure outlined in step 3, page 16, the equation for $\varphi_i^{(2)}(x, \epsilon)$ is

$$\left(\epsilon a_i \frac{\partial^2}{\partial \epsilon^2} + \epsilon \frac{\partial}{\partial \epsilon} + 1\right) \varphi_i^{(2)}(x, \epsilon) = - \frac{\epsilon}{a_i} e^{-\epsilon/a_i} \frac{d^2 f_i(x)}{dx^2} . \qquad (39)$$

The particular solution to equation 39 is of the form

$$- \frac{d^2 f_i(x)}{dx^2} e^{-\epsilon/a_i} \left\{1 - \frac{\epsilon}{a_i} \ln \frac{\epsilon}{a_i} + c_1 \frac{\epsilon}{a_i} + c_2 \frac{\epsilon}{a_i} \int_{-\infty}^{\epsilon/a_i} \frac{e^t}{t^2} dt\right\}, \qquad (40)$$

where c_1 and c_2 are constants multiplying the solutions to the homogeneous equation. It is impossible to select c_1 and c_2 so that the particular solution 40 satisfies both energy boundary conditions 35 and 36. For instance, if $c_2 = 0$ so that 36 is satisfied, then 40 is different from zero at $\epsilon = 0$ and therefore does not satisfy 35. Therefore, the only way that $\varphi_i^{(2)}(x, \epsilon)$ can simultaneously satisfy both energy boundary conditions 35 and 36 is to require the particular solution to be zero; that is

$$\frac{d^2 f_i(x)}{dx^2} = 0 , \qquad i = 0, 1, \qquad (41)$$

or

$$f_i(x) = A_i + B_i x \quad , \quad i = 0,1, \tag{42}$$

where A_i and B_i are constants. The boundary condition 32 at $x = \infty$ and the symmetry about $x = -1/2$ yield

$$B_1 = B_o = 0 \; ,$$
$$A_o = \frac{1}{T_o} . \tag{42}$$

Therefore, the interior approximations are

$$\frac{\epsilon}{T_o} e^{-\epsilon} \; , \qquad \text{for } 0 \leq x < \infty \; ,$$
$$A_1 \frac{\epsilon}{a_1} e^{-\epsilon/a_1} , \text{ for } -1/2 \leq x < 0. \tag{43}$$

Note that if $A_1 = 1/T_1$, then the interior approximation in each region would be a Maxwellian distribution characterized by the temperature of that region.

The interior approximations 43 satisfy the boundary conditions at $x = \infty$, $\epsilon = 0$, and $\epsilon = \infty$, but they do not satisfy the interface conditions. Therefore, to the interior solutions near $x = 0$ must be added boundary layer corrections on each side of the interface so that the continuity of flux and current is maintained. According to the previous arguments the equation for the boundary layer corrections near $x = 0$ must have a positive value of α. We further require that α have a definite value so that the transformation 27 will be known explicitly.

It is seen from the α, β diagram, page 19, that there is only one definite positive value of α, $\alpha = 1$, for which there are two choices of β, $\beta = 0$ or $\beta < 0$. The choice $\alpha = 1$, $\beta = 0$ leads to the exact solution to the diffusion equation, which, as mentioned in the introduction, is cumbersome. The equation with $\alpha = 1$, $\beta < 0$ will be used for the boundary layer correction for two reasons. First, it is desirable to have a tractable solution, even if approximate, so that the character of the results can be investigated. (The exact solution to diffusion theory is difficult to investigate because the coefficients of the eigenfunction expansion cannot be solved for explicitly.) Secondly, the equation with $\beta < 0$ should approximate the situation better at high energies than at low energies (see page 16). This is exactly the place where the expansions of the energy transfer and scattering cross sections are valid and where the heavy gas model is best.

Using the subscript b to denote the boundary layer correction term, the equation for $\alpha = 1$, $\beta < 0$ is

$$\frac{\partial^2 \varphi_{bi}(\xi, \eta)}{\partial \xi^2} + \eta \frac{\partial \varphi_{bi}(\xi, \eta)}{\partial \eta} + \varphi_{bi}(\xi, \eta) = 0 , \quad i = 0, 1. \tag{44}$$

If $\xi < 0$ then

$$\xi = \xi_1 = \lambda_1 x ; \quad \eta = \eta_1 = \lambda_1^{\beta} \epsilon , \tag{45}$$

and if $\xi > 0$ then

$$\xi = \xi_o = \lambda_o x ; \quad \eta = \eta_o = \lambda_o^{\beta} \epsilon , \tag{46}$$

by the transformations 27.

The energy boundary conditions will be the same as those for the interior solution, namely

$$\varphi_{bi}(\xi, 0) = 0 \;, \qquad i = 0, 1, \tag{47}$$

and that

$$\int_0^{\infty} \varphi_{bi}(\xi, \eta)\, d\epsilon, \qquad i = 0, 1, \tag{48}$$

exists for all ξ.

The boundary layer correction term is added to the interior approximation for the purpose of satisfying the interface conditions. Thus, the continuity of flux condition 33 becomes

$$\frac{\epsilon e^{-\epsilon}}{T_o} + \varphi_{bo}(0,\eta) = A\,\frac{\epsilon}{a}\, e^{-\epsilon/a} + \varphi_{b1}(0,\eta)\,, \tag{49}$$

or the sum of the interior approximation and boundary layer correction is continuous at the interface. Since the interior approximations are constant in space, the continuity of current condition 34 becomes

$$\frac{\lambda_o}{\sigma_o}\,\frac{\partial \varphi_{bo}(0, \eta)}{\partial \xi} = \frac{\lambda_1}{\sigma_1}\,\frac{\partial \varphi_{b1}(0, \eta)}{\partial \xi}\;, \tag{50}$$

which is consistent with the m^{-1} approximation because m has been taken as a constant throughout space.

In addition to boundary conditions 47 through 50, exponential decay in the ξ direction on both sides of the interface is required so that the effects of the boundary layer correction, $\varphi_{bi}(\xi, \eta)$, will be confined to a narrow zone (or boundary layer) near the interface. Notice that the equation and the boundary conditions are independent of the choice of β; therefore, it is expected that the solution will be independent of β, which is indeed the case.

The boundary value problem described by equations 44 - 50 is solved in appendix A with the aid of Fourier transforms. The solution satisfying boundary conditions 48, 49, and 50 is

$$\varphi_{bi} = \frac{(-1)^i \epsilon \xi}{2\sqrt{\pi}} \int_0^{\infty} \left(\frac{A}{a} e^{-\epsilon u/a} - \frac{1}{T_o} e^{-\epsilon u} \right) u^2 e^{-t^2 \xi^2/4} \, dt, \tag{51}$$

where $u = e^{1/t^2}$.

The constant A from the interior approximation remaining in the result is determined by integrating the interface condition 49 over all ϵ

$$\frac{1}{T_o} + \int_0^{\infty} \varphi_{bo}(\xi, \epsilon)\, d\epsilon = aA + \int_0^{\infty} \varphi_{b1}(\xi, \eta)\, d\epsilon . \tag{52}$$

The integral of the boundary layer correction term can be calculated by integrating equation 44 over all energies and applying the energy boundary conditions 47 and 48 to obtain

$$\frac{d^2}{d\xi^2} \int_0^{\infty} \varphi_{bi}(\xi, \epsilon)\, d\epsilon = 0, \qquad i = 0, 1, \tag{53}$$

or

$$\int_0^{\infty} \varphi_{bi}(\xi, \epsilon)\, d\epsilon = c_1\xi + c_2 = 0, \quad i = 0, 1, \tag{54}$$

because of the exponential decay in ξ. Hence,

$$A = \frac{1}{aT_o} = \frac{1}{T_1} . \tag{55}$$

Because equation 44 is first order in η, only one energy boundary condition (i.e. at a given value of η) could be imposed. This was selected to the high energy boundary condition 48. Equation 44, which governs the boundary layer correction, is known to be most accurate at high energies since $\epsilon = \lambda^{-\beta}\eta$, and β is negative. Thus, satisfying the high energy boundary condition 48 is consistent with the equation employed to describe the boundary layer correction. The discussion of the situation at small energy is deferred until Part IV. It should be pointed out that the integral of the boundary layer correction, equation 51, over all ϵ gives zero, a result which agrees with equation 54.

The approximation to the solution obtained by this argument is

$$\varphi_o(z, E) = \frac{\epsilon e^{-\epsilon}}{T_o} + \varphi_{bo}(\xi, \epsilon) , \tag{56}$$

for $0 \leq z < \infty$, and

$$\varphi_1(z, E) = \frac{\epsilon a^{-\epsilon/a}}{T_1 a_1} + \varphi_{b1}(\xi, \epsilon) , \tag{57}$$

for $-W/2 \leq z \leq 0$, where

$$\xi = \begin{cases} \sigma_o(6/m)^{1/2}z & \text{if } z > 0\ , \\ \sigma_1(6/m)^{1/2}z & \text{if } z < 0\ , \end{cases} \tag{57}$$

and $\varphi_{bi}(\xi,\epsilon)$ is given by equation 51.

C. Absorbing Case in Diffusion Theory

The formalism of the approximation procedure employed in the scattering case carries over to the absorbing case; however, the boundary conditions must be changed. As mentioned earlier, the presence of absorption requires a neutron source so that a steady state neutron distribution can be maintained. The source term may be included either in the transport equation 1 or imposed as a boundary condition.

In this thesis it is assumed that the source provides high energy neutrons (~ 1 Mev) from either fissions or independent sources symmetrically distributed about $x = -1/2$. These high energy neutrons migrate through the medium colliding with the nucleii until they attain thermal energy (~ 0.025 eV). Because the source neutrons have such high energies compared to the average nuclear energy, the initial collisions can be considered as ones between the neutrons and nucleii which are at rest. (Only 10^{-10^5} of the nucleii have energies greater than 1 kev.) Therefore, the spatial distribution of the high energy neutrons in the intermediate energy range, (below source energies and above thermal energies), say 100 kev to 1 kev, can be adequately described by the Fermi Age model or one-velocity diffusion theory.

The assumption of stationary nucleii for the high energy collisions leads to the characteristic flux inversely proportional to the energy at large energies (11, 17, 18). The large energy boundary condition used in the scattering case will be replaced here by requiring that the flux have a prescribed spatial distribution (symmetric about $x = -1/2$) at a certain high energy, say ϵ_o. Hence, ϵ is restricted to the range 0 to ϵ_o. Because the flux is known to be inversely proportional to the energy, for large energy, it would be convenient if the flux were $O(1/\epsilon)$ for large energies, even those outside the above range. If this were the case, a smooth fit for the flux would occur at $\epsilon = \epsilon_o$.

The zero energy boundary condition will remain as in the scattering case; that is, the flux is required to vanish at $\epsilon = 0$. It is known that the flux is zero at zero energy in the non-absorbing case, and the presence of an absorber, with an absorption cross section inversely proportional to the neutron velocity, should not alter this property of the flux.

For the absorbing case the differential equations to which the approximation procedure will be applied are

$$\frac{1}{\lambda_o^2}\frac{\partial^2\varphi_o(x,\epsilon)}{\partial x^2} + \epsilon\frac{\partial^2\varphi_o(x,\epsilon)}{\partial\epsilon^2} + \epsilon\frac{\partial\varphi_o(x,\epsilon)}{\partial\epsilon} + (1 - \Delta_o\epsilon^{-1/2})\varphi_o(x,\epsilon) = 0 \quad , \tag{58}$$

for $0 \leq x < \infty$ and

$$\frac{1}{\lambda_1^2}\frac{\partial^2\varphi_1(x,\epsilon)}{\partial x^2} + \epsilon a_1 \frac{\partial^2\varphi_1(x,\epsilon)}{\partial\epsilon^2} + \epsilon\frac{\partial\varphi_1(x,\epsilon)}{\partial\epsilon}$$

$$+ (1 - \Delta_1(\epsilon/a_1)^{-1/2})\varphi_1(x,\epsilon) = 0 \ , \qquad (59)$$

for $-1/2 \leq x \leq 0$. The absorption is represented by the parameter Δ_i (see equation 24).

The energy boundary conditions in the absorbing case are taken to be

$$\varphi_i(x, 0) = 0 \ , \qquad i = 0, 1, \qquad (60)$$

for all x, and

$$\varphi_i(x, \epsilon_o) = f(x) \ , \qquad (61)$$

where $f(x)$ is the prescribed spatial distribution of the flux at $\epsilon = \epsilon_o$. The interface conditions, continuity of flux and current,* remain the same as in the scattering case; that is

$$\varphi_o(0, \epsilon) = \varphi_1(0, \epsilon) \ , \qquad (62)$$

$$\frac{1}{\sigma_o}\frac{\partial\varphi_o(0,\epsilon)}{\partial x} = \frac{1}{\sigma_1}\frac{\partial\varphi_1(0,\epsilon)}{\partial x} \ , \qquad (63)$$

for all ϵ in the range 0 to ϵ_o.

Again the interior equation is solved first. From the α, β diagram, page 19, the interior equation ($\alpha = \beta = 0$) is

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* For the large mass assumption $D_i = 1/3\sigma_i$. See page 57, equation 141.

$$\left\{\epsilon a_i \frac{\partial^2}{\partial\epsilon^2} + \epsilon \frac{\partial}{\partial\epsilon} + 1 - \Delta_i(\epsilon/a_i)^{-1/2}\right\}\varphi_i(x,\epsilon) = 0 \ , \qquad (64)$$

$$i = 0, 1.$$

The solution to equation 64, which is identical with the equation for an infinite medium composed of a heavy monatomic gas, is known to be (2, 13, 15, 16)

$$\varphi_i(x,\epsilon) = \frac{f(x)}{K_i}\left\{\frac{\epsilon}{a_i} e^{-\epsilon/a_i} \sum_{n=0}^{\infty} b_n^i \left(\frac{\epsilon}{a_i}\right)^{n/2}\right\}, \ i = 0, 1 \ , \qquad (65)$$

where

$$b_o^i = 1 \quad , \qquad b_1^i = \frac{4\Delta_i}{3} \quad , \qquad (66)$$

$$b_n^i = \frac{1}{n(n+2)}\left\{4\Delta_i b_{n-1}^i + 2(n-2)b_{n-2}^i\right\}; \quad n \geq 2 \ . \qquad (67)$$

The constant K_i is chosen to be equal to the sum in brackets evaluated at $\epsilon = \epsilon_o$, so that boundary conditions 60 and 61 are satisfied. For the sake of brevity define

$$\varphi_i(\epsilon) = \frac{1}{K_i} \cdot \frac{\epsilon}{a_i} e^{-\epsilon/a_i} \sum_{n=0}^{\infty} b_n^i \left(\frac{\epsilon}{a_i}\right)^{n/2}, \ i = 0, 1 \ , \qquad (68)$$

which is the solution to the infinite medium heavy monatomic gas equation, 64, normalized in such a way as to have the value unity at $\epsilon = \epsilon_o$.

The interior approximations satisfy the large and zero energy boundary conditions, but they do not satisfy the interface conditions. Therefore, a boundary layer correction is required near the interface. For the same reasons as in the scattering case, the differential equation, 44, with $\alpha = 1$, $\beta < 0$ is used to describe the boundary layer correction near the interface. The equation is

$$\frac{\partial^2 \varphi_{bi}(\xi, \eta)}{\partial \xi^2} + \eta \frac{\partial \varphi_{bi}(\xi, \eta)}{\partial \eta} + \varphi_{bi}(\xi, \eta) = 0, \quad i = 0, 1. \tag{69}$$

The addition of the boundary layer correction to the interior solution makes it possible to satisfy the interface conditions which are

$$f(0)\varphi_o(\epsilon) + \varphi_{bo}(0, \eta) = f(0)\varphi_1(\epsilon) + \varphi_{b1}(0, \eta), \tag{70}$$

$$\frac{1}{\sigma_o} \frac{\partial f(0)}{\partial x} \varphi_o(\epsilon) + \frac{\lambda_o}{\sigma_o} \frac{\partial \varphi_{bo}(0, \eta)}{\partial \xi} = \frac{1}{\sigma_1} \frac{\partial f(0)}{\partial x} \varphi_1(\epsilon) + \frac{\lambda_1}{\sigma_1} \frac{\partial \varphi_{b1}(0, \eta)}{\partial \xi}, \tag{71}$$

for all $0 \le \epsilon \le \epsilon_o$. Equation 71 has terms of order λ^1 and λ^0 and according to step 3, page 16, which says that only the terms with coefficients of the highest power in λ are kept in the boundary conditions, equation 71, the continuity of current condition, becomes

$$\frac{\lambda_o}{\sigma_o} \frac{\partial \varphi_{bo}(0,\eta)}{\partial \xi} = \frac{\lambda_1}{\sigma_1} \frac{\partial \varphi_{b1}(0, \eta)}{\partial \xi} . \tag{72}$$

The large and zero energy boundary conditions are

$$\varphi_{bi}(\xi, 0) = 0 , \quad i = 0,1, \tag{73}$$

$$\varphi_{bi}(\xi, \epsilon_o) = 0 , \quad i = 0,1, \tag{74}$$

for all ξ. In addition, exponential decay in the ξ direction away from the interface is required so that the effects of the boundary layer corrections are confined to a narrow zone near the interface. That is,

$$\varphi_{bi}(\xi,\eta) \sim e^{-c|\xi|} , \quad \text{as } \xi \to \pm\infty , \tag{75}$$

for some positive c, which may be a function of energy.

The method of solving the boundary layer correction in the absorbing case is very similar to that used in the scattering case. This boundary value problem described by equations 69 through 75 is solved in appendix A. The result, satisfying boundary conditions 70, 72, 74, and 75, is

$$\varphi_{bi}(\xi,\eta) = \frac{(-1)^i f(0)\xi}{2\sqrt{\pi}} \int_{[\ln(\epsilon_o/\epsilon)]^{-1/2}}^{\infty} (\varphi_1(\epsilon u)-\varphi_o(\epsilon u))ue^{-\xi^2 t^2/4}\, dt,$$

$$i = 0,1, \tag{76}$$

where

$$u = e^{1/t^2} , \tag{77}$$

and $\varphi_o(\epsilon)$ and $\varphi_1(\epsilon)$ are the interior approximations given by equations 65, 66, and 67 in power series form. Since the only singularities of the differential equation 64 for the interior approximation are at $\epsilon = 0$ and $\epsilon = \infty$, the power series certainly converges in the interval of interest, $0 \leq \epsilon \leq \epsilon_o$. Since power series are uniformly convergent within every closed disc interior to the circle of convergence, the integrations in equation 76 may be done term by term. The discussion of the situation at small energy is deferred until Part IV.

The approximate flux given by the boundary layer technique for the absorbing case is

$$\varphi_o(x,\epsilon) = f(x)\varphi_o(\epsilon) - \frac{\xi f(0)}{2\sqrt{\pi}} \int_{\infty}^{(\ln \epsilon_o/\epsilon)^{-1/2}} (\varphi_1(\epsilon u) - \varphi_o(\epsilon u))ue^{-\xi^2 t^2/4}\, dt, \qquad (78)$$

for $0 \leq x < \infty$, and

$$\varphi_1(x,\epsilon) = f(x)\varphi_1(\epsilon) + \frac{\xi f(0)}{2\sqrt{\pi}} \int_{\infty}^{(\ln \epsilon_o/\epsilon)^{-1/2}} (\varphi_1(\epsilon u) - \varphi_o(\epsilon u))ue^{-\xi^2 t^2/4}\, dt, \qquad (79)$$

for $-1/2 \leq x \leq 0$. The $\varphi_i(\epsilon)$ terms are given by equation 68, ξ is given by equation 57, and $u = e^{1/t^2}$.

Most of the discussion of these results will be deferred until Part IV. There are two points that should be made at the present stage. First, the flux at the interface, $x = \xi = 0$, can be obtained in the scattering case by setting $\xi = 0$ in equation 56 or 57. The integrations can be performed explicitly to give

$$\varphi(0,\epsilon) = \frac{1}{2}\left\{\frac{\epsilon}{T_o} e^{-\epsilon} + \frac{\epsilon}{a_1 T_1} e^{-\epsilon/a_1}\right\}. \qquad (80)$$

In the absorbing case the same operations on equation 78 or 79 gives

$$\varphi(0,\epsilon) = \frac{f(0)}{2}\left\{\varphi_o(\epsilon) + \varphi_1(\epsilon)\right\}. \qquad (81)$$

Equations 80 and 81 state that the flux at the interface, in this approximation, is the average of the interior approximations extrapolated to the interface. The energy dependence of the interior approximations for $x > 0$ is the same as would exist in an infinite homogeneous medium composed of the same material. The same is true for the interior approximation for $x < 0$. Thus, in the slab problem where one infinite medium solution is blended into the other across the interface, it would be expected that the energy dependence of the flux at the interface would depend in some manner on the infinite medium solutions. Therefore, the averages obtained above are very reasonable results.

The second point is that diffusion theory is an approximation to the actual physical process which is taking place. The assumption that all moments of the angular flux higher than the first could be neglected, which is the basis of the diffusion theory model, is not necessarily valid near places where material properties change rapidly. At such places the angular flux is very likely to be anisotropic and consequently the higher moments may not be neglected (18).

In this problem the region of greatest interest is near the interface which is the place where diffusion theory may not be valid. A priori it is not known whether the approximation constructed here is better or poorer than an exact answer to the diffusion theory equations in the sense of yielding a result which is closer or further from the actual flux occurring in the physical problem at and near the interface.

III. TRANSPORT THEORY

A. Introduction

The purpose of Part III is to find an approximate solution to the transport equation 1 using the technique introduced in Part II. The transport equation will be solved for slab geometry, the slab occupying the space from $z = -W$ to $z = 0$. The nucleii of the media present are assumed to be monatomic gases in Maxwellian energy distributions characterized by different temperatures for the slab and the surrounding medium. From the analysis of Part II we expect that the exact solution to the transport equation will be approximated by the sum of an interior approximation and a boundary layer correction which will make an appreciable contribution to the flux only near the interfaces.

In terms of the dimensionless variables

$$x = z/W, \qquad \epsilon = E/T_o , \tag{19}$$

the transport equation is

$$\frac{\mu}{\lambda_o} \frac{\partial \varphi_o(x,\epsilon,\mu)}{\partial x} + \left\{ \frac{\sigma_s^o(\epsilon)}{\sigma_o} + \frac{2\Delta_o}{m} \epsilon^{-1/2} \right\} \varphi_o(x,\epsilon,\mu)$$
$$= \int_0^{\infty} d\epsilon' \int_{-1}^{+1} d\mu' \frac{\sigma_s^o(\epsilon',\mu' \rightarrow \epsilon,\mu)}{\sigma_o} \varphi_o(x,\epsilon',\mu') , \tag{82}$$

for $0 \le x < \infty$, and

$$\frac{\mu}{\lambda_1}\frac{\partial\varphi_1(x,\epsilon,\mu)}{\partial x}+\left\{\frac{\sigma_s^1(\epsilon)}{\sigma_1}+\frac{2\Delta_1}{m}(\epsilon/a_1)^{-1/2}\right\}\varphi_1(x,\epsilon,\mu)$$

$$=\int_0^\infty d\epsilon'\int_{-1}^{+1}d\mu'\,\frac{\sigma_s^1(\epsilon',\mu'\to\epsilon,\mu)}{\sigma_2}\,\varphi_1(x,\epsilon',\mu'), \qquad (83)$$

for $-1/2 \le x \le 0$. The subscript 1 denotes quantities in the slab and the subscript o denotes quantities in the surrounding medium. In terms of the dimensionless variables the scattering cross section is

$$\frac{\sigma_s^i(\epsilon)}{\sigma_i} = 1+\frac{a_i}{2m\epsilon}\ \mathrm{erf}\,(m\epsilon/a_i)^{1/2}+\frac{e^{-m\epsilon/a_i}}{(\pi m\epsilon/a_i)^{1/2}}\,, \quad i=0,1, \qquad (84)$$

where erf (x) is defined by equation 5.

The energy transfer cross section is

$$\frac{\sigma_s^i(\epsilon',\mu'\to\epsilon,\mu)}{\sigma_i}=\frac{1}{8\pi^2}\left(1+\frac{1}{m}\right)^2\left(\frac{\epsilon}{\epsilon'}\right)^{1/2}\int_{-\infty}^{\infty}dt\int_0^{2\pi}d\psi\,e^{it(\epsilon-\epsilon')}$$

$$\times\ \exp\left\{\frac{it-a_it^2}{m}\,(\epsilon+\epsilon'-2\mu_o(\epsilon\epsilon')^{1/2}\right\},\quad i=0,1, \qquad (85)$$

where

$$\mu_o=\mu\mu'+\left[(1-\mu^2)(1-\mu'^2)\right]^{1/2}\cos\psi\ . \qquad (4)$$

The parameters used in equations 82 to 85 are

$$a_i=T_i/T_o\,,\qquad \lambda_i=\sigma_iW\,,\qquad i=0,1\,, \qquad (86)$$

and for an absorption cross section inversely proportional to the neutron velocity,

$$\Delta_i = \frac{m\sigma_2^i(\epsilon)}{2\sigma_i} (\epsilon/a_i)^{1/2} , \qquad i = 0,1, \qquad (24)$$

is a constant.

The angular flux in the rest of space is obtained by the symmetry about $x = -1/2$

$$\varphi(x, \epsilon, \mu) = \varphi(-1-x, \epsilon, -\mu) , \qquad x > -1/2 , \qquad (87)$$

At the interface, $x = 0$, the angular flux is to be continuous,

$$\varphi_1(0, \epsilon, \mu) = \varphi_o(0, \epsilon, \mu) , \qquad (88)$$

for all energies ϵ and angles $\cos^{-1} \mu$. At zero energy the angular flux is to vanish,

$$\varphi_i(x, 0, \mu) = 0 , \qquad i = 0,1, \qquad (89)$$

for all x and angles $\cos^{-1} \mu$. The large energy boundary condition will again depend on whether or not absorption is present. In the scattering case $(\Delta_i = 0)$ the angular flux will be required to go to zero at large energies in such a way that

$$\int_0^\infty \varphi_i(x, \epsilon, \mu) \, d\epsilon , \qquad i = 0,1, \qquad (90)$$

exists for all x and angles $\cos^{-1} \mu$. If absorption is present the energy range will be restricted to $0 \leq \epsilon \leq \epsilon_o$ and the angular flux will be required to agree with a prescribed spatial and angular distribution of flux at ϵ_o. These are the same energy boundary conditions that were used for the scattering and absorbing cases in the treatment based on the diffusion theory model.

We again assume that λ_i is a large quantity, implying that the slab width is much greater than the mean free scattering length. In order to obtain the equations which are approximately valid in the different regions of the x, ϵ plane, the change of variables

$$\xi = \lambda^{\alpha} x \quad , \qquad \eta = \lambda^{\beta} \epsilon \tag{91}$$

is introduced into equations 82 to 85. We then pass to the limit of infinite λ . The resulting equations for different pairs of α, β will govern the first approximations to the flux in various regions of the x, ϵ plane. This is the same procedure that was used in the treatment of the diffusion theory model to obtain the equations governing first approximations. The results of this operation on the transport equation are displayed in the α, β plane, figure 2. The only new symbol used in figure 2 is given by

$$\frac{\bar{\sigma}^i(\eta', \mu' \rightarrow \eta, \mu)}{\sigma_i} = \frac{1}{8\pi^2}\left(1 + \frac{1}{m}\right)^2 \left(\frac{\eta}{\eta'}\right)^{1/2} \int_{-\infty}^{\infty} dt \int_0^{2\pi} d\psi \, e^{it(\eta - \eta')}$$

$$\cdot \exp\left\{\frac{it}{m}\left(\eta + \eta' - 2\mu_o (\eta\eta')^{1/2}\right)\right\}, \quad i = 0, 1, \tag{92}$$

where μ_o is given by equation 4. The equation for $\alpha = 1$, $\beta = 0$ has been omitted from the diagram. It can be obtained by adding $\mu(\partial\varphi_i(\xi, \epsilon, \mu)/\partial\xi)$ to the left hand side of the equation for $\alpha < 1$, $\beta = 0$.

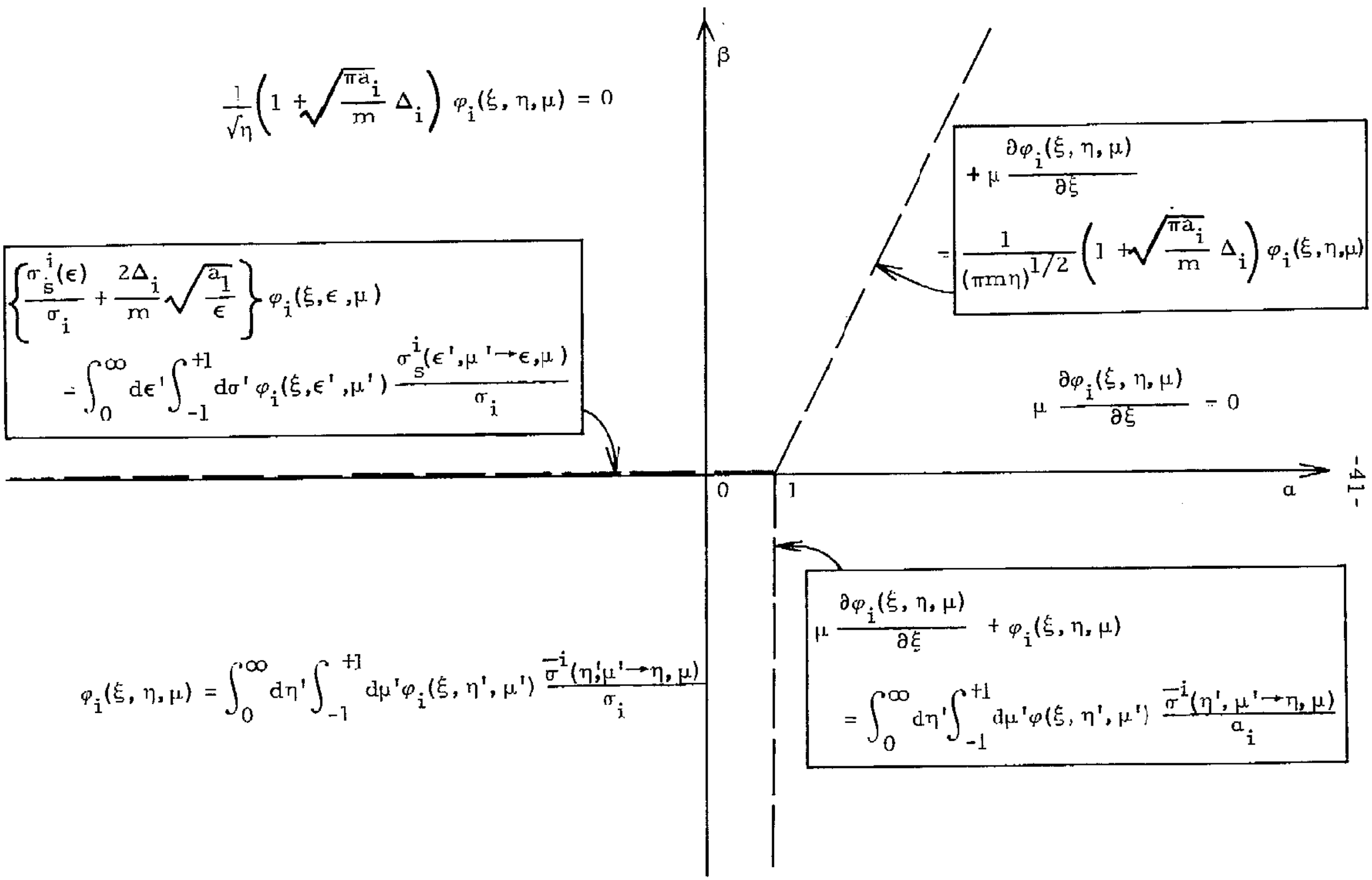

Figure 2. α, β plane for transport theory

B. Scattering Case

1. Formulation of the boundary layer problem

For the scattering case $(\Delta_i = 0)$ the angular flux is required to be Maxwellian for all μ at infinite distance from the interface. That is

$$\varphi_o(x,\epsilon,\mu) \sim \frac{\epsilon}{2T_o} e^{-\epsilon}, \qquad \text{as } x \rightarrow \infty . \tag{93}$$

The factor of 1/2 is included so that the integral of the angular flux over all μ is the same for large x as that used in diffusion theory.

According to the procedure established in Part II the first step in obtaining an approximate solution is to solve the interior equation. For the scattering case in transport theory the interior equation $(\alpha = \beta = 0)$ is

$$\frac{\sigma_s^i(\epsilon)}{\sigma_i} \varphi_i(x,\epsilon,\mu) = \int_0^{\infty} d\epsilon' \int_{-1}^{+1} d\mu' \varphi_i(x,\epsilon',\mu') \frac{\sigma_s^i(\epsilon',\mu' \rightarrow \epsilon,\mu)}{\sigma_i}, \tag{94}$$

$$i = 0, 1,$$

where the scattering cross section, $\sigma_s^i(\epsilon)$, and the energy transfer cross section, $\sigma_s^i(\epsilon',\mu' \rightarrow \epsilon,\mu)$ are given by equations 84 and 85 respectively.

The energy and angular dependence of the solution of equation 94 may be determined by either of two methods. For the first method we recognized that equation 94 is identical with the transport equation for an infinite homogeneous non-absorbing medium. Therefore the flux is an isotropic Maxwellian distribution characterized by the temperature of the medium. For the second method m is assumed large and an expansion in powers of m^{-1} is performed on equation 94 using the Dirac delta function indentification equation 11. The resulting equation to order m^{-1} is

$$\left(1+\frac{a_i}{2m\epsilon}\right)\varphi_i(x,\epsilon,\mu)$$
$$= -\frac{\mu}{m}\left(\epsilon a_i\frac{\partial^2}{\partial\epsilon^2}+\epsilon\frac{\partial}{\partial\epsilon}\right)\int_{-1}^{+1}\mu'\varphi_i(x,\epsilon,\mu')\,d\mu'$$
$$+\frac{1}{2}\left(1+\frac{2}{m}+\frac{a_i}{2m\epsilon}+\frac{2\epsilon a_i}{m}\frac{\partial^2}{\partial\epsilon^2}+\frac{2\epsilon}{m}\frac{\partial}{\partial\epsilon}\right)\int_{-1}^{+1}\varphi_i(x,\epsilon,\mu')\,d\mu',$$
$$i=0,1. \tag{95}$$

The right-hand side of equation 95 tells us that $\varphi_i(x,\epsilon,\mu)$ is a linear function of μ, say

$$\varphi_i(x,\epsilon,\mu)=\varphi_{0i}(x,\epsilon)+\mu\varphi_{1i}(x,\epsilon),\qquad i=0,1. \tag{96}$$

This implies that the diffusion or P_1 approximation is consistent with the large mass assumption for the interior approximation. Therefore, $\varphi_{0i}(x,\epsilon)$ may be identified with the flux and φ_{1i} with the current (see equations 8 and 9). The equation for φ_{0i} is

$$\epsilon a_i\frac{\partial^2\varphi_{0i}(x,\epsilon)}{\partial\epsilon^2}+\epsilon\frac{\partial\varphi_{0i}(x,\epsilon)}{\partial\epsilon}+\varphi_{0i}(x,\epsilon)=0,\quad i=0,1, \tag{97}$$

and the equation for φ_{1i} is

$$\frac{\epsilon a_i}{m}\frac{\partial^2\varphi_{1i}(x,\epsilon)}{\partial\epsilon^2}+\frac{\epsilon}{m}\frac{\partial\varphi_{1i}(x,\epsilon)}{\partial\epsilon}+\frac{3}{2}\left(1+\frac{a_i}{2m\epsilon}\right)\varphi_{1i}(x,\epsilon)=0,$$
$$i=0,1. \tag{98}$$

The solution to equation 98 to order m^{-1} is

$$\varphi_{1i}(x, \epsilon) = 0, \qquad i = 0, 1. \tag{99a}$$

The remaining equation 97 for $\varphi_{0i}(x, \epsilon)$ is identical with the equation used for the interior approximation in the treatment of the diffusion theory model. Therefore, by either method the solution to the interior equation satisfying the energy boundary conditions 89 and 90 is

$$\varphi_i(x, \epsilon, \mu) = f_i(x) \frac{\epsilon}{a_i} e^{-\epsilon/a_i}, \qquad i = 0, 1, \tag{99b}$$

where $f_i(x)$ is a function of x to be determined.

The functions $f_i(x)$ are determined exactly as they were in the treatment of the scattering case based on diffusion theory. We again find that the particular solution to the equation for the first order term in the flux expansion (see equation 28) must be zero in order to satisfy both the large and small energy boundary conditions. This implies that

$$\frac{df_i(x)}{dx} = 0, \qquad i = 0, 1, \tag{100}$$

or

$$f_o(x) = \frac{1}{2T_o}, \qquad f_1(x) = A, \tag{101}$$

where the constant $f_o(x)$ has been chosen to satisfy boundary condition 93.

These results, equations 99 and 101, could be obtained in a completely equivalent manner by arguing that diffusion theory is adequate for the interior approximation. It has already been shown that the large mass assumption for the interior equation derived from transport theory is equivalent to a P_1 or diffusion approximation. Davison (18) shows that the error in the flux using the diffusion theory approximation is of the order of $e^{-\sigma d}$ where d is the distance to the closest boundary and σ is the total cross section. Since the results obtained by the approximation plan are correct to order $\lambda^{-1} = (\sigma W)^{-1}$, the error in the flux caused by using diffusion theory for the interior solution is less than the error inherent in the approximation scheme away from the boundaries of the region in which the interior solution is valid. Therefore, we could have started with the diffusion theory results of Part II for the interior approximation. The detailed derivation using the approximation scheme has been included to show this equivalence between the interior approximation and the diffusion approximation for the large mass assumption.

The interior approximations are therefore

$$\frac{\epsilon}{2T_o} e^{-\epsilon}, \qquad \text{for} \quad 0 \leq x < \infty, \tag{102}$$

$$A \frac{\epsilon}{a_1} e^{-\epsilon/a_1}, \qquad \text{for} \quad -1/2 \leq x \leq 0, \tag{103}$$

which satisfy the small energy boundary condition 89, the large energy boundary condition 90, and the boundary condition 93 at $x = \infty$. These interior approximations do not satisfy the interface condition 88. Hence, to the interior approximations must be added boundary layer corrections, which make an appreciable contribution to the flux only near the interface, so that the interface condition can be satisfied to order λ^{-1}.

For the boundary layer correction the equation with $\alpha = 1$, $\beta < 0$ will again be used. From the arguments by which the equations were derived and the fact that β is negative, this equation is expected to be most accurate for large energies. From the α, β diagram, figure 2, this equation is

$$\mu \frac{\partial \varphi_{bi}(\xi, \eta, \mu)}{\partial \xi} + \varphi_{bi}(\xi, \eta, \mu)$$

$$= \int_0^{\infty} d\eta' \int_{-1}^{+1} d\mu' \varphi_{bi}(\xi, \eta', \mu') \frac{\overline{\sigma}^i(\eta', \mu' \to \eta, \mu)}{\sigma_i}, \quad i = 0, 1, \qquad (104)$$

where $\overline{\sigma}^i(\eta', \mu' \to \eta, \mu)$ is given by equation 92. We now treat this equation approximately by assuming that m is large. The kernel of the integral, $\overline{\sigma}^i(\eta', \mu' \to \eta, \mu)/\sigma_i$, is expanded in powers of m^{-1} and the resulting terms are identified with the Dirac delta function and its derivatives, equation 11. The result of keeping all terms with coefficients of zeroth and first power of m^{-1} is

$$\mu \frac{\partial \varphi_{bi}(\xi, \eta, \mu)}{\partial \xi} + \varphi_{bi}(\xi, \eta, \mu)$$

$$= \left(\frac{1}{2} + \frac{1}{m} + \frac{\eta}{m} \frac{\partial}{\partial \eta} \right) \int_{-1}^{+1} \varphi_{bi}(\xi, \eta, \mu') d\mu'$$

$$- \frac{\mu\eta}{m} \frac{\partial}{\partial \eta} \int_{-1}^{+1} \mu' \varphi_{bi}(\xi, \eta, \mu')\, d\mu' + O\left(\frac{1}{m^2}\right), \quad i = 0, 1 . \qquad (105)$$

The energy boundary conditions 89 and 90 are taken to be the same as those for the interior solution. The boundary layer correction is added to the interior approximation so that the interface condition 88 can be satisfied to order λ^{-1}; that is

$$\frac{\epsilon e^{-\epsilon}}{2T_o} + \varphi_{b0}(0,\eta,\mu) = A\frac{\epsilon}{a_1}e^{-\epsilon/a_1} + \varphi_{b1}(0,\eta,\mu) \ , \qquad (106)$$

for all ϵ and μ. In addition, exponential decay as $|\xi| \to \infty$ is required, so that φ_{b0} and φ_{b1} will only be significant near the interface.

The constant A remaining from the interior approximation can now be determined in the same manner as it was in the treatment of the scattering case in diffusion theory. After integrating the interface condition 106 over all ϵ and μ and using equation 105 to determine the integrals of the boundary layer corrections, the result is

$$A = \frac{1}{2T_1} \ . \qquad (107)$$

Hence, to first order the interior approximations are again Maxwellians characterized by the temperature of the respective media.

Several points can now be made before we consider the construction of the solution of equation 105. First, the equation 105 and boundary conditions 89, 90, and 106 are independent of the choice of β, the negative constant which determines the energy scale on which we are working. Therefore, the boundary layer correction, φ_{bi}, will be independent of β. (This was also the case in the diffusion theory treatment.) Consequently, from now on we will use ϵ instead of η *as the energy variable in the boundary layer correction.*

Secondly, if the boundary layer correction is expanded in Legendre polynomials and only the first two Legendre coefficients are kept as in diffusion theory, the resulting boundary layer equation is identical to the boundary layer equation 44 used in the diffusion theory model. This at least indicates consistency between the two treatments.

Thirdly, if the limit $m \to \infty$ is formally carried out on the boundary layer equation 105 the resulting equation is

$$\mu \frac{\partial \varphi_{bi}(\xi, \epsilon, \mu)}{\partial \xi} + \varphi_{bi}(\xi, \epsilon, \mu) = \frac{1}{2} \int_{-1}^{+1} \varphi_{bi}(\xi, \epsilon, \mu') \, d\mu', \quad i=0,1, \quad (108)$$

which is the one-velocity transport equation with multiplication equal to one. The interface condition 106 remains the same. It can be interpreted as a jump condition for each fixed ϵ. It is known (18, 19) that the one-velocity equation 108 does not have a solution which simultaneously decays exponentially with distance from the interface and satisfies a jump condition at the interface. This is related to the fact that the limit $m \to \infty$ removes the energy derivatives from the boundary layer equation 105. The energy derivatives arise in the boundary layer equation 105 because of the expansion of the kernel in equation 104. Thus, the limit $m \to \infty$ removes the mechanism of energy exchange between the neutrons and the nucleii for those neutrons crossing the interface. Therefore, the m^{-1} terms must be kept in the boundary layer equation 105 in order to account for the energy exchange. The retention of the m^{-1} terms allows fulfillment of the exponential decay requirement. This point will be further discussed in Part IV.

2. Solution of the boundary layer equation

The boundary layer equation 105 will be treated by using a technique similar to that introduced by Case (19) for treating the one-velocity transport equation. We first consider solutions to the equations 105 of the special form

$$e^{-\xi/\nu}\psi(\nu, \epsilon, \mu) , \tag{109}$$

where ν is a parameter. Solutions of this form will not in general satisfy the interface conditions for any choice of ν. However, the solution to equation 105 which also satisfies the interface conditions will then be constructed by a superposition of the special forms 109 over all admissible values of ν. The substitution of 109 for $\varphi_{bi}(\xi, \eta, \mu)$ in equation 105 gives

$$\frac{\nu-\mu}{\nu}\ \psi\ (\nu,\epsilon\ ,\mu) = \frac{m+2}{2m}\ a(\nu,\epsilon) + \frac{\epsilon}{m}\ \frac{\partial a(\nu, \epsilon)}{\partial\epsilon} - \frac{\mu\epsilon}{m}\ \frac{\partial b(\nu, \epsilon)}{\partial\epsilon}, \tag{110}$$

where

$$a(\nu, \epsilon) = \int_{-1}^{+1} \psi(\nu, \epsilon, \mu')\ d\mu' , \tag{111}$$

$$b(\nu, \epsilon) = \int_{-1}^{+1} \mu'\psi(\nu, \epsilon, \mu')\ d\mu' . \tag{112}$$

Since μ is real and in the range -1 to $+1$, either ν is in the same interval, so that $\nu = \mu$ is a possibility, or ν is not in the interval. The functional equation 110 for $\psi(\nu, \epsilon, \mu)$ must be investigated separately for these two cases.

Case (i) ν real and $-1 \leq \nu \leq 1$

For ν in this range the solution to equation 110 is

$$\psi(\nu, \epsilon, \mu) = \frac{\nu}{\nu-\mu}\left\{\frac{m+2}{2m}\, a(\nu, \epsilon) + \frac{\epsilon}{m}\frac{\partial a(\nu, \epsilon)}{\partial \epsilon} - \frac{\mu\epsilon}{m}\frac{\partial b(\nu, \epsilon)}{\partial \epsilon}\right\}$$

$$+ \lambda(\nu, \epsilon)\,\delta(\nu-\mu) \, , \qquad (113)$$

where $\delta(\nu-\mu)$ is the Dirac delta function. It is now required that result 113 be consistent with equations 111 and 112. This gives the following two equations for a, b and λ.

$$b(\nu, \epsilon) = -\frac{2\nu}{m}\left(a(\nu, \epsilon) + \epsilon\frac{\partial a(\nu, \epsilon)}{\partial \epsilon}\right) , \qquad (114)$$

$$\lambda(\nu, \epsilon) = a(\nu, \epsilon) - \frac{2\nu\epsilon}{m}\frac{\partial b(\nu, \epsilon)}{\partial \epsilon}$$

$$- \left\{\frac{\nu}{2}\left(\frac{m+2}{m}\, a(\nu, \epsilon) + \frac{2\epsilon}{m}\frac{\partial a(\nu, \epsilon)}{\partial \epsilon}\right) - \frac{\nu^2\epsilon}{m}\frac{\partial b(\nu, \epsilon)}{\partial \epsilon}\right\}\int_{-1}^{+1}\frac{d\mu}{\nu-\mu} \, .$$

(115)

From equations 114 and 115*, two of the unknown functions $a(\nu, \epsilon)$, $b(\nu, \epsilon)$ or $\lambda(\nu, \epsilon)$ may be determined in terms of the remaining one. $a(\nu, \epsilon)$ will be chosen as the unknown function. Eventually the

*All integrals are evaluated in the principal value sense when necessary.

interface condition 106 will yield a functional equation which will determine $a(\nu, \epsilon)$.

Equation 114 indicates that $b(\nu, \epsilon)$ is of order m^{-1}, consequently $\frac{\epsilon}{m} \frac{\partial b(\nu, \epsilon)}{\partial \epsilon}$ is of order m^{-2}. To be consistent with the m^{-1} approximation the term $\frac{\epsilon}{m} \frac{\partial b(\nu, \epsilon)}{\partial \epsilon}$ should be eliminated from equation 105 for ν in the interval $(-1, 1)$ because it is of order m^{-2}. If this is done, $\lambda(\nu, \epsilon)$ as given by equation 114 becomes

$$\lambda(\nu, \epsilon) = a(\nu, \epsilon) - \nu\left\{\left(\frac{m+2}{2m}\right) a(\nu, \epsilon) + \frac{\epsilon}{m} \frac{\partial a(\nu, \epsilon)}{\partial \epsilon}\right\} \int_{-1}^{+1} \frac{d\mu}{\nu - \mu}, \tag{116}$$

so that

$$\psi(\nu, \epsilon, \mu) = \frac{\nu}{\nu - \mu}\left\{\frac{m+2}{2m} a(\nu, \epsilon) + \frac{\epsilon}{m} \frac{\partial a(\nu, \epsilon)}{\partial \epsilon}\right\}$$
$$+ \left\{a(\nu, \epsilon) - \left(\frac{\nu(m+2)}{2m} a(\nu, \epsilon) + \frac{\nu\epsilon}{m} \frac{\partial a(\nu, \epsilon)}{\partial \epsilon}\right) \int_{-1}^{+1} \frac{d\mu'}{\nu - \mu'}\right\} \delta(\nu - \mu). \tag{117}$$

Case (ii) ν not in the interval $(-1, 1)$

The solution to equation 110 for ν in this range is

$$\psi(\nu, \epsilon, \mu) = \frac{\nu}{\nu - \mu}\left\{\frac{m+2}{2m} a(\nu, \epsilon) + \frac{\epsilon}{m} \frac{\partial a(\nu, \epsilon)}{\partial \epsilon} - \frac{\mu\epsilon}{m} \frac{\partial b(\nu, \epsilon)}{\partial \epsilon}\right\}. \tag{118}$$

The substitution of this result into equation 112 again yields equation 114 for $b(\nu, \epsilon)$ in terms of $a(\nu, \epsilon)$. We again conclude that $\frac{\epsilon}{m} \frac{\partial b(\nu, \epsilon)}{\partial \epsilon}$ is of order m^{-2} and, therefore, should be eliminated from equation 105 for ν in this range. Then equation 118 becomes

$$\psi(\nu, \epsilon, \mu) = \frac{\nu}{\nu-\mu}\left\{\frac{m+2}{2m}\, a(\nu,\epsilon) + \frac{\epsilon}{m}\, \frac{\partial a(\nu,\epsilon)}{\partial \epsilon}\right\} . \tag{119}$$

The substitution of 119 into equation 111 gives a first order differential equation for $a(\nu, \epsilon)$,

$$a(\nu, \epsilon) = \nu \tanh^{-1}\left(\frac{1}{\nu}\right)\left\{\frac{m+2}{2m}\, a(\nu,\epsilon) + \frac{\epsilon}{m}\, \frac{\partial a(\nu,\epsilon)}{\partial \epsilon}\right\} . \tag{120}$$

The solution to this equation is

$$a(\nu, \epsilon) = V(\nu) \quad \exp\left\{\frac{m \ln \epsilon}{2}\left(1 - \frac{m+2}{m}\, \nu \tanh^{-1}\left(\frac{1}{\nu}\right)\right)\right\} , \tag{121}$$

where $V(\nu)$ is an arbitrary function of ν to be determined.

Since the boundary layer correction $\varphi_{bi}(\xi, \epsilon, \mu)$ will be constructed as a superposition of special solutions of the form $e^{-\xi/\nu}\psi(\nu, \epsilon, \mu)$ over all admissible values of ν, $\psi(\nu, \epsilon, \mu)$ will obey the same boundary conditions at $\epsilon = 0$ and $\epsilon = \infty$ as $\varphi_{bi}(\xi, \epsilon, \mu)$. Because of the definition 111, $a(\nu, \epsilon)$ is required to obey the same boundary conditions at $\epsilon = 0$ and $\epsilon = \infty$ as $\psi(\nu, \epsilon, \mu)$ and consequently of $\varphi_{bi}(\xi, \epsilon, \mu)$. To satisfy the condition at zero energy we must have

$$\mathrm{Re}\left(1 - \frac{m+2}{m}\, \nu \tanh^{-1}\left(\frac{1}{\nu}\right)\right) > 0 , \tag{122}$$

so that $a(\nu, 0) = 0$. To satisfy the condition at large energies we must have

$$\mathrm{Re}\left(1 - \frac{m+2}{m}\, \nu \tanh^{-1}\left(\frac{1}{\nu}\right)\right) < -1 , \tag{123}$$

so that the integral of $a(\nu, \epsilon)$ over all ϵ exists. Hence, there are no values of ν in this range which satisfy both conditions simultaneously unless $V(\nu) = 0$. Thus, the only admissible values are those of case (i); i.e., ν real and $-1 \leq \nu \leq 1$.

We now superpose solutions of the form 109 over all values of ν in the interval $(-1, 1)$ and obtain in this way the boundary layer corrections

$$\varphi_{bi}(\xi, \epsilon, \mu) = \int_{-1}^{+1} W_i(\nu) e^{-\xi/\nu} \psi(\nu, \epsilon, \mu)\, d\nu , \quad i = 0, 1, \tag{124}$$

where $W_i(\nu)$ is an arbitrary function of ν to be determined and $\psi(\nu, \epsilon, \mu)$ is given by equation 117 in terms of $a(\nu, \epsilon)$ which also must be determined. The requirement of exponential decay of the boundary layer corrections as $|\xi| \to \infty$ is satisfied by selecting

$$W_o(\nu) = \begin{cases} +1 , & \text{if } \nu > 0 , \\ 0 , & \text{if } \nu < 0 , \end{cases} \tag{125}$$

since $i = 0$ implies $\xi \geq 0$, and

$$W_1(\nu) = \begin{cases} 0 , & \text{if } \nu > 0 , \\ -1 , & \text{if } \nu < 0 , \end{cases} \tag{126}$$

since $i = 1$ implies $\xi \leq 0$. All further ν dependence is expressed in $e^{-\xi/\nu} \psi(\nu, \epsilon, \mu)$. Thus, the boundary layer corrections become

$$\varphi_{b0}(\xi, \epsilon, \mu) = \int_0^1 e^{-\xi/\nu} \psi(\nu, \epsilon, \mu)\, d\nu , \tag{127}$$

for $\xi \geq 0$, and

$$\varphi_{b1}(\xi, \epsilon, \mu) = -\int_{-1}^{0} e^{-\xi/\nu} \psi(\nu, \epsilon, \mu)\, d\nu , \tag{128}$$

for $\xi \leq 0$.

The interface condition 106 then becomes

$$\frac{\epsilon}{2T_o}\left(\frac{e^{-\epsilon/a}}{a^2} - e^{-\epsilon}\right) = \int_{-1}^{+1} \psi(\nu, \epsilon, \mu)\, d\nu$$

$$= a(\mu, \epsilon) - \left(\frac{m+2}{2m}\, a(\mu, \epsilon) + \frac{\epsilon}{m}\, \frac{\partial a(\mu, \epsilon)}{\partial \epsilon}\right) \mu \int_{-1}^{+1} \frac{d\nu}{\mu - \nu}$$

$$+ \int_{-1}^{+1} \frac{\nu}{\nu - \mu} \left(\frac{m+2}{2m}\, a(\nu, \epsilon) + \frac{\epsilon}{m}\, \frac{\partial a(\nu, \epsilon)}{\partial \epsilon}\right) d\nu , \tag{129}$$

with the aid of equation 117 which gives $\psi(\nu, \epsilon, \mu)$ in terms of $a(\nu, \epsilon)$. Equation 129, which must determine $a(\nu, \epsilon)$, is treated in detail in appendix B. The result is

$$a(\mu, \epsilon) = \frac{-\epsilon}{\pi \mu T_o} \int_0^{\infty} dt \left(\frac{e^{-\epsilon u/a}}{a^2} - e^{-\epsilon u}\right) u^2 e^{-\theta t}$$

$$\times (\chi \cos \chi t - \theta \sin \chi t), \tag{130}$$

where

$$u = e^{-t/m}, \tag{131}$$

$$\chi = \frac{\pi}{4\mu} \left[(\tanh^{-1} \mu)^2 + \frac{\pi^2}{4}\right]^{-1} , \tag{132}$$

$$\theta = \frac{1}{2} \left(1 - \frac{4}{\pi} \chi \tanh^{-1} \mu\right) . \tag{133}$$

Therefore, the approximate solution for the angular flux using the approximation scheme is, from 127,

$$\varphi_o(x, \epsilon, \mu) = \frac{\epsilon e^{-\epsilon}}{2T_o} + \int_0^1 e^{-\xi/\nu} \psi(\nu, \epsilon, \mu)\, d\nu \ , \tag{134}$$

for $0 \leq x < \infty$, and, from 128,

$$\varphi_1(x, \epsilon, \mu) = \frac{\epsilon e^{-\epsilon/a}}{2aT_1} - \int_{-1}^0 e^{-\xi/\nu} \psi(\nu, \epsilon, \mu)\, d\nu \ , \tag{135}$$

for $-1/2 \leq x \leq 0$. $\psi(\nu, \epsilon, \mu)$ is given by equation 117. The integral of the angular flux $\varphi(x, \epsilon, \mu)$ over all μ, called the flux $\varphi(x, \epsilon)$, is

$$\varphi_o(x, \epsilon) = \frac{\epsilon e^{-\epsilon}}{T_o} + \int_0^1 e^{-\xi/\nu} a(\nu, \epsilon)\, d\nu \ , \tag{136}$$

for $0 \leq x < \infty$, and

$$\varphi_1(x, \epsilon) = \frac{\epsilon e^{-\epsilon/a}}{aT_1} - \int_{-1}^0 e^{-\xi/\nu} a(\nu, \epsilon)\, d\nu \ , \tag{137}$$

for $-1/2 \leq x \leq 0$, where $a(\nu, \epsilon)$ is given by equation 130. The flux from transport theory, equations 136 and 137, is to be compared with the flux from diffusion theory, equations 56 and 57.

The approximate flux at the interface $x = \xi = 0$ is

$$\begin{aligned} \varphi(0, \epsilon) &= \frac{\epsilon e^{-\epsilon}}{T_o} + \int_0^1 a(\nu, \epsilon)\, d\nu \\ &= \frac{\epsilon e^{-\epsilon}}{T_o} + \frac{1}{2}\int_{-1}^{+1} a(\nu, \epsilon)\, d\nu \ , \end{aligned} \tag{138}$$

since $a(\nu, \epsilon)$ is an even function of ν. Using 130 to 133 the integration may be performed explicitly to give

$$\varphi(0, \epsilon) = \frac{1}{2}\left(\frac{\epsilon e^{-\epsilon}}{T_o} + \frac{\epsilon e^{-\epsilon/a}}{aT_1}\right), \qquad (139)$$

which is the same result for the interface flux as that obtained on the basis of diffusion theory.

Various consequences of the result represented by equations 136 and 137 will be discussed in Part IV.

C. Absorption Case

The case with absorption present is very similar to the scattering case. As in the treatment in Part II based on diffusion theory, the energy variable is restricted to the range $0 \leq \epsilon \leq \epsilon_o$. We must determine an appropriate boundary condition for the angular flux at $\epsilon = \epsilon_o$. In Part II it was argued that the Fermi age model or one-velocity diffusion theory was adequate to describe the high energy neutrons. The same arguments hold in the present case. Thus, at intermediate energies all moments of the angular flux higher than the first may be neglected.

Then from one-velocity diffusion theory, the boundary condition for the angular flux at $\epsilon = \epsilon_o$ is

$$\varphi_i(x, \epsilon_o, \mu) = \frac{1}{2}\left\{f(x) - \mu D_i \frac{df(x)}{dx}\right\}, \quad i = 0, 1, \qquad (140)$$

where D_i is the diffusion constant at $\epsilon = \epsilon_o$ and $f(x)$ is the prescribed function for the neutron flux (see equation 61). The diffusion constant is given by

$$D_i = \frac{1}{3\sigma_s^i(\epsilon_o)} = \frac{1}{3\sigma_i}\left(1 + O(\frac{1}{m})\right), \quad i = 0,1, \qquad (141)$$

where the last part of equation 141 follows from equation 15. For the large mass assumption the boundary condition 140 becomes

$$\varphi_i(x, \epsilon_o, \mu) = \frac{1}{2}\left\{f(x) - \frac{\mu}{3\sigma_i}\frac{df(x)}{dx}\right\}, \quad i = 0,1, \qquad (142)$$

to order m^{-1}.

At zero energy the angular flux is required to be zero

$$\varphi_i(x, 0, \mu) = 0 \quad , \qquad (143)$$

for all x and μ. At the interface the angular flux is to be continuous,

$$\varphi_o(0, \epsilon, \mu) = \varphi_1(0, \epsilon, \mu) \, , \qquad (144)$$

for all $0 \leq \epsilon \leq \epsilon_o$ and $-1 \leq \mu \leq 1$.

We again start the approximation procedure by solving the interior equation. From the analysis of the scattering case in transport theory it is known that the large mass assumption is consistent with diffusion theory for the interior approximation. With the large mass assumption the interior equation is

$$\epsilon a_i \frac{\partial^2 \varphi_i(x, \epsilon, \mu)}{\partial \epsilon^2} + \epsilon \frac{\partial \varphi_i(x, \epsilon, \mu)}{\partial \epsilon} + (1 - \Delta_i(\epsilon/a_i)^{-1/2})\varphi_i(x, \epsilon, \mu) = 0,$$

$$i = 0,1. \qquad (145)$$

Equation 145 may be obtained by expanding the equation with $\alpha = \beta = 0$ from figure 2 for large m, or from the treatment of the absorbing case in diffusion theory, equation 64. The solution to equation 145 satisfying boundary conditions 142 and 143 is

$$\varphi_i(x, \epsilon, \mu) = \frac{1}{2}\left\{f(x) - \frac{\mu}{3\sigma_i} \frac{df(x)}{dx}\right\} \varphi_i(\epsilon), \quad i = 0, 1, \tag{146}$$

where $\varphi_i(\epsilon)$ is given by 68.

The solutions given in 146 satisfy the required conditions at zero energy and for large energy, but do not satisfy the interface condition 144. Therefore, a boundary layer correction, again determined from the equation for $\alpha = 1$, $\beta < 0$ from figure 2, must be added to the interior approximation so that the interface condition is satisfied to order λ^{-1}. The equation governing these boundary layer corrections (with the large mass assumption) is derived in the manner illustrated in the previous cases. It turns out to be

$$\mu \frac{\partial\varphi_{bi}(\xi, \epsilon, \mu)}{\partial} + \varphi_{bi}(\xi, \epsilon, \mu) = -\mu \frac{\epsilon}{m}\int_{-1}^{+1} \mu' \frac{\partial\varphi_{bi}(\xi, \epsilon, \mu')}{d\epsilon}\, d\mu'$$

$$+ \int_{-1}^{+1}\left(\frac{m+2}{2m} \varphi_{bi}(\xi, \epsilon, \mu') + \frac{\epsilon}{m} \frac{\partial\varphi_{bi}(\xi, \epsilon, \mu')}{\partial\epsilon}\right) d\mu',$$

$$i = 0, 1, \tag{147}$$

which is the same as equation 104 which was used to determine the boundary layer correction for the scattering case in transport theory.

The boundary conditions are

$$\varphi_{bi}(\xi, 0, \mu) = 0, \qquad i = 0, 1, \tag{148}$$

$$\varphi_{bi}(\xi, \epsilon_o, \mu) = 0, \qquad i = 0, 1, \tag{149}$$

and the interface condition 144, with the addition of the boundary layer corrections becomes

$$\varphi_o(0, \epsilon, \mu) + \varphi_{bo}(0, \epsilon, \mu) = \varphi_1(0, \epsilon, \mu) + \varphi_{b1}(0, \epsilon, \mu) \quad , \tag{150}$$

for all $0 \leq \epsilon \leq \epsilon_o$ and $-1 \leq \mu \leq 1$. The $\varphi_i(0, \epsilon, \mu)$ terms are given by equation 146. In addition to 148, 149, and 150, exponential decay of φ_{bi} as $|\xi| \to \infty$ is required so that the effect of φ_{bi} is limited to the region near the interface.

The preliminary steps in solving for the boundary layer correction by the method introduced by Case (19) are identical to those in the treatment of the scattering case in transport theory. We again look for solutions to equation 147 of the form

$$e^{-\xi/\nu}\,\psi(\nu, \epsilon, \mu) , \tag{151}$$

and the boundary layer correction is then given by a superposition of the special forms 151 over all admissible values of ν. It is again found that the term $\frac{\epsilon}{m}\int_{-1}^{+1}\mu' \frac{\partial\psi(\nu, \epsilon, \mu')}{\partial\epsilon}\, d\mu'$ is of order m^{-2} for all values of ν and, therefore, should be eliminated from equation 147 as being inconsistent with the m^{-1} approximation. For ν in the interval $(-1, 1)$, $\psi(\nu, \epsilon, \mu)$ is given by

$$\psi(\nu, \epsilon, \mu) = \frac{\nu}{\nu-\mu}\left(\frac{m+2}{2m}\, a(\nu, \epsilon) + \frac{\epsilon}{m}\,\frac{\partial a(\nu, \epsilon)}{\partial\epsilon}\right) + \left\{a(\nu, \epsilon) - \nu\left(\frac{m+2}{2m}\, a(\nu, \epsilon) + \frac{\epsilon}{m}\,\frac{\partial a(\nu, \epsilon)}{\partial\epsilon}\right)\int_{-1}^{+1}\frac{d\mu'}{\nu-\mu'}\right\} \times \delta(\nu-\mu) , \tag{152}$$

where $a(\nu, \epsilon)$ is a function which will eventually be determined by the interface condition 150.

For ν not in the interval $(-1, 1)$ $\psi(\nu, \epsilon, \mu)$ is given by equation 121. We must again have

$$\text{Re}\left[1 - \frac{m+2}{m}\,\nu \tanh^{-1}\left(\frac{1}{\nu}\right)\right] > 0 \ , \tag{153}$$

in order to satisfy 148 that the boundary layer correction vanish at zero energy. From the discussion in Part II of the absorbing case in diffusion theory, it is known that the flux at high energies is inversely proportional to the energy. Since $\psi(\nu, \epsilon, \mu)$ must have the same energy behavior as the flux, we must have

$$\text{Re}\left[1 - \frac{m+2}{m}\,\nu \tanh^{-1}\left(\frac{1}{\nu}\right)\right] \leq -1 \ , \tag{154}$$

in order that the boundary layer correction be less than or equal to a constant times ϵ^{-1} for large ϵ. Thus, again the only admissible values of ν are those in the interval $(-1, 1)$.

To satisfy the requirement of exponential decay in the ξ direction, we again find the boundary layer correction is of the form

$$\varphi_{b0}(\xi, \epsilon, \mu) = \int_0^1 e^{-\xi/\nu}\psi(\nu, \epsilon, \mu)\, d\nu, \tag{155}$$

for $\xi > 0$, and

$$\varphi_{b1}(\xi, \epsilon, \mu) = -\int_{-1}^0 e^{-\xi/\nu}\psi(\nu, \epsilon, \mu)\, d\nu\ , \tag{156}$$

for $\xi < 0$. $\psi(\nu, \epsilon, \mu)$ is given by equation 152. The interface condition 150 becomes

$$\varphi_1(0, \epsilon, \mu) - \varphi_0(0, \epsilon, \mu) = \int_{-1}^{+1} \psi(\nu, \epsilon, \mu)\, d\nu , \tag{157}$$

which after the substitution of 152 for $\psi(\nu, \epsilon, \mu)$ becomes a functional equation for $a(\nu, \epsilon)$. This functional equation is

$$\varphi_1(0, \epsilon, \mu) - \varphi_0(0, \epsilon, \mu) = a(\mu, \epsilon) - \left(\frac{m+2}{2m}\, a(\mu, \epsilon) + \frac{\epsilon}{m} \frac{\partial a(\mu, \epsilon)}{\partial \epsilon} \right) \mu \int_{-1}^{+1} \frac{d\nu}{\mu - \nu}$$

$$+ \int_{-1}^{+1} \frac{\nu}{\nu - \mu} \left(\frac{m+2}{2m}\, a(\nu, \epsilon) + \frac{\epsilon}{m} \frac{\partial a(\nu, \epsilon)}{\partial \epsilon} \right) d\nu . \tag{158}$$

Equation 158, which determines $a(\nu, \epsilon)$, is treated in appendix B. The result is

$$a(\nu, \epsilon) = \frac{-1}{\pi\nu} \int_0^\infty dt \left\{ f(0) \left(\varphi_1(\epsilon u) - \varphi_0(\epsilon u) \right) - \frac{\nu}{3} \frac{df(0)}{dx} \left(\frac{\varphi_1(\epsilon u)}{\sigma_1} - \frac{\varphi_0(\epsilon u)}{\sigma_0} \right) \right\}$$

$$\times\; u e^{-\theta t} (\chi \cos \chi t - \theta \sin \theta t) , \tag{159}$$

where

$$u = e^{-t/m} , \tag{131}$$

and χ and θ are functions of ν given by equations 132 and 133.

The approximate angular flux which results from using the boundary layer technique is then

$$\varphi_0(x, \epsilon, \mu) = \frac{1}{2} \left(f(x) - \frac{\mu}{3\sigma_o} \frac{df(x)}{dx} \right) \varphi_o(\epsilon) + \int_0^1 e^{-\xi/\nu} \psi(\nu, \epsilon, \mu) d\nu , \tag{160}$$

for $0 \leq x < \infty$, and

$$\varphi_1(x,\epsilon,\mu) = \frac{1}{2}\left(f(x) - \frac{\mu}{3\sigma_1}\frac{df(x)}{dx}\right)\varphi_1(\epsilon) - \int_{-1}^{0} e^{-\xi/\nu}\psi(\nu,\epsilon,\mu)\, d\nu, \tag{161}$$

for $-1/2 \leq x \leq 0$. $\psi(\nu,\eta,\mu)$ is given by equation 152.

The integral of the angular flux, equation 160 and 161, over all μ, called the flux, is

$$\varphi_0(x,\epsilon) = f(x)\varphi_o(\epsilon) + \int_0^1 e^{-\xi/\nu}\, a(\nu,\epsilon)\, d\nu, \tag{162}$$

for $0 \leq x < \infty$, and

$$\varphi_1(x,\epsilon) = f(x)\varphi_1(\epsilon) - \int_{-1}^{0} e^{-\xi/\nu} a(\nu,\epsilon)\, d\nu, \tag{163}$$

for $-1/2 \leq x < 0$. $a(\nu,\epsilon)$ is given by equation 158. This flux, equations 162 and 163, is to be compared with that obtained from diffusion theory, equations 78 and 79.

It should be noted that solutions 160 and 161 do not satisfy boundary condition 142. If the term in brackets in equation 159 is expanded about $t = 0$ at $\epsilon = \epsilon_0$, the resulting expansion is

$$a(\mu,\epsilon_0) = \frac{-2\epsilon_0}{\pi m\mu}\frac{d}{d\epsilon}\left\{ f(0)(\varphi_1(\epsilon_0)-\varphi_0(\epsilon_0)) - \frac{\mu}{3}\frac{df(0)}{dx}\left(\frac{\varphi_1(\epsilon_0)}{\sigma_1} - \frac{\varphi_0(\epsilon_0)}{\sigma_0}\right)\right\}$$

$$\times \frac{\chi\left(\theta^2 + \chi^2 - \frac{1}{m^2}\right)}{\left\{\left(\frac{1}{m}+\theta\right)^2 + \chi^2\right\}^2} + O\left(\frac{1}{m^2}\right). \tag{164}$$

The integral of $a(\mu,\epsilon_0)$ over all μ, which is greater than the term which enters in reaction rate calculations, is of order m^{-2}.

Therefore, the amount by which 160 and 161 fail to satisfy boundary condition 142 is of order m^{-2} and, hence, is within the error involved in the large mass approximation of the equations. Therefore, no additional boundary layer correction will be added to the approximation obtained.

The approximate flux at the interface may be calculated by setting $\xi = 0$ in equation 161. The integral over $a(\nu, \epsilon)$ may be performed giving

$$\varphi(0, \epsilon) = \frac{f(0)}{2} (\varphi_0(\epsilon) + \varphi_1(\epsilon)), \tag{165}$$

where $\varphi_0(\epsilon)$ and $\varphi_1(\epsilon)$ are given by equation 68.

IV. DISCUSSION OF ASSUMPTIONS AND RESULTS

A. Discussion of Assumptions

In applying this or any other analysis to an actual reactor calculation, it must be ascertained that the initial assumptions of the analysis are satisfied by the actual system. For the present analysis to be applied to an actual system both m and λ must be large and the step discontinuities in material properties must be well approximated. At the core-reflector interface the step discontinuity in cross sections is applicable; however, the step discontinuity in temperature is applicable only for certain reactors. If the temperature changes from one value to another in a distance less than one mean free scattering length, (or equivalently, a small fraction of λ), then the step function description of the temperature is a good approximation since most of the neutrons in the region of rapidly changing temperature would come from a region of uniform temperature.

If the core and reflector are in contact, the heat generated in the core is conducted to the reflector. In this case the temperature would not be well approximated by a step function since the temperature would most likely be changing continuously over a distance of several mean free scattering lengths. In some reactors there is a gap between the core and reflector. The heat generated in the core is removed by a coolant circulating through the core. In such systems there is little heat transferred from the core to the reflector. Consequently, the step function description of the temperature should be a good approximation for such systems. For the case of gas cooled reactors, where the temperature does change rapidly across the solid-coolant interface, this approximation method would be applicable only if the coolant channel is wide (i.e. λ large). The assumption of the step discontinuity in temperature is a useful starting point for analytical analysis of the problem of neutron distributions in materials with spatial temperature variation.

The assumption that λ be large is not too restrictive. σ, the free atomic cross section, is given by (13)

$$\sigma = 4\pi R^2 N \, , \tag{166}$$

where R, the nuclear radius, equals $1.2 \times 10^{-13} m^{1/3}$ centimeters (20) and N is the number of nucleii per cubic centimeter. For diffusion theory λ is

$$\lambda_D = 0.266 \; \rho m^{-5/6} \; W, \tag{167}$$

and for transport theory

$$\lambda_T = 0.109 \; \rho m^{-1/3} \; W, \tag{168}$$

where ρ is the density in grams per cubic centimeter and W is the slab width in centimeters. For example, with carbon ($m = 12$, $\rho = 1.6$) the λ's are

$$\begin{aligned} \lambda_D &= 0.0536 \; W, \\ \lambda_T &= 0.0763 \; W \, . \end{aligned} \tag{169}$$

Thus, for a carbon system 200 cm. wide, λ is of order 10.

From equations 167 and 168 we see that for the same W and the same material, λ_T is larger than λ_D. Since the boundary layer arguments imply that the error from the actual flux is of order λ^{-1}, the flux derived from transport theory has a smaller error than the approximate flux derived from diffusion theory for the same slab width, W.

The assumption of a heavy gaseous medium is the most unrealistic of the assumptions because very few reactor materials are heavy gases. Most reactor materials are crystalline solids, hence the collisions occur between a neutron and a bound nucleus. The energy exchange cross section is considerably more complicated if the effects of chemical binding are taken into account. The heavy gas energy exchange cross section is the only one that is amenable to an analytic attack.

Aamodt <u>et al</u>. (12) have shown that all energy exchange cross sections approach that of the heavy gas at high neutron energies ($E/T > 1/m$). Nelkin's (21) analysis shows a weak dependence of the thermal spectrum on the choice of the model used to calculate the energy exchange cross sections for heavy nucleii. The equations 44 and 105 used to calculate the boundary layer correction were derived from an argument which assumed that λ was large. This argument implied that the equations were better approximations at high neutron energies. For these reasons the results obtained in this thesis are expected to be better, in the sense of being closer to the actual flux that exists in the physical problem, at high neutron energies ($E/T > 1/m$).

The assumption of large λ and the subsequent α, β argument leads to the equations used for the different regions of the x, ϵ plane. This is equivalent to establishing different models for the different regions. *For instance, the interior equation* ($\alpha = \beta = 0$) is identical with the infinite medium equation. This expresses the fact that neutrons far from the interface are not affected by the presence of the interface. It is interesting that the boundary layer equations, 44 and 105, have constant cross section; implying that the energy dependence of the cross sections is not important for that portion of the flux attributed to the boundary layer corrections. Absorption and the temperature ratio enter the boundary layer correction calculation only through the boundary conditions at the interface. These are consequences of the assumption of large λ and the α, β argument.

Two large parameters, m and λ, are present in the equations. The α, β argument was applied to the equations using λ. At first sight there is no reason why m can not be used for the α, β argument. However, the equations correctly describe the neutron migration regardless of the size of λ, even infinite λ. This is not so with m since the linear transport equation does not correctly describe the situation for infinite mass. For infinite mass the linear transport equation allows for no means of energy transfer because it neglects neutron-neutron collisions. Also for infinite mass the slowing down time is infinite with the linear transport theory model. For these two reasons an equilibrium distribution can never be established in the case of infinite mass with the linear transport theory model. We must, therefore, limit our considerations to large but finite mass. Hence, m may not be used for the α, β argument.

B. Discussion of Results

In Parts II and III, four different problems were considered: scattering and absorbing media for both the diffusion theory and transport theory models. In all four cases an approximate flux, composed of two parts, was constructed using a boundary layer technique. The energy dependence of one part, called the interior approximation, was found to be the same as that which would exist in an infinite medium. The other part, called a boundary layer correction, made an appreciable contribution to the flux only near the interface.

1. Boundary Conditions

For the scattering case the flux was required to be zero at zero energy. At large energies the flux was required to go to zero in such a way that the integral of the flux over all energies existed. Far from the interface in either direction the flux approaches a Maxwellian distribution characterized by the temperature of the medium. The above energy boundary conditions on the flux hold because the flux must be intermediate between the two Maxwellian distributions, each of which has these characteristics.

For the absorbing case the flux is still required to be zero at zero energy because the presence of the absorber should not alter this property of the flux. At a fixed large energy ϵ_o the flux was required to attain a certain prescribed spatial distribution, which is equivalent to a neutron source. The interior approximations were constructed to satisfy these energy boundary conditions; therefore, only the boundary layer corrections need to be investigated.

The transport theory boundary layer corrections are superpositions of solutions of the form $e^{-\xi/\nu}\psi(\nu, \epsilon, \mu)$ over all allowable values of the parameter ν. It was necessary to use both the zero energy and large energy boundary conditions in order to eliminate values of ν except those in the interval -1 to $+1$. To determine a unique solution to the functional equation which arose from the requirement of continuity of flux at the interface, only the small energy boundary condition was satisfied. It was shown in appendix B that the large energy boundary condition was satisfied for the scattering case. It was shown in Part III that, for the absorbing case, the boundary condition at $\epsilon = \epsilon_o$ failed to be satisfied by an amount of order m^{-2}. It is also quite obvious from the form of the solutions, equations 134 and 135, that the condition of exponential decay in the ξ direction is satisfied.

In the treatment based on diffusion theory, the situation is quite different. Here only the large energy boundary condition was satisfied. The differential equation 44 governing the boundary layer correction is a partial differential equation which is of first order in the energy variable; therefore, only one energy boundary condition could be imposed. The corresponding equation in transport theory, equation 105, is a functional equation involving energy and spatial derivatives and integrals over all μ. Both energy boundary conditions are used until the problem is reduced to a first order differential equation in the energy variable. At that stage, again only one energy boundary condition could be satisfied. The solutions to the respective boundary layer equations are determined uniquely only if the boundary conditions mentioned above are selected as the ones to be satisfied for the respective theories.

It remains to investigate the diffusion theory boundary layer corrections for small energies. At the same time exponential decay in the ξ direction will be demonstrated.

We define

$$I(\xi,\epsilon) = \frac{\epsilon\xi}{2\sqrt{\pi}} \int_0^{\infty} \exp\left(-\epsilon e^{1/t^2} + \frac{2}{t^2} - \frac{\xi^2 t^2}{4}\right) dt, \tag{170}$$

for $\xi \geq 0$. According to equation 61, the boundary layer correction for $\xi \geq 0$ is then given by

$$\varphi_{bo}(\xi,\epsilon) = \frac{1}{T_1} I(\xi,\epsilon/a) - \frac{1}{T_o} I(\xi,\epsilon), \tag{171}$$

for the scattering case. We will investigate 170, which is only one term of the boundary layer correction. The behavior of the boundary layer correction can then be obtained from equation 171.

The integral 170 exists for $\epsilon, \xi > 0$ because the integrand is continuous and exponentially small for large t. At $t = 0$ the integrand is zero if $\epsilon > 0$, since $\epsilon e^{1/t^2}$ dominates at small t. With the change of integration variables $y = \xi t$, the integration may be performed at $\xi = 0$, to give

$$I(0, \epsilon) = \frac{\epsilon}{2} e^{-\epsilon} . \tag{172}$$

To investigate the situation for small ϵ, we may not set $\epsilon = 0$ in the integrand, since the integral is divergent because of the behavior of the integrand at small t. L'Hospital's rule cannot be applied to find the limit as ϵ goes to zero, because the resulting integral is still divergent when $\epsilon = 0$.

If $\epsilon > 2$, we may use the inequality

$$e^{1/t^2} \geq \left(1 + \frac{1}{t^2}\right) \quad ; \quad t > 0 \tag{173}$$

in the first term of the exponential of equation 170 to obtain

$$I(\xi, \epsilon) \leq \frac{\epsilon \xi}{2\sqrt{\pi}} e^{-\epsilon} \int_0^\infty \exp\left(\frac{-(\epsilon - 2)}{t^2} - \frac{\xi^2 t^2}{4} \right) dt$$

$$= \frac{\epsilon}{2} e^{-\epsilon} e^{-\xi\sqrt{\epsilon - 2}} . \tag{174}$$

Equation 174 shows the exponential decay in the ξ direction for $\epsilon < 2$; the larger the value of ϵ, the greater the rate of decay. Therefore, the width of the boundary layer correction decreases as ϵ increases. This is to be expected since at large energies the boundary layer corrections are required to do very little smoothing of the interior approximations across the interface.

If $0 < \epsilon < 4$ we again use inequality 173 to obtain

$$I(\xi, \epsilon) \leq \frac{\epsilon\xi}{2\sqrt{\pi}} \left[\exp\left(-\frac{\epsilon}{2} e^{1/t^2} + \frac{2}{t^2}\right)\right]_{max} e^{-\epsilon/2} \int_0^\infty \exp\left(\frac{-\epsilon}{2t^2} - \frac{\xi^2 t^2}{4}\right) dt$$

$$= \frac{16e^{-2}}{\epsilon} \; e^{-\epsilon/2} \, e^{-\xi\sqrt{\epsilon/2}} . \qquad (175)$$

Again for $\epsilon > 0$, there is exponential decay in the ξ direction, although it is quite slow for small ϵ.

It is now possible to determine the region in the z, ϵ plane in which the boundary layer correction $\varphi_{bo}(\xi, \epsilon)$ makes an appreciable contribution to the flux. Suppose we require the flux $\varphi_o(z, \epsilon)$, for $z > 0$, to be described to within a certain percentage, say five per cent, of the Maxwellian interior approximation, so that

$$\left| \frac{\varphi_o(z, \epsilon)}{T_o^{-1}\epsilon e^{-\epsilon}} - 1 \right| = \left| \frac{\varphi_{bo}(\xi, \epsilon)}{T_o^{-1}\epsilon e^{-\epsilon}} \right| \leq 0.05 , \qquad (176)$$

where $\xi = \sigma_o(6/m)^{1/2} z$.

If $\epsilon > \max(2, 2a)$ equations 171 and 174 show that 176 will hold for those values of ξ and ϵ for which*

$$\frac{1}{2} a^{-2} \exp\left[-\epsilon\left(\frac{1}{a} - 1\right) - \xi\sqrt{\frac{\epsilon}{a} - 2}\right] + \frac{1}{2} \exp\left(-\xi\sqrt{\epsilon - 2}\right) \leq 0.05 \qquad (177)$$

*We require $1/2 < a < 1$, so that the exponentials in equation 177 are not growing with increasing ϵ. This limits the range of temperature ratios "a" considered. If $a > 1$, a different argument is used.

On the other hand, if $0 < \epsilon < \min(4, 4a)$, we obtain from 171 and 175 the result that 176 will hold if

$$\frac{16 e^{\epsilon(1-\frac{1}{2a})}}{\epsilon^2 e^2} e^{-\xi\sqrt{\epsilon/2a}} + \frac{16 e^{\epsilon/2}}{\epsilon^2 e^2} e^{-\xi\sqrt{\epsilon/2}} < 0.05 \qquad (178)$$

is satisfied. Now if the temperature ratio "a" is in the range $1/2 < a < 2$, the energy intervals $\epsilon > \max(2, 2a)$ and $0 < \epsilon < \min(4, 4a)$ overlap.

Equations 177 and 178 define a region in the z, ϵ plane in which the boundary layer correction contributes less than 5 per cent of the total flux. The general nature of this region is indicated by the shaded area in figure 3. Since upper bounds were used for the integral $I(\xi, \epsilon)$ in deriving 177 and 178, the shaded region indicated in figure 3 is actually contained within the precise region in which φ_B contributes less than 5 per cent of the total flux. In this sense the shaded region is a conservative estimate.

Equation 178, or alternatively figure 3, indicate the possibility that the flux may not vanish at zero energy. To investigate this possibility, a lower bound to the integral 170 is needed. A lower bound may be constructed to show that

$$I(\epsilon, \xi) > \frac{e^{-2}\xi^3 e^{-\xi^2/4\ln(2/\epsilon)}}{\pi\ \epsilon(\ln 2/\epsilon)^3} , \qquad (179)$$

for $0 < \epsilon < 2$. For $\epsilon \to 0$, we obtain from 179, that $I(\epsilon, \xi) \to \infty$. However, this does not mean that the boundary layer correction necessarily violates the zero energy boundary condition because

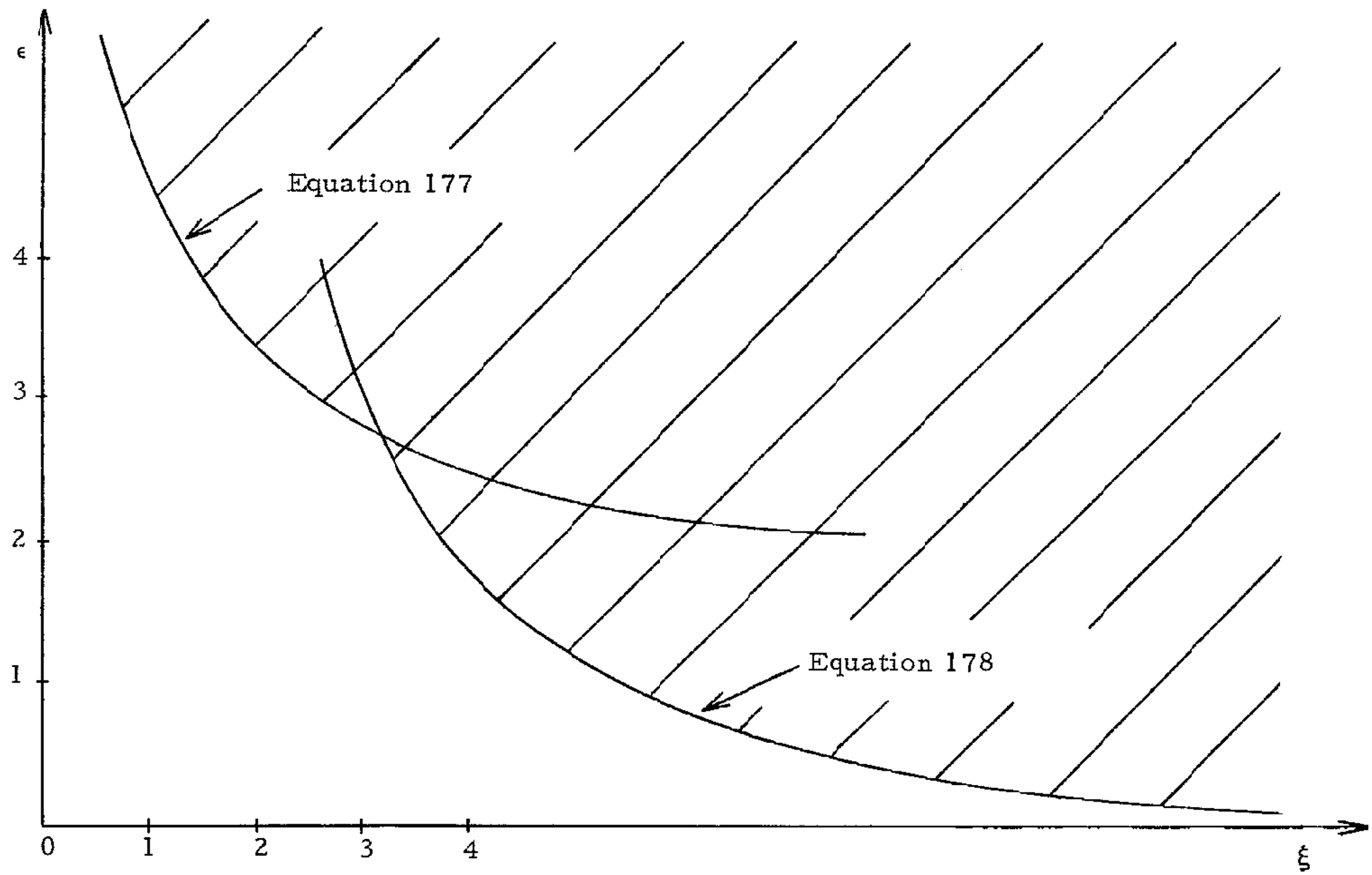

Figure 3. A conservative estimate of the region in ϵ, ξ plane in which $\varphi_{Bo}(\xi, \epsilon)$ contributes less than 5% of the flux.

there may be cancellation between $I(\xi, \epsilon)$ and $I(\xi, \frac{\epsilon}{a})$ as ϵ goes to zero. It has been impossible to show this one way or the other, because of the complicated form of the integrals 170. It would not be too surprising if the zero energy boundary condition was violated, because the boundary layer equation is expected to be a good approximation only at high energies.

It would be even more difficult to show the character of the flux for small energies in the absorbing case. The flux is represented by an infinite series of terms of the form 68. For small energies the upper bound for each term would behave as in 175, and the lower bound as in 179. There would, of course, be different constants multiplying each term, but the energy behavior of each term would be the same. In the absorbing case the same cancellation at small energies might occur because of the infinite series representation of the interior approximations. Again it has been impossible to show whether or not the zero energy boundary condition is satisfied.

2. Flux at the Interface

There exists only one analytic solution reported in the literature with which comparisons of the present results can be made. This is the solution to the diffusion equation 16 for two semi-infinite media at different temperatures in the pure scattering case. Using the same boundary conditions as used in this thesis, Kottwitz (4) gives the flux as

$$\varphi_o(z,\epsilon) = \frac{\epsilon e^{-\epsilon}}{T_o}\left[1+\sum_{n=1}^{\infty} C_n(1-a)^n L_n^1(\epsilon) e^{-\sqrt{n}\,\xi_o}\right] \tag{180}$$

for $z \geq 0$, and

$$\varphi_1(z,\epsilon) = \frac{\epsilon e^{-\epsilon/a}}{a T_1}\left[1+\sum_{n=1}^{\infty} C_n\left(1-\frac{1}{a}\right)^n L_n^1\left(\frac{\epsilon}{a}\right) e^{+\sqrt{n}\,\xi_1}\right] \tag{181}$$

for $z \leq 0$. The ξ_i variables are related to z by

$$\xi_o = \sigma_o (6/m)^{1/2} z, \tag{182}$$

$$\xi_1 = \sigma_1 (6/m)^{1/2} z . \tag{183}$$

The $L_n^1(\epsilon)$'s are the Laguerre polynomials of first order and degree n. The C_n's are constants to be determined by the recursion relation

$$1 + \sum_{k=1}^{n} \binom{n}{k} (-1)^k \left(1 + \sqrt{k/n}\right) C_n = 0, \quad n \geq 1 . \tag{184}$$

The symbol "a" denotes the temperature ratio. Thus, the notation in equations 180 and 181 is the same as that used in the present work.

Equations 180 and 181 are to be compared to the approximate flux obtained by the boundary layer technique, equation 56 for diffusion theory, or equation 136 for transport theory, for the case of large λ. Large λ implies large slab width, so that the geometry of the problem is essentially that of two semi-infinite media.

The most interesting place to compare the flux is at the interface, since away from the interface the flux is the same as that which exists in an infinite medium. The solution given by Kottwitz evaluated at the interface is

$$\varphi_K(0,\epsilon) = \frac{\epsilon e^{-\epsilon}}{T_o}\left[1 + \sum_{n=1}^{\infty} C_n(1-a)^n L_n^1(\epsilon)\right]$$

$$= \frac{\epsilon e^{-\epsilon/a}}{aT_1}\left[1 + \sum_{n=1}^{\infty} C_n\left(1 - \frac{1}{a}\right)^n L_n^1\left(\frac{\epsilon}{a}\right)\right] . \tag{185}$$

The approximate flux at the interface using the boundary layer technique employed in the present work is

$$\varphi_{BL}(0,\epsilon) = \frac{1}{2}\left\{\frac{\epsilon}{T_o} e^{-\epsilon} + \frac{\epsilon}{aT_1} e^{-\epsilon/a}\right\}$$

$$= \frac{\epsilon e^{-\epsilon}}{T_o}\left[1 + \frac{1}{2}\sum_{n=1}^{\infty} (1-a)^n L_n^1(\epsilon)\right] . \tag{186}$$

This result follows from equation 81 in the case of diffusion theory, or from equation 139 for transport theory.

Based on Kottwitz' calculation of the first twenty C_n's, it seems reasonable to assume that

$$\frac{1}{n+1} \leq C_n \leq 0.06 + \frac{0.94}{n+1} , \tag{187}$$

for all $n \geq 1$. With assumption 187 it can be shown that for small ϵ

$$\frac{\epsilon}{T_o}\,\frac{1}{a} \leq \varphi_K(0,\epsilon) \leq \frac{\epsilon}{T_o a}\left(0.94 + \frac{0.06}{a}\right) . \tag{188}$$

for $1/2 < a < 2$.

The approximate flux at the interface, from the boundary layer treatment, for small ϵ is

$$\varphi_{BL}(0,\epsilon) \simeq \frac{\epsilon}{2T_o}(1 + \frac{1}{a^2}) \text{ .} \tag{189}$$

Consequently, for small ϵ

$$\varphi_{BL}(0,\epsilon) \geq \varphi_K(0,\epsilon) \text{ ,} \tag{190}$$

for $1/2 < a < 2$.

For large ϵ we are unable to make a rigorous comparison of $\varphi_K(0,\epsilon)$ to $\varphi_{BL}(0,\epsilon)$ because of difficulties in obtaining the asymptotic form of the C_n's for large n. (Equation 187 is not adequate for large energy considerations.) This is due to the complicated nature of the recursion relation 184. However, because the integral over all ϵ of φ_K is the same as that of φ_{BL} and since φ_{BL} is greater than φ_K for small ϵ, it may be conjectured that φ_K should be greater than φ_{BL} for large ϵ.

Figure 4 is a plot of $\varphi_K(0,\epsilon)$ and $\varphi_{BL}(0,\epsilon)$ vs. ϵ for $a = 3/2$, $T_o = 1$. From figure 4 it can be seen that the above relationships of φ_{BL} to φ_K hold for this particular value of a.

It is interesting that the approximate flux at the interface is the average of the interior approximations extrapolated to the interface, for both the scattering and absorbing cases. It would be expected that the interface flux would be, in some sense, intermediate between the values of the fluxes for the infinite media. The average of the

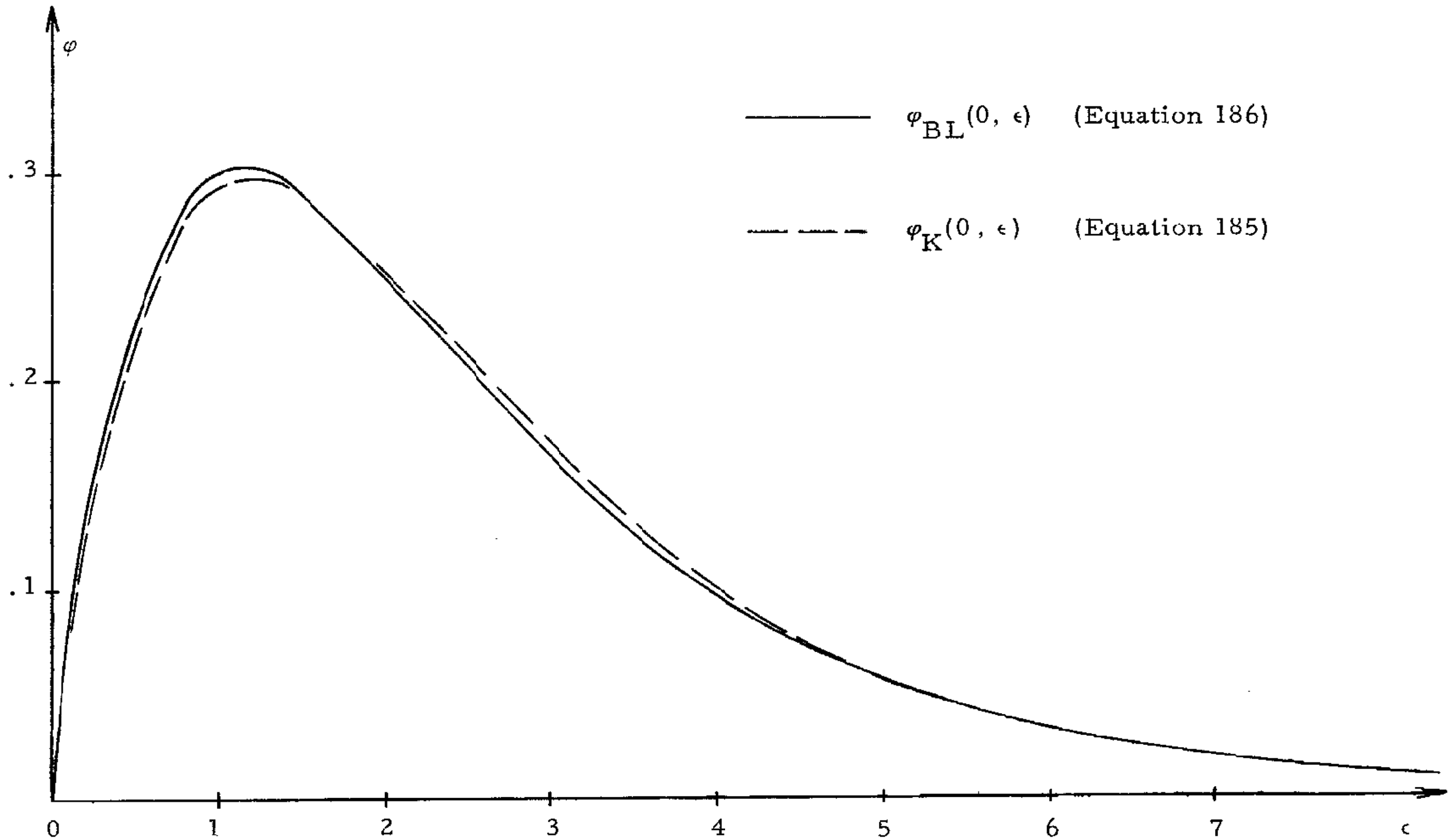

Figure 4. Plot of $\varphi_{BL}(0, \epsilon)$ and $\varphi_K(0, \epsilon)$ vs. ϵ .

two infinite media fluxes is, therefore, a very reasonable result.

It is not surprising that the approximate method applied to the diffusion equation yields a different interface flux than the exact answer to the diffusion equation by Kottwitz. It is surprising that the approximation method yields the same approximate interface flux in both the diffusion theory and transport theory models. Diffusion theory itself is an approximation to transport theory and the quality of this approximation is poorest near the interface (11, 17, 18). However, a small distance from the interface the diffusion theory result and the transport theory result are different as the preceding analysis of the small energy behavior has demonstrated.

3. Neutron Current at the Interface

The neutron current, when calculated according to diffusion theory, is given by equation 7 as

$$j_i(z,\epsilon) = \frac{-1}{3\sigma_i}\frac{\partial\varphi_i(z,\epsilon)}{\partial\xi} = -\left(\frac{2}{3m}\right)^{1/2}\frac{\partial\varphi_i(z,\epsilon)}{\partial\xi}, \quad i = 0,1, \qquad (191)$$

where

$$\xi = \sigma_i\left(\frac{m}{6}\right)^{1/2} z . \qquad (192)$$

The flux, $\varphi_i(z,\epsilon)$, for the scattering case is given by equation 56. The approximate neutron current in the pure scattering case is

$$j_o(z,\epsilon) = -\left(\frac{2}{3m\pi}\right)^{1/2}\frac{\epsilon}{2T_o}\int_0^{\infty}\left(\frac{e^{-\epsilon u/a}}{a^2} - e^{-\epsilon u}\right)u^2\left(1-\frac{\xi^2 t^2}{2}\right)e^{-\xi^2 t^2/4}dt, \qquad (193)$$

for $\xi > 0$, where

$$u = e^{1/t^2} . \tag{194}$$

It may be noted that ξ cannot be set equal to zero directly in 193 because the resulting integral is divergent. We, therefore, make the change of variable $y = \xi t/2$ and recognize that

$$\int_0^\infty (1-2y^2)e^{-y^2}\, dy = 0 . \tag{195}$$

The current may then be written as

$$j(z,\epsilon) = \frac{\epsilon}{\sqrt{6\pi m}\, T_o \xi} \int_0^\infty \left\{ v^2\left(e^{-\epsilon v} - \frac{e^{-\epsilon v/a}}{a^2}\right) - \left(e^{-\epsilon} - \frac{e^{-\epsilon/a}}{a^2}\right) \right\}$$

$$\times \quad (1 - 2y^2)e^{-y^2}\, dy , \tag{196}$$

where

$$v = e^{4\xi^2/y^2} .$$

An application of L'Hospitals rule in 196 gives

$$j(z,\epsilon) = \left(\frac{2}{3m\pi}\right)^{1/2} \frac{\epsilon}{T_o} \int_0^\infty \left\{ u^2\left(e^{-\epsilon u} - \frac{e^{-\epsilon u/a}}{a^2}\right) - \left(e^{-\epsilon} - \frac{e^{-\epsilon/a}}{a^2}\right) \right\} dt, \tag{197}$$

where $u = e^{1/t^2}$. The integral in this equation exists for $\epsilon > 0$, because at large t the integrand is $O(1/t^2)$.

In transport theory the neutron current is given by equation 9 to be

$$j(z,\epsilon) = \int_{-1}^{+1} \mu\varphi(z,\epsilon,\mu)\, d\mu$$

$$= -\frac{2}{m}\frac{\partial}{\partial\epsilon}\int_0^1 e^{-\xi/\nu}\, \nu\epsilon a(\nu,\epsilon)\, d\nu \qquad (198)$$

for $z > 0$, where

$$\xi = \sigma_o z\ , \qquad (199)$$

and $a(\nu,\epsilon)$ is given by equation 130 for the scattering case. In the scattering case the approximate neutron current at the interface is

$$j(z,\epsilon) = \frac{2\epsilon}{m}\int_0^\infty \int_0^1 \nu \left[(2-\epsilon u)e^{-\epsilon u} - \frac{1}{a^2}(2-\frac{\epsilon u}{a})e^{-\epsilon u/a}\right]$$

$$\times\ u^2 e^{-\theta t}(\theta \sin\chi t - \chi\cos\chi t)\, d\nu\, dt\ , \qquad (200)$$

where

$$u = e^{-t/m}\ , \qquad (131)$$

$$\chi = \frac{\pi}{4\nu}\left[(\tanh^{-1}\nu)^2 + \frac{\pi^2}{4}\right]^{-1}, \qquad (132)$$

$$\theta = \frac{1}{2}(1 - \frac{\pi}{4}\chi\ \tanh^{-1}\nu)\ . \qquad (133)$$

Because of the form of the integrals in equations 197 and 200, it is difficult to find either the sign of the current or the behavior for large ϵ.

The coefficient of the neutron current from diffusion theory is $m^{-1/2}$, while that from transport theory is m^{-1}. Thus, the magnitude of the approximate neutron current at the interface is different for the two theories. From this we conclude that the approximate fluxes near the interfaces are quite different, even though the approximate fluxes at the interface are the same. The analysis of the small energy behavior also indicates this to be the case.

From the above analysis it would seem that the first moment of the angular flux is small and, therefore, diffusion theory would be adequate even though the interface is present. However, there is no reason to suspect that the second, third, etc. moments of the angular flux can be neglected when compared to both the zeroth and first moments.

4. Further Remarks

For the problem of a large sphere or cylinder the same boundary layers should be added to the appropriate interior solutions, since a large sphere or cylinder looks the same as a slab for a neutron near the interface. Other energy dependent cross sections can be treated by the same method presented in this thesis. If in the limit of infinite energy the absorption cross section is zero, the boundary layer equations will remain the same. Thus, the only requirement for obtaining an analytic solution is that the interior equations have an analytic solution.

The analysis of the transport theory model would seem to be the most reliable result, because fewer assumptions are involved. Also, transport theory should be inherently better than diffusion theory near the interface. The transport theory results are no more difficult to obtain than those of diffusion theory.

This method of analyzing energy dependent problems seems useful for the case where flux transients, represented by the boundary layer corrections, are introduced by inhomogeneities of material properties. This is the first time, to the authors knowledge, that inhomogeneities of material properties and non-constant cross section have been treated simultaneously. The results should be useful for preliminary reactor calculations to take into account the effects of interfaces on reaction rates.

APPENDIX A

SOLUTION OF THE BOUNDARY LAYER EQUATION IN DIFFUSION THEORY

In applying the boundary layer technique to the diffusion theory model it was found necessary to add boundary layer corrections to the interior approximations near the interface, $x = 0$, in order to satisfy the requirement of continuity of flux at the interface. The boundary value problem determining the boundary layer correction is given by equations 44 through 50 for the scattering case and by equations 69 through 74 for the absorbing case. These two cases may be combined in the following manner.

The relevant equation is

$$\frac{\partial^2 \varphi(\xi, \eta)}{\partial \xi^2} + \eta \frac{\partial \varphi(\xi, \eta)}{\partial \eta} + \varphi(\xi, \eta) = 0 \ , \qquad \text{(A1)}$$

for $\xi \neq 0$. If $\xi < 0$ then $\xi = \xi_1 = \lambda_1 \chi$, $\varphi(\xi, \eta) = \varphi_{b1}(\xi, \eta)$, and $\eta = \lambda_1^{\beta} \epsilon$. If $\xi > 0$ then $\xi = \xi_o = \lambda_o \chi$, $\varphi(\xi, \eta) = \varphi_{bo}(\xi, \eta)$, and $\eta = \lambda_o^{\beta} \epsilon$. β is the negative constant which determines the energy scale on which we are working.

The boundary conditions for large ξ are

$$\varphi(\xi, \eta) \sim e^{-c|\xi|} \quad \text{as} \quad \xi \to \pm \infty \ , \qquad \text{(A2)}$$

for some $c > 0$, where c may be a function of energy.

At $\xi = 0$ the boundary conditions are

$$\frac{\partial \varphi(0^+, \eta)}{\partial \xi} = \frac{\partial \varphi(0^-, \eta)}{\partial \xi} \ , \qquad \text{(A3)}$$

and

$$\varphi(0^+, \eta) - \varphi(0^-, \eta) = h(\epsilon) = h(\lambda^{-\beta}\eta) \tag{A4}$$

In the scattering case, the function h is given by

$$h(\epsilon) = \frac{A\epsilon}{a} e^{-\epsilon/a} - \frac{\epsilon}{T_o} e^{-\epsilon} , \tag{A5}$$

while in the absorbing case

$$h(\epsilon) = f(0)(\varphi_1(\epsilon) - \varphi_o(\epsilon)) , \tag{A6}$$

where $\varphi_1(\epsilon)$ and $\varphi_o(\epsilon)$ are the interior approximations given by equation 68.

The boundary condition at zero energy is that

$$\varphi(\xi, 0) = 0 . \tag{A7}$$

In the scattering case, $\varphi(\xi, \eta)$ is to go to zero for large η in such a way that

$$\int_0^\infty \varphi(\xi, \eta)\, d\epsilon \tag{A8}$$

exists for all ξ. In the absorbing case, ϵ is limited to the range 0 to ϵ_o. At $\epsilon = \epsilon_o$,

$$\varphi(\xi, \epsilon_o) = 0 \tag{A9}$$

Because the differential equation A1 is first order in the energy variable, only one energy boundary condition can be imposed. Since the arguments which lead to equation A1 implied that the equation was most accurate at high energies, the large energy boundary condition

A8, for the scattering case, or A9, for the absorbing case, is the natural one to impose on φ.

Taking the Fourier transform of equation A1 gives

$$\eta \frac{\partial \overline{\varphi}(\rho, \eta)}{\partial \eta} + (1-\rho^2)\overline{\varphi}(\rho, \eta) = - i\rho h(\lambda^{-\beta}\eta) , \qquad \text{(A10)}$$

where

$$\overline{\varphi}(\rho, \eta) = \int_0^\infty e^{i\xi\rho} \varphi(\xi, \eta) e\eta + \int_{-\infty}^0 d^{i\xi\rho}\varphi(\xi, \eta) d\xi. \qquad \text{(A11)}$$

The general solution of the first order differential equation A10 is

$$\overline{\varphi}(\rho, \eta) = - i\rho\eta^{\rho^2-1} \int_\gamma^\eta y^{-\rho^2} h(y\lambda^{-\beta}) dy + C(\rho)\eta^{-\rho^2-1} , \qquad \text{(A12)}$$

where $C(\rho)$ is an arbitrary function of ρ introduced by integrating Equation A10. With the change of integration variables, $y = \lambda^\beta s$, equation A12 becomes

$$\overline{\varphi}(\rho, \eta) = - i\rho\epsilon^{\rho^2-1} \int_\gamma^\epsilon s^{-\rho^2} h(s) ds + C(\rho)\eta^{\rho^2-1} . \qquad \text{(A13)}$$

In equation A13, γ and $C(\rho)$ are to be selected so that boundary condition A8, for the scattering case, or A9, for the absorbing case, is satisfied. We now consider the scattering and absorbing cases separately.

Case (i) <u>Scattering Case</u>

For the scattering case, boundary condition A8 is satisfied by selecting

$$C(\rho) = 0 \,, \tag{A14}$$

because the integral of η^{ρ^2-1} does not exist for any ρ over all η. Since $h(s)$ is an exponential function, we select

$$\gamma = \infty \,, \tag{A15}$$

so that the integral in equation A13 is exponentially small for large ϵ. Therefore, the integral of $\overline{\varphi}(\rho, \eta)$ over all η exists.

The Fourier inversion theorem now provides the solution φ of Equation A1 as

$$\varphi(\xi, \eta) = \frac{\text{Sgn}\,(\xi)}{2\sqrt{\pi}} \int_{\epsilon}^{\infty} \frac{s}{\epsilon} \left(\frac{A}{a}\, e^{-s/a} - \frac{e^{-s}}{T_o} \right) \frac{\xi e^{-\xi^2/4 \ln (s/\epsilon)}}{\ln \frac{s}{\epsilon}^{\;3/2}}\, ds. \tag{A16}$$

With the change of integration variables $s = \epsilon e^{1/t^2}$, equation A16 becomes

$$\varphi(\xi, \eta) = \frac{\xi\epsilon\ \text{Sgn}\,(\xi)}{2\sqrt{\pi}} \int_0^{\infty} \left(\frac{A}{a}\, e^{-\epsilon u/a} - \frac{e^{-\epsilon u}}{T_o} \right) u^2 e^{-t^2 \xi^2/4}\, dt, \tag{A17}$$

where

$$u = e^{1/t^2} . \tag{A18}$$

Case (ii) <u>Absorbing Case</u>

For the absorbing case, boundary condition A9 is satisfied by selecting

$$C(\rho) = 0 \,, \tag{A19}$$

and

$$\gamma = \epsilon_o , \tag{A20}$$

then $\varphi(\xi, \epsilon_o) = 0$. The Fourier inversion theorem then gives

$$\varphi(\xi, \eta) = \frac{\xi \operatorname{Sgn} \xi}{2\sqrt{\pi}\, T_o} \int_{[\ln(\epsilon_o/\epsilon)]^{-1/2}}^{\infty} (\varphi_1(\epsilon u) - \varphi_o(\epsilon u))\, u^2 e^{-t^2\xi^2/4}\, dt, \tag{A21}$$

where the change of integration variables $s = \epsilon e^{1/t^2}$ has been introduced, and u is given by equation A18. $\varphi_o(\epsilon)$ and $\varphi_1(\epsilon)$ are given by equation 68.

If we had chosen to satisfy the zero energy boundary condition, A7, instead of the high energy boundary condition, A8 or A9, it would have been impossible to determine $C(\rho)$. If $\rho > 1$, the term $C(\rho)\eta^{\rho^2-1}$, in the general solution A12, always goes to zero as η goes to zero. Therefore, $C(\rho)$ would remain undetermined for $\rho > 1$. We might then try to impose the high energy boundary condition, but we would find that it would be impossible to satisfy it after the zero energy boundary condition has been satisfied. Thus the requirements $\varphi \to 0$ as $\eta \to 0$ and $\int^{\infty} \varphi \, d\eta < \infty$ are incompatible for the differential equation A10.

The change of variables

$$\eta = e^{-\tau} , \qquad \psi(\xi, \tau) = \eta\varphi(\xi, \eta) , \tag{A22}$$

converts equation A1 into the heat equation

$$\frac{\partial^2 \psi(\xi, \tau)}{\partial \xi^2} = \frac{\partial \psi(\xi, \tau)}{\partial \tau} \, .$$

Therefore, the high energy boundary conditions correspond to initial conditions. It is known that not both initial and final values of the solution to the heat equation can be prescribed. Therefore, only one energy boundary condition can be prescribed for the solution to equation A1.

APPENDIX B

SOLUTION OF THE INTERFACE CONDITION IN TRANSPORT THEORY

In the treatment of the first approximation for the boundary layer correction in transport theory, the interface condition 106 yielded the functional equation 129 (in the scattering case) or 158 (in the absorbing case) for $a(\mu, \epsilon)$. The equations are of the form

$$h(\epsilon) + \mu k(\epsilon) - \int_{-1}^{+1} \left(\frac{m+2}{2m} a(\nu, \epsilon) + \frac{\epsilon}{m} \frac{\partial a(\nu, \epsilon)}{\partial \epsilon} \right) d\nu$$

$$= a(\mu, \epsilon) + \mu \left(\frac{m+2}{2m} a(\mu, \epsilon) + \frac{\epsilon}{m} \frac{\partial a(\mu, \epsilon)}{\partial \epsilon} \right) \int_{-1}^{+1} \frac{d\nu}{\nu - \mu}$$

$$+ \frac{\mu}{2} \int_{-1}^{+1} \frac{d\nu}{\nu - \mu} \left(\frac{m+2}{2m} a(\nu, \epsilon) + \frac{\epsilon}{m} \frac{\partial a(\nu, \epsilon)}{\partial \epsilon} \right) . \quad \text{(B1)}$$

In the scattering case, h and k are

$$h(\epsilon) = \frac{\epsilon}{2T_o} \left(\frac{e^{-\epsilon/a}}{a^2} - e^{-\epsilon} \right) , \quad \text{(B2)}$$

$$k(\epsilon) = 0 . \quad \text{(B3)}$$

In the absorbing case, they have the values

$$h(\epsilon) = \frac{1}{2} f(0)(\varphi_1(\epsilon) - \varphi_o(\epsilon)) , \quad \text{(B4)}$$

$$k(\epsilon) = - \frac{1}{6} \frac{\partial f(0)}{\partial x} \left(\frac{\varphi_1(\epsilon)}{\sigma_1} - \frac{\varphi_o(\epsilon)}{\sigma_o} \right) , \quad \text{(B5)}$$

where $\varphi_i(\epsilon)$ is given by equation 68. The boundary condition at zero energy is

$$a(\mu, 0) = 0 , \tag{B6}$$

for all μ.

Equation B1 will be solved using boundary condition B6 by making use of the techniques for treating singular integral equations given by Muskhelishvili (22). All integrals are to be evaluated in the principal value sense when necessary.

Integrating equation B1 for all μ yields

$$h(\epsilon) = \frac{1}{2}\int_{-1}^{+1} a(\mu, \epsilon)\, d\mu . \tag{B7}$$

Thus the left-hand side of equation B1 becomes

$$-\frac{2h(\epsilon)}{m} - \frac{2\epsilon}{m}\frac{dh(\epsilon)}{d\epsilon} + \mu k(\epsilon) . \tag{B8}$$

We define the following functions

$$A(z, \epsilon) = \frac{1}{2\pi i}\int_{-1}^{+1} \frac{a(\nu, \epsilon)}{\nu - z}\, dz , \tag{B9}$$

$$H(z, \epsilon) = \frac{1}{2\pi i}\int_{-1}^{+1}\left(\frac{-2h(\epsilon)}{m} - \frac{2\epsilon}{m}\frac{dh(\epsilon)}{d\epsilon} + \nu k(\epsilon)\right)\frac{d\nu}{\nu - z} , \tag{B10}$$

$$R(z) = \int_{-1}^{+1} \frac{d\nu}{z - \nu} , \tag{B11}$$

where z is complex.

The functions A, H, and R are analytic in the z plane cut from -1 to +1 and are zero at infinity. As z approaches the cut from above or below the Plemelj formula gives

$$A^{\pm}(\mu,\epsilon) = \pm \frac{1}{2} a(\mu,\epsilon) + \frac{1}{2\pi i}\int_{-1}^{+1} \frac{a(\nu,\epsilon)}{\nu-\mu}\, d\nu , \qquad \text{(B12)}$$

$$H^{\pm}(\mu,\epsilon) = \pm \frac{1}{2}\left(\frac{-2h(\epsilon)}{m} - \frac{2\epsilon}{m}\frac{dh(\epsilon)}{d\epsilon} + \mu k(\epsilon)\right)$$

$$+ \frac{1}{2\pi i}\int_{-1}^{+1}\left(\frac{-2h(\epsilon)}{m} - \frac{2\epsilon}{m}\frac{dh(\epsilon)}{d\epsilon} + \nu k(\epsilon)\right)\frac{d\nu}{\nu-\mu} , \qquad \text{(B13)}$$

$$R^{\pm}(\mu) = \quad \pi i + \int_{-1}^{+1} \frac{d\nu}{\mu-\nu} , \qquad \text{(B14)}$$

where the upper or lower sign indicates that z approaches the cut from above or below, respectively. We, therefore, have

$$A^{+}(\mu,\epsilon) - A^{-}(\mu,\epsilon) = a(\mu,\epsilon) , \qquad \text{(B15)}$$

$$A^{+}(\mu,\epsilon) + A^{-}(\mu,\epsilon) = \frac{1}{2\pi i}\int_{-1}^{+1} \frac{a(\nu,\epsilon)}{\nu-\mu}\, d\nu , \qquad \text{(B16)}$$

$$H^{+}(\mu,\epsilon) - H^{-}(\mu,\epsilon) = \frac{-2h(\epsilon)}{m} - \frac{2\epsilon}{m}\frac{dh(\epsilon)}{d\epsilon} + \mu k(\epsilon) , \qquad \text{(B17)}$$

$$R^{+}(\mu) - R^{-}(\mu) = -\, 2\pi i , \qquad \text{(B18)}$$

$$R^{+}(\epsilon) + R^{-}(\mu) = -\, 2\int_{-1}^{+1} \frac{d\nu}{\nu-\mu} . \qquad \text{(B19)}$$

With the help of B8 and B15 through B19 equation B1 may now be written as

$$H^{+}(\mu,\epsilon) - H^{-}(\mu,\epsilon) = A^{+}(\mu,\epsilon) - A^{-}(\mu,\epsilon)$$

$$- \frac{\mu}{2}\left(R^{+}(\mu) + R^{-}(\mu)\right)\left[\frac{m+2}{2m}\left(A^{+}(\mu,\epsilon) - A^{-}(\mu,\epsilon)\right) + \frac{\epsilon}{m}\frac{\partial}{\partial\epsilon}\left(A^{+}(\mu,\epsilon) - A^{-}(\mu,\epsilon)\right)\right]$$

$$- \frac{\mu}{2}\left(R^{+}(\mu) - R^{-}(\mu)\right)\left[\frac{m+2}{2m}\left(A^{+}(\mu,\epsilon) + A^{-}(\mu,\epsilon)\right) + \frac{\epsilon}{m}\frac{\partial}{\partial\epsilon}\left(A^{+}(\mu,\epsilon) + A^{-}(\mu,\epsilon)\right)\right] ,$$

(B20)

where it has been assumed in the last term that differentiation with respect to ϵ and integration with respect to ν can be interchanged. Upon multiplying out the terms of equation B20 we obtain

$$H^+(\mu,\epsilon)-A^+(\mu,\epsilon)+\mu R^+(\mu)\left[\frac{m+2}{2m}\;A^+(\mu,\epsilon)+\frac{\epsilon}{m}\frac{\partial A^+(\mu,\epsilon)}{\partial\epsilon}\right]$$

$$= H^-(\mu,\epsilon)-A^-(\mu,\epsilon)+\mu R^-(\mu)\left[\frac{m+2}{2m}\;A^-(\mu,\epsilon)+\frac{\epsilon}{m}\frac{\partial A^-(\mu,\epsilon)}{\partial\epsilon}\right]. \qquad \text{(B21)}$$

Now the function

$$F(z,\epsilon) = H(z,\epsilon)-A(z,\epsilon)+zR(z)\left[\frac{m+2}{2m}\,A(z,\epsilon)+\frac{\epsilon}{m}\;\frac{\partial A(z,\epsilon)}{\partial\epsilon}\right], \qquad \text{(B22)}$$

is zero at infinity since H and A are zero at infinity and zR(z) tends to two as z tends to infinity. Furthermore, $F(z,\epsilon)$ is analytic everywhere in the z plane except possibly at the cut from -1 to +1 because H, A, and R are analytic everywhere except at the cut. However, the difference in $F(z,\epsilon)$ across the cut is zero by equation B21. Therefore, $F(z,\epsilon)$ is analytic everywhere and zero at infinity and consequently it must be zero everywhere by Liouville's theorem. Equation B22 then becomes the first order inhomogeneous differential equation

$$\epsilon\,\frac{\partial A(z,\epsilon)}{\partial\epsilon} + \left(1+\frac{m}{2}-\frac{m}{zR(z)}\right)A(z,\epsilon) = -\,H(z,\epsilon)\,. \qquad \text{(B23)}$$

From the definition B9, $A(z,\epsilon)$ will obey the same energy boundary condition B6 that $a(\mu,\epsilon)$ does; $a(\mu,\epsilon)$ will then be determined from equation B15. The general solution of equation B23 is

$$A(z,\epsilon) = \frac{-m\epsilon^{-g(z)}}{zR(z)} \int_0^{\epsilon} y^{g(z)-1} H(z, y)\, dy + c(z)\epsilon^{-g(z)} , \tag{B24}$$

where c(z) is an arbitrary function of z introduced by integrating equation B23. The function g(z) is given by

$$g(z) = 1 + \frac{m}{2} - \frac{m}{zR(z)} . \tag{B25}$$

In order to satisfy the zero energy boundary condition B6, c(z) must be zero since $\text{Re}\{g(z)\} > 1$. If we had chosen to satisfy the large energy boundary condition, c(z) would remain undetermined. Therefore, we must satisfy the zero energy boundary condition in order to determine the solution uniquely.

Equation B10 may be rewritten as

$$H(z, \epsilon) = \frac{R(z)}{m\pi i} \frac{d(\epsilon h(\epsilon))}{d\epsilon} + \frac{k(\epsilon)}{\pi i}\left(1 - \frac{z}{2} R(z)\right) . \tag{B26}$$

Substitution of B26 into B24 and integration by parts on the first term gives

$$A(z, \epsilon) = \frac{1}{2\pi i}\left\{- h(\epsilon) + (g(z)-1) \int_0^{\epsilon} \left(\frac{y}{\epsilon}\right)^{g(z)} h(y) \frac{dy}{y}\right\}$$
$$+ \frac{1}{\pi i} (g(z)-1) \int_0^{\epsilon} \left(\frac{y}{\epsilon}\right)^{g(z)} k(y) \frac{dy}{y} . \tag{B27}$$

$a(\mu, \epsilon)$ is now determined from equation B15. $g^{+}(\mu)$ and $g^{-}(\mu)$

are determined from equations B25 and B14. The result for the scattering case after the change of variables $t = -m \ln y/\epsilon$ is

$$a(\mu, \epsilon) = \frac{\epsilon}{\pi\mu T_o} \int_0^\infty dt \left(\frac{e^{-\epsilon u/a}}{a^2} - e^{-\epsilon u} \right) u^2 e^{-\theta t}$$

$$(\theta \sin \chi t - \chi \cos \chi t) \;, \qquad \text{(B28)}$$

where

$$u = e^{-t/m} \;, \qquad \text{(B29)}$$

$$\chi = \frac{\pi}{4\mu} \left[(\tanh^{-1} \mu)^2 + \frac{\pi^2}{4} \right]^{-1}, \qquad \text{(B30)}$$

$$\theta = \frac{1}{2} (1 - \frac{4}{\pi} \chi \tanh^{-1} \mu) \;. \qquad \text{(B31)}$$

If equation B28 is integrated over all ϵ, the $\int^\infty a(\mu, \epsilon)\, d\epsilon$ exists because the remaining integral over t exists. The integral over t exists because θ, as given by equation B31, is positive for all μ.

For the absorbing case the result is

$$a(\mu, \epsilon) = \frac{1}{\pi\mu} \int_0^\infty dt \left[f(0)(\varphi_1(\epsilon u) - \varphi_o(\epsilon u)) - \frac{1}{3} \frac{\partial f(0)}{\partial x} \left(\frac{\varphi_1(\epsilon u)}{\sigma_1} - \frac{\varphi_o(\epsilon u)}{\sigma_o} \right) \right]$$

$$\times\; u e^{-\theta t} (\theta \sin \chi t - \chi \cos \chi t) \;. \qquad \text{(B32)}$$

The results B28 and B32 may be verified by substitution into equation B1.

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