

1964

# Temperature dependent neutron thermalization

Varada P.T Charyulu  
*Iowa State University*

Follow this and additional works at: <https://lib.dr.iastate.edu/rtd>

 Part of the [Nuclear Commons](#)

## Recommended Citation

Charyulu, Varada P.T, "Temperature dependent neutron thermalization " (1964). *Retrospective Theses and Dissertations*. 2731.  
<https://lib.dr.iastate.edu/rtd/2731>

This Dissertation is brought to you for free and open access by the Iowa State University Capstones, Theses and Dissertations at Iowa State University Digital Repository. It has been accepted for inclusion in Retrospective Theses and Dissertations by an authorized administrator of Iowa State University Digital Repository. For more information, please contact [digirep@iastate.edu](mailto:digirep@iastate.edu).

This dissertation has been        65-3788  
microfilmed exactly as received

CHARYULU, Varada P. T., 1934-  
TEMPERATURE DEPENDENT NEUTRON  
THERMALIZATION.

Iowa State University of Science and Technology  
Ph.D., 1964  
Physics, nuclear

University Microfilms, Inc., Ann Arbor, Michigan

TEMPERATURE DEPENDENT NEUTRON THERMALIZATION

by

Varada P. T. Charyulu

A Dissertation Submitted to the  
Graduate Faculty in Partial Fulfillment of  
The Requirements for the Degree of  
DOCTOR OF PHILOSOPHY

Major Subject: Nuclear Engineering

Approved:

Signature was redacted for privacy.  
In Charge of Major Work

Signature was redacted for privacy.  
Head of Major Department

Signature was redacted for privacy.  
Dean of Graduate College

Iowa State University  
Of Science and Technology  
Ames, Iowa

1964

## TABLE OF CONTENTS

	Page
INTRODUCTION	1
REVIEW OF LITERATURE	3
STATEMENT OF THE PROBLEM	10
RIGOROUS SOLUTION	12
APPROXIMATE SOLUTIONS	38
DISCUSSION	65
CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER INVESTIGATION	71
LITERATURE CITED	73
ACKNOWLEDGMENTS	75

## INTRODUCTION

During the preliminary stages of reactor design, a knowledge of the reactor flux spectrum is essential in order to evaluate a set of properly averaged nuclear parameters such as cross sections. It is customary in elementary reactor theory to treat thermal neutrons as a monoenergetic group and then to use in the design calculations a properly averaged set of absorption and scattering cross sections of the medium assuming that the neutrons have Maxwellian distribution of velocity characterized by the temperature of the medium. This treatment cannot be expected to be rigorous as absorption per se, if not any other factor, disturbs the equilibrium by removing neutrons from the medium. In addition to absorption if the temperature variation in the medium is considered, the simpler theory is hardly valid. The reactor designer does often encounter situations which involve two adjacent media with markedly different temperatures and/or compositions. As an example one may consider a lattice cell containing a high temperature fuel element and relatively cooler medium surrounding it. The purpose of the present investigation is to present a theoretical method suited to solving the problem of the thermal flux spectrum in two adjacent media at different temperatures with and without absorption. Both rigorous and approximate expressions have been developed for

the flux spectrum in such media with  $\frac{1}{V}$  absorption.

It is felt that the problem of thermalization in media with non-uniform temperature will achieve increased importance as reactors with strong temperature gradients become more common. Although the problem considered in the present investigation may be too idealized to be of direct use in reactor applications, it is felt that the availability of an analytic or even an approximate solution will be of help in checking numerical methods developed for use in more complicated problems.

## REVIEW OF LITERATURE

In nuclear reactors neutrons are produced, primarily by fission, with energies large compared to the energy of thermal motion of the moderator. These neutrons while slowing down undergo three processes in succession: moderation, thermalization and diffusion. The term moderation is usually applied to the case of neutrons slowing down to an energy range somewhat above that in which the neutron energy and moderator energy are comparable. This theory of moderation is well established and has been well presented by Weinberg and Wigner (1).

Thermalization is the process of slowing down below the energy limit just mentioned, in which the neutrons are approaching thermal equilibrium with the moderator but cannot quite do so due to absorption while being thermalized. During the process of thermalization neutrons lose as well as gain energy through collisions with the atoms of the moderator, which have a distribution of velocities and are bound, in the case of solids or liquids. The neutron thermalization continues until the neutrons attain an asymptotic energy distribution characterized by the energy exchange scattering kernel and by the absorption and leakage of neutrons. In weakly absorbing media thermalization will be almost complete and there will be a large group of neutrons with approximately Maxwellian energy distribution.

The process of diffusion follows the thermalization process. During diffusion the shape of the asymptotic energy spectrum is not altered but only the amplitude decreases with time. Eventually this process is terminated by the absorption or leakage of neutrons from the medium.

The scope of the present investigation is limited to the thermalization theory which is concerned with the calculation of neutron energy distribution in the energy region from zero to a few electron volts. In this energy region, the thermal motion and the chemical binding of the moderating nuclei influence the energy transfer properties although the nuclear scattering amplitudes for all moderating materials are independent of neutron energy as well as scattering angle (2). The energy interchange between neutrons and the moderator is of such a nature that the neutrons can reach thermal equilibrium with the moderator only if the average number of scattering collisions of a thermal neutron before absorption is sufficiently large. As mentioned earlier, the neutron must be able to gain as well as lose energy in collisions with the moderating nuclei, so that the scattering leads to thermal equilibrium. This is the essential difference between the phenomenon of neutron thermalization and neutron slowing down. The purpose of calculating the neutron spectrum is to determine the deviations of the thermal spectrum from an equilibrium Maxwellian distribution. The thermal spectrum is governed by the

energy change cross section,  $\sigma (E \rightarrow E')$ , of the moderating material. The calculation of this cross section is rather complicated for all moderating media of practical interest. Hence a simplifying assumption is made that the medium is a heavy monoatomic gas in which case  $\sigma (E \rightarrow E')$  can be calculated. Several studies on moderators of practical interest, which are chemically bound in either the crystalline state or the liquid state, have indicated that the chemical binding effect is not large (3). However, these results are either purely numerical in nature or are based on fragmentary experimental information, and as yet the physical understanding of the conditions under which the chemical binding effects are important is vague. Hence in the present investigation the medium is assumed to be a monoatomic gas.

Wigner and Wilkins (4) were the first to derive and discuss the integral equation for the energy distribution of neutrons in an infinite homogeneous medium when the moderator is a monoatomic gas. They were able to reduce the integral equation to a differential equation and solve by numerical methods for a hydrogen moderator. By the use of Monte Carlo techniques Coveyou, Bate and Osborne (5) have solved the integral equation in the monoatomic case, for a large range of nuclear masses and absorption to scattering ratios. This technique is time consuming even on large computing machines. However, this may be useful if space

dependence is also included.

Wilkins (6) was successful in reducing the integral equation to a second order differential equation in the limit of large moderator mass on general mathematical grounds. Later Hurwitz, Nelkin and Habetler (7) also formed a second order differential equation from the integral equation on better physical grounds. They have calculated, numerically, the energy distribution and migration area of neutrons in an infinite homogeneous medium with  $1/V$  absorption. Similar work has been accomplished by Cohen (8) but on an analytic basis. There is considerable overlap in these two later papers, but Cohen has primarily investigated the mathematical properties of Wilkin's equation where as Hurwitz et al. have dwelt on the physical nature of the heavy gas model.

All the work cited so far has been for a medium with uniform properties. Space-energy distribution of neutrons was not considered except briefly by Hurwitz et al., where the space-energy distribution function is examined for the region of relatively high energies. A more general case has been treated by Kazarnovsky, Stepanov and Shapiro (9). By including extraneous sources in a non-absorbing medium of variable mass and variable neutron mean free path with position, they have derived an age-type equation for the space-energy distribution. Besides, they have formulated another method of approaching similar problems by expanding

the neutron distribution function in terms of energy groups. The two specific cases they have examined are a) a finite or infinite moderator of uniform properties and b) a medium composed of two dissimilar contiguous plates of infinite extensions, the neutron sources being located on the interface. This latter method is particularly suited for the solution of problems in which the source emits neutrons with energies close to thermal or when a knowledge of the precise shape of the neutron energy spectrum is not known. Examples of such problems are when the steady state neutron diffusion at a large distance from the source is desired or when the neutron diffusion at a large distance from a pulse source is desired after long time.

The problem of finding the steady state space energy distribution of flux when the sources of neutrons are distributed in space was solved by Michale (10). From the general form of the solution he was able to show that the space-wise asymptotic distribution depends upon the distribution of sources and is governed by the extent of the sources. More specifically, for a source with larger extent than the thermal diffusion length the asymptotic spectra are dependent on the energy distribution of the source while for sources of limited extent, the asymptotic distribution is independent of the source spectra.

However, the studies on the space energy distribution cited thus far have been confined only to the variation of

the mass of the medium with position or the variation of the source with position. Very few investigators have considered the temperature of the medium as a function of position. The first breakthrough in this area came about when Kottwitz (11) was able to solve analytically the problem of a thermal neutron flux spectrum in a medium with a temperature discontinuity. He considered an infinite homogeneous non-absorbing medium which has an absolute temperature  $T_1$ , in one half space and  $T_2$  in the other and arrived at the steady state solution for neutron flux distribution when the ratio of the two temperatures was 2:1. He has compared his solution with those based on two other approximate schemes giving simple analytical results. One of the approximation schemes employs the concept of neutron temperature, the other method utilizes the two thermal group approximation, which is a special case of Selengut's method (12). Basically, Selengut's method consists of approximating the actual neutron distribution by a superposition of overlapping thermal groups. The thermal groups chosen are those in equilibrium with each region of uniform temperature in the system. The rate of transfer of neutrons in the non-equilibrium groups into the local equilibrium group can be calculated in a simple manner for the case of heavy gas moderator. This calculation will be considered in greater detail in later sections. Another work of interest in this area is due to de Ladonchamps and

Grossman (13). They have investigated the space energy distribution of neutrons diffusing in a source-free non-absorbing medium possessing a temperature gradient. They were able to do this by solving the appropriate Boltzmann equation to a second order approximation using the expansion technique of Chapman and Enskog. They found that the neutron current increased in the direction of negative temperature gradient.

However, the work reviewed so far for the medium of non-uniform temperature has been restricted to non-absorbing media and also to a temperature distribution of idealized type. The present investigation is directed toward a consideration of the effect of a non-uniform temperature of the medium on the thermal neutron flux spectrum, when the medium itself has  $\frac{1}{V}$  type absorption.

## STATEMENT OF THE PROBLEM

The purpose of the present investigation is to study the effect of temperature, as a function of position, on the thermal neutron flux spectrum in a source-free absorbing medium.

For mathematical simplicity, the medium is assumed to be infinite in extent, consisting of two semi-infinite regions with a common boundary plane. Positions are denoted by a single coordinate indicating distances from the common plane. For further analytical simplicity, the temperature is assumed to be a constant in one half of the medium and a different constant in the other half of the medium. In other words, the temperature is a step function of position. The scattering cross section is assumed to be independent of energy while the absorption cross section is assumed to obey the  $\frac{1}{v}$  law. Further, the entire medium is treated as a heavy monoatomic gas so that the chemical binding and crystalline effects are eliminated. As a result of this assumption the scattering is considered to be isotropic in the laboratory system of coordinates and also, the energy transfer in a single collision is taken to be small. The transport aspects of the problem are considered in the P<sub>1</sub> approximation of the Boltzman equation and the associated boundary conditions at the interface between the hot and cold halves of the medium.

Analytical solutions are presented for the second-order partial differential equation which results from the stated assumptions. The boundary conditions imposed on the system are that the flux shall vanish at zero energy and have finite energy moments everywhere in the medium. Also, far from the interface of the two temperature regions, the flux spectrum shall be independent of position, i.e., the effect of one temperature on the other is not felt at large distances from the interface. In addition to these conditions there are the conditions that at the temperature interface the flux together with the first derivative shall be continuous.

An analytical solution is developed in the next section by solving the equation separately in the two regions by the method of separation of variables and matching the resulting solutions for each region at the temperature discontinuity by the conditions at the interface.

Approximate solutions are developed to the same problem as well as a similar problem in a non-absorbing medium using the method of Galerkin.

## RIGOROUS SOLUTION

In order to be able to calculate deviations from a Maxwellian energy distribution, a particular model for the medium must be assumed. The simplest model is the mono-atomic heavy gaseous moderator with a Maxwellian distribution of nuclear velocities. The advantage of this model is that it bypasses the less well understood chemical binding and crystalline effects but does retain the essential features of neutron thermalization. This model will be valid in every case at sufficiently high temperatures.

Based on this model a partial differential equation has been derived in the diffusion approximation by Hurwitz, Nelkin and Habetler (7). In a form suitable to the present investigation it is

$$\frac{D}{2\mu\Sigma_s} (\nabla^2\phi) + \left[ 1 - a'(E) + E \frac{\partial}{\partial E} + E \theta(r) \frac{\partial^2}{\partial E^2} \right] \phi = 0 \quad (1)$$

which gives the steady state neutron flux spectrum in a homogeneous, isotropic medium without extraneous sources, where,

$\phi (r, E)$  = flux per unit energy interval.

$D$  = diffusion coefficient of the medium

$\mu$  = ratio of neutron mass to that of the moderator nucleus

$\theta(r)$  = temperature of the medium times Boltzmann's  
constant, i.e.  $kT$

$$a' = \frac{\Sigma_a}{2\mu\Sigma_s}$$

$\Sigma_a$  = macroscopic absorption cross section

$\Sigma_s$  = macroscopic scattering cross section

Due to the presence of the term  $\theta(r)$ , this partial differential equation cannot be solved by the usual technique of separation of variables, except in a few special cases. If the medium is assumed to be infinite in extent and the temperature of the medium is a constant in one half space and a different constant in the other half space, it will be possible to obtain an analytical solution to the above equation for each region. The solutions thus obtained for each region can be matched at the interface by suitable boundary conditions and the solution continued from one region to the other.

Without loss of generality, only one dimensional case for the spatial dependence can be considered. Further, it will be assumed that the scattering cross section is independent of energy, which is a valid assumption for the monoatomic heavy gas model. Thus, the Equation 1 for the case of  $\frac{1}{V}$  absorption can be written as,

$$\frac{D}{2\mu\Sigma_s} \frac{\partial^2 \Phi}{\partial z^2} + \left[ 1 - \frac{a}{\sqrt{E}} + E \frac{\partial}{\partial E} + E \theta(z) \frac{\partial^2}{\partial E^2} \right] \Phi = 0 \dots (2)$$

$$\text{where, } \theta(z) = \begin{cases} \theta_1 & \text{for } z < 0 \\ \theta_2 & \text{for } z > 0 \end{cases} \quad (3)$$

Since Equation 2 is an elliptic second order equation, the boundary conditions on  $\mathfrak{S}$  or its normal derivative along the entire perimeter of the relevant region in the  $x, E$  plane are necessary to determine a unique physical solution to the problem. For this problem the boundary conditions are

$$\frac{\partial \phi}{\partial z} (\pm \infty, E) = 0 \quad (4)$$

$$\phi(z, 0) = 0 \quad (5)$$

$$E^n \phi(z, E) \longrightarrow 0 \quad \text{as } E \longrightarrow \infty \text{ for all } z \text{ and } n. \quad (6)$$

Also, at the interface, which is taken to be at the origin,

$$\phi(0^-, E) = \phi(0^+, E) \quad (7)$$

$$\frac{\partial \phi(0^-, E)}{\partial z} = \frac{\partial \phi(0^+, E)}{\partial z} \quad (8)$$

Physically the boundary conditions have the following meaning. Equation 4 reflects the absence of sources everywhere in the medium. The condition (5) and (6) guarantee the flux to be finite and meaningful. The conditions at the interface given by Equations 7 and 8 provide for the continuity of flux and the neutron current to the zeroth order approximation in  $\mu$  to the exact equation expressing the continuity of neutron current across the interface. Besides,

far from the interface the flux spectrum is independent of position as the effect of the temperature of one region on the other is little. This condition is implicit in Equation 4.

It is convenient to write Equation 2 in dimensionless form by introducing a new set of variables as follows:

$$y = \sqrt{\frac{2\mu\Sigma_s}{D}} z \quad (9)$$

and

$$x^2 = \frac{E}{\theta}$$

The differential Equation 2 then becomes

$$\frac{\partial^2 \phi}{\partial y^2} + \left[ x \frac{\partial^2 \phi}{\partial x^2} + (2x^2 - 1) \frac{\partial \phi}{\partial x} + (4x - 4a)\phi \right] \frac{1}{4x} = 0 \quad (10)$$

Now, assuming a product solution of the form

$$\phi(x, y) = f(x) \cdot h(y)$$

and using the standard procedure of introducing a separation constant  $n$  Equation 10 results in two ordinary differential equations.

$$h'' - nh = 0 \quad (11)$$

$$xf'' + (2x^2 - 1)f' + 4 \left[ (n+1)x - a \right] f = 0 \quad (12)$$

In view of boundary condition stated in Equation 4 the

acceptable solutions to Equation 11 are restricted to

$$h(y) = \exp(-\sqrt{n} |y|) \quad (13)$$

where  $\sqrt{n}$  is the root in the positive real part. From Equation 12 it will be convenient to factor out a Maxwellian component by letting

$$f = x^2 e^{-x^2} N(x) \quad (14)$$

Substitution of Equation 14 into Equation 12 and simplifying results in

$$xN'' + (3-2x^2) N' + 4(nx-a) N = 0 \quad (15)$$

Inspection of Equation 15 shows that the origin is a regular singular point and that an irregular singular point exists at infinity. Equation 15 can be solved by assuming a power series solution of the form

$$N = \sum_{p=0}^{\infty} C_p x^{p+\lambda} \quad (16)$$

Substitution of Equation 16 into Equation 15 yields

$$\begin{aligned} \sum C_p (p+\lambda)(p+\lambda+2) x^{p+\lambda-1} - \sum C_p \cdot 4n \cdot x^{p+\lambda} \\ - \sum C_p \cdot 2(p+\lambda-2n) x^{p+\lambda+1} = 0 \end{aligned} \quad (17)$$

From Equation 17 the indicial equation obtained is

$$C_0(\lambda+2) \lambda = 0 \quad (18)$$

which gives  $\lambda = 0$  or  $\lambda = -2$ . The coefficients are obtained as

$$C_1 = \frac{4a}{(1+\lambda)(3+\lambda)} C_0 \quad \text{with } C_0 \neq 0$$

$$C_2 = \frac{1}{(\lambda+2)(\lambda+4)} \left[ 2(\lambda-2n) C_0 + 4aC_1 \right]$$

$$C_3 = \frac{1}{(\lambda+3)(\lambda+5)} \left[ 2(\lambda+1-2n) C_1 + 4aC_2 \right]$$

. . . etc.

The recursion relation is given by

$$C_p = \frac{1}{(p+\lambda)(p+\lambda+2)} \left[ 2(p-2+\lambda-2n) C_{p-2} + 4aC_{p-1} \right] \quad (19)$$

for  $p > 3$

Two linearly independent solutions to Equation 15 can be obtained from Equation 16 whose coefficients are given by Equation 19, where each solution corresponds to one of the two  $\lambda$ 's. The three term recursion relation given by Equation 19 is hard to solve in general. However, the first few terms can be evaluated easily, correct up to an order  $a^2$  for  $\lambda=0$ . These are

$$\begin{aligned} C_1 &= \frac{4a}{3} C_0 \\ C_2 &= \frac{C_0}{6} \left[ 4a^2 - 3n \right] \\ C_3 &= \frac{2a}{45} \left[ 4 - 11n \right] \end{aligned} \quad (20)$$

$$\begin{aligned}
c_4 &= \left[ \frac{19}{135} a^2 - \frac{26n}{135} a^2 + \frac{n(n-1)}{12} \right] c_0 \\
c_5 &= \frac{4a}{35} \left[ \frac{4}{15} + \frac{n^2}{12} - \frac{91}{180} n \right] c_0 \\
c_6 &= \frac{2a^2}{3} \left[ \frac{953}{37800} + \frac{n^2}{420} - \frac{182}{4725} n \right] c_0
\end{aligned} \tag{20}$$

and

$$c_p = \frac{1}{p(p+2)} \left[ 2 (p-2-2n) c_{p-2} + 4a c_{p-1} \right]$$

Now, the second solution can be obtained by setting  $do = [\lambda+2] c_0$  in each of the coefficients given by Equation 20, after differentiating with respect to  $\lambda$  and evaluating the corresponding coefficients at  $\lambda = -2$ . However, much labor can be saved by considering the solution for the case  $\lambda = -2$ , when there is no absorption present, for reasons which will become obvious consequently. For the case when  $a = 0$ , the solution of Equation 15 for the root  $\lambda = -2$ , is found to be of the form, given by Cohen (8),

$$N_n = K_n \left[ x^2 e^{-x^2} E_i(x^2) - 1 \right]$$

which for  $x = 0$ , a boundary condition given by Equation 5 is negative. Hence  $K_n$  must be set equal to zero for a physically meaningful solution. It may be noted here that Wilkins (6) also has considered the Equation 15 with  $n = 0$ , i.e. space independent problem. He has obtained two independent solutions which he has examined in the limit of

small  $x$  and found that one of the two solutions, which corresponds to the second solution in the present work, gives a negative slowing down density at  $x = 0$ , while the other gives a value of zero for the slowing down at  $x = 0$ , as expected on physical grounds. The solution accepted by Wilkins corresponds to the first solution in the present work.

For the case  $a = 0$ , i.e. without absorption, the Equation 15 gives Laguerre polynomials of order one as solutions, viz.  $l'n(x^2)$ . This is indeed true, for in Equation 15 setting  $a = 0$  results in

$$x N'' + (3-2x^2) N' + 4nxN = 0 \quad (21)$$

Substituting  $x^2 = u$  in Equation 21 leads to

$$u \frac{dN}{du^2} + (2-u) \frac{dN}{du} + nN(u) = 0 \quad (22)$$

The general solution of Equation 22 is

$$N(u) = C_1 H(-n|2|u) + C_2 G(-n|2|u) \quad (23)$$

where  $H$  is a confluent hypergeometric function and  $G$  is a Gordon function as given by Morse and Feshbach (14). Since a Gordon function leads to non-vanishing flux at  $u = 0$ , i.e. at  $E = 0$ , in violation of Equation 5, it is rejected.

The hypergeometric functions are satisfactory at  $u = 0$  but must be inspected as  $u$  tends to be large. The asymptotic

nature of this equation will be discussed in the following paragraphs, but from the results obtained there, it is to be concluded that Laguerre polynomials of order one, are the correct solution to the Equation 21 consistent with the boundary conditions stated in Equations 5 and 6.

By following the method suggested by Ince (15) and Erdelyi (16) for the point at  $\infty$  as an irregular singular point, two asymptotic series for the Equation 12 can be obtained as follows:

$$f_{1Asy} \sim x^{-2(n+1)} \left\{ 1 + \frac{(n+1)(n+2)}{x^2} + \dots \right\} \\ + x^{-2(n+1)} \left\{ \frac{2a^2}{x^2} + \frac{a}{6x^3} \left[ 4(n+1)(3n+8) - 8a^2 \right] \right. \\ \left. + \dots \right\} \quad (24)$$

and

$$f_{2Asy} \sim x^{2(n+1)} e^{-x^2} \left\{ 1 + \frac{2a}{x} + \frac{2a^2(-n(n+1))}{x^2} + \dots \right\} \quad (25)$$

For large values of  $x$ ,  $f_{1Asy} \ll f_{2Asy}$ . Also, it is evident from physical considerations that at high energies slowing down density cannot vanish and hence  $f_{1Asy}$  is the valid asymptotic solution for Equation 12.

It can be observed that Equation 24 which is the valid asymptotic solution to Equation 12 is written in two parts, one of which is independent of the absorption parameter 'a' and the other dependent on 'a'. Setting  $a = 0$  in Equation 24

should lead to the asymptotic nature of Equation 22. This is in effect the asymptotic behavior of Equation 15, but for the factor  $x^2 e^{-x^2}$  which was taken out. Hence consideration of the asymptotic form of  $H(-n|2|x)$ , shows that, except for a discreet set of values of  $n$ , the flux would vary asymptotically as an inverse power of  $x$  and thus would not vanish fast enough to satisfy the boundary condition stated in Equation 6, that all energy moments tend to zero for large values of energy. However, for positive integral values of  $n$ , i.e.  $n = 0, 1, 2, 3 \dots$  etc. this would lead to a satisfactory behavior of the flux at large energies. For integral values of  $n$   $H(-n|2|x)$  is Laguerre polynomial.

Even when absorption is present, the asymptotic nature should satisfy Equation 6, and both the parts of Equation 24 should simultaneously lead to vanishing energy moments for large  $x$ . Hence  $n$  is restricted to integral values.

The asymptotic series obtained not only permits the determination of the proper solutions but is also useful for computational purposes when  $x$  is large. In order to calculate the flux at large values of  $x$ , the arbitrary constant,  $C_a, n$ , associated with Equation 24 should be evaluated. To evaluate  $C_a, n$  it is found convenient to multiply Equation 12 by  $L_n(x^2)$ , Laguerre polynomial of order one, which gives

$$xL_n f'' + (2x^2 - 1) L_n f' + 4(n+1) n L_n f = 4a L_n f \dots (26)$$

The left hand side of Equation 26 is found to be an exact differential, for, Equation 26 can be written as

$$\begin{aligned} (x L_n f')' + \left[ (2x^2-1) L_n - x L_n' - L_n \right] f' \\ + 4(n+1) x L_n f = 4a L_n f \end{aligned} \quad (27)$$

Equation 27 after rearrangement gives

$$\begin{aligned} (x L_n f')' + \left[ \left\{ (2x^2-1) L_n - x L_n' \right\} f \right]' \\ + f \left[ 4nL_n + (3-2x^2) L_n' + x L_n'' \right] = 4aL_n f \dots (28) \end{aligned}$$

The last expression on the left hand side drops out since it is a form of the Laguerre equation as shown previously.

After integrating Equation 28 once and noting that for  $n = 0$ ,  $f = 0$  it can be shown that

$$xL_n f' + \left[ (2x^2-2) L_n - x L_n' \right] f = 4a \int_0^x L_n f dx \dots (29)$$

Now, for  $x$  tending to infinity let

$$x^{2n+2} f_{1Asy} \sim Ca, n \quad (30)$$

It is shown by Morse and Feshbach (14) that

$$L_n(x^2) \sim b_n x^{2n} \quad (31)$$

when  $b_n$  is known. In view of Equation 31 it can be observed

that terms  $xL_n f'$ ,  $2L_n f$  and  $xL_n' f$  tend to zero for  $x$  tending to infinity. Hence, the only contribution comes from the term  $2x^2 L_n$ , for

$$2x^2 L_n f \longrightarrow 2x^2 \cdot b_n x^{2n} \cdot \frac{C_{a,n}}{x^{2n+2}} \longrightarrow 2 b_n C_{a,n}$$

From Equation 29 and the inferences drawn above,  $C_{a,n}$  is given by

$$C_{a,n} = \frac{2a}{b_n} \int_0^{\infty} L_n f \, dn \quad (32)$$

with the relevant results from Equations 13, 14, 16 and 20 the complete solution to Equation 10, subject to the boundary conditions stated in Equations 4, 5 and 6 can be written, formally, for each region of temperature as,

$$\begin{aligned} \psi_1(x, y) &= \sum_{n=0}^{\infty} A_n e^{\sqrt{n} y} x_1^2 e^{-x_1^2} N_n(x_1) \\ &\dots (y \leq 0) \end{aligned} \quad (33)$$

and

$$\begin{aligned} \psi_2(x, y) &= \sum_{n=0}^{\infty} B_n e^{-\sqrt{n} y} x_2^2 e^{-x_2^2} N_n(x_2) \\ &(y \geq 0) \end{aligned} \quad (34)$$

which, when written in terms of the energy variable,  $E$ , by means of Equation 9, will be

$$\psi_1(E, y) = \sum_{n=0}^{\infty} \frac{A_n}{\theta_1} e^{\sqrt{n} y} \frac{E}{\theta_1} e^{-E/\theta_1} N_n\left(\frac{E}{\theta_1}\right) \quad (35)$$

$$\psi_2 (E, y) = \sum_{n=0}^{\infty} \frac{A_n}{\theta_2} e^{-\sqrt{n}} y \frac{E}{\theta_2} e^{-E/\theta_2} N_n \left( \frac{E}{\theta_2} \right) \quad (36)$$

where

$$N_n \left( \frac{E}{\theta_1} \right) = \sum_{p=0}^{\infty} C_p \left( \frac{E}{\theta_1} \right)^{p/2} \quad (i = 1, 2) \quad (37)$$

where  $C_p$  is given by Equation 19 and the first few coefficients are given explicitly by Equation 20. Since Equation 12 does not have any singularities for finite  $z$ , but for the origin, the power series given by  $N(x)$ , converges uniformly and absolutely for all finite values of  $x$ . If it is multiplied by  $x^2 e^{-x^2}$  and rearranged, Equation 15 can be written in Sturm-Liouville form

$$\frac{d}{dx} \left[ x^3 e^{-x^2} \frac{dN_n}{dx} \right] - \left[ 4ax^2 e^{-x^2} + 4x^2 e^{-x^2} n \right] N_n = 0 \quad (38)$$

Similarly an equation for  $N_m$  can be formed

$$\frac{d}{dx} \left[ x^3 e^{-x^2} \frac{dN_m}{dx} \right] - \left[ 4ax^2 e^{-x^2} + 4x^2 e^{-x^2} m \right] N_m = 0 \quad (39)$$

Multiplying Equation 38 by  $N_m$  and Equation 39 by  $N_n$  and subtracting, gives

$$\begin{aligned} (n-m) 4 x^3 e^{-x^2} N_m N_n &= N_m \frac{d}{dx} \left[ x^3 e^{-x^2} \frac{dN_n}{dx} \right] \\ &\quad - N_n \frac{d}{dx} \left[ x^3 e^{-x^2} \frac{dN_m}{dx} \right] \\ &= \frac{d}{dx} \left[ N_m x^3 e^{-x^2} \frac{dN_n}{dx} - N_n x^3 e^{-x^2} \frac{dN_m}{dx} \right] \quad (40) \end{aligned}$$

Integrating both members of Equation 40 over the interval 0 to  $\infty$ , with respect to  $x$ , gives

$$4(n-m) \int_0^{\infty} x^3 e^{-x^2} N_m N_n dx = \left[ N_m x^3 e^{-x^2} \frac{dN_n}{dx} - N_n x^3 e^{-x^2} \frac{dN_m}{dx} \right]_0^{\infty} \quad (41)$$

Since  $m-n \neq 0$ , it follows that

$$\int_0^{\infty} x^3 e^{-x^2} N_m N_n dx = 0 \quad (42)$$

which establishes the orthogonality and completeness of the set  $N_n$  in the range (0 to  $\infty$ ).

Further, with the aid of Equation 8 transforming the variable  $x$  to  $E$  Equation 42 results in

$$\int_0^{\infty} \left(\frac{E}{\theta}\right) e^{-E/\theta} N_m N_n \frac{dE}{\theta} = 0 \quad m \neq n \quad (43)$$

At  $y = 0$ , the boundary condition given by Equations 7 and 8 lead to

$$\sum_{n=0}^{\infty} \frac{A_n}{\theta_1} \frac{E}{\theta_1} e^{-E/\theta_1} N_n \left(\frac{E}{\theta_1}\right) = \sum_{n=0}^{\infty} \frac{B_n}{\theta_2} \frac{E}{\theta_2} e^{-E/\theta_2} N_n \left(\frac{E}{\theta_2}\right) \quad (44)$$

and

$$\sum_{n=0}^{\infty} \frac{A_n}{\theta_1} \frac{E}{\theta_1} e^{-E/\theta_1} \sqrt{n} N_n \left(\frac{E}{\theta_1}\right) = \sum_{n=0}^{\infty} \frac{B_n}{\theta_2} \frac{E}{\theta_2} e^{-E/\theta_2} 2\sqrt{n} N_n \left(\frac{E}{\theta_2}\right) \quad (45)$$

To determine the constants  $A_n$  and  $B_n$ , Equations 44 and 45 are each multiplied by  $N_m \left( \frac{E}{\theta_1} \right)$  and integrated over  $E$ . That is,

$$\begin{aligned} \int_0^{\infty} \sum_{m=0}^{\infty} A_n \frac{E}{\theta_1} e^{-E/\theta_1} N_n \left( \frac{E}{\theta_1} \right) \cdot N_m \left( \frac{E}{\theta_1} \right) \cdot \frac{1}{\theta_1} \cdot dE \\ = \int_0^{\infty} \sum_{n=0}^{\infty} B_n \frac{E}{\theta_2} e^{-E/\theta_2} N_n \left( \frac{E}{\theta_2} \right) \cdot N_m \left( \frac{E}{\theta_1} \right) \frac{1}{\theta_2} dE \end{aligned} \quad (46)$$

and

$$\begin{aligned} \int_0^{\infty} \sum_{n=0}^{\infty} \sqrt{n} A_n \frac{E}{\theta_1} e^{-E/\theta_1} N_n \left( \frac{E}{\theta_1} \right) N_m \left( \frac{E}{\theta_1} \right) \frac{1}{\theta_1} dE \\ = \int_0^{\infty} \sum_{n=0}^{\infty} -\sqrt{n} B_n \frac{E}{\theta_2} e^{-E/\theta_2} N_n \left( \frac{E}{\theta_2} \right) N_m \left( \frac{E}{\theta_1} \right) \frac{1}{\theta_2} dE \end{aligned} \quad (47)$$

In view of orthogonality relations for the functions  $N_n$ 's, the left hand members of Equations 46 and 47 can be written as

$$\int_0^{\infty} \sum_{n=0}^{\infty} A_n \frac{E}{\theta_1} e^{-E/\theta_1} N_n \left( \frac{E}{\theta_1} \right) \cdot N_m \left( \frac{E}{\theta_1} \right) \frac{1}{\theta_1} dE = K_m A_m \quad (48)$$

and

$$\int_0^{\infty} \sum_{n=0}^{\infty} n A_n \frac{E}{\theta_1} e^{-E/\theta_1} N_n \left( \frac{E}{\theta_1} \right) N_m \left( \frac{E}{\theta_1} \right) \frac{1}{\theta_1} dE = \sqrt{m} K_m A_n \quad (49)$$

where  $K_m$  is the value of the integral. Similarly, assuming that  $N \left( \frac{E}{\theta_1} \right)$  can be expressed in terms of  $N \left( \frac{E}{\theta_2} \right)$ , the right hand members of Equations 46 and 47 can be written as,

$$\int_0^{\infty} \sum_{n=0}^{\infty} B_n \frac{E}{\theta_2} e^{-E/\theta_2} N_n \left( \frac{E}{\theta_2} \right) N_m \left( \frac{E}{\theta_1} \right) \frac{1}{\theta_2} \cdot dE = \sum_{n=0}^{\infty} B_n J_{mn} \quad (50)$$

and

$$\int_0^\infty \sum_{n=0}^\infty n B_n \cdot \frac{E}{\theta_2} \cdot e^{-E/\theta_2} N_n\left(\frac{E}{\theta_2}\right) N_m \frac{E}{\theta_1} \frac{1}{\theta_2} dE = \sum_{n=0}^\infty \sqrt{n} B_n J_{mn} \tag{51}$$

Thus Equations 46 and 47 can be written as

$$K_m A_m = \sum B_n J_{mn} \tag{52}$$

$$\sqrt{m} K_m A_m = \sum - \sqrt{n} B_n J_{mn} \tag{53}$$

From Equation 52 substitution for  $K_m A_m$  in Equation 53 leads to

$$\sqrt{m} \sum_n B_n J_{mn} = \sum_n - \sqrt{n} B_n J_{mn} \tag{54}$$

Expanding Equation 54 and simplifying results in

$$\begin{aligned} 0 \cdot B_0 + J_{01} B_1 + \sqrt{2} J_{02} B_2 + \sqrt{3} J_{03} B_3 + \dots &= 0 \\ J_{01} B_0 + 2 J_{11} B_1 + (1 + \sqrt{2}) J_{12} B_2 + (1 + \sqrt{3}) J_{13} B_3 + \dots &= 0 \\ 2 J_{02} B_0 + (1 + \sqrt{2}) J_{12} B_1 + (2 \cdot \sqrt{2}) J_{22} B_2 + (\sqrt{2} + \sqrt{3}) J_{23} B_3 + \dots &= 0 \\ 3 J_{03} B_0 + (1 + \sqrt{3}) J_{13} B_1 + (\sqrt{2} + \sqrt{3}) J_{23} B_2 + (2 \cdot \sqrt{3}) J_{33} B_3 + \dots &= 0 \\ \dots &= 0 \\ \dots &= 0 \end{aligned} \tag{55}$$

From the set of Equations 55,  $B_i$ , ( $i = 1, 2, 3, \dots$ ) can be solved for in terms of arbitrary coefficient  $B_0$ , provided

$J_{mn}$  are evaluated.

Examination of the integrals defining  $J_{mn}$ , given by Equations 50 and 51, reveals that the functions  $N_n(\frac{E}{\theta_2})$  and  $N_m(\frac{E}{\theta_1})$  appearing in the integrand are function of different variables. Hence evaluating them is slightly harder. However, much labor can be saved by observing that the function  $N_n$  can be split up into parts composed of functions independent of 'a' and dependent on 'a' and  $a^2$ . Expressing  $N_j$  in this fashion gives,

$$N_j(\zeta_1) = L_j(\zeta_i) + a \left[ \frac{4}{3} \zeta_i^2 + \frac{2}{45} (4-11j) \zeta_i^{3/2} + \dots \right] \\ + a^2 \left[ \frac{2}{3} \zeta_i + \left( \frac{19}{135} - \frac{26j}{135} \right) \zeta_i^2 + \dots \right] \quad (56)$$

where  $L_j$  is the Laguerre polynomial of order one which is the solution when  $a = 0$ , as discussed earlier, and  $\zeta_i = E/\theta_i$  ( $i = 1, 2$ ). Since the temperature of the two regions can be related through a ratio given by

$$\frac{\theta_2}{\theta_1} = R \quad (57)$$

it is possible to express the terms in the right hand member of Equation 56 when  $\zeta = E/\theta_1$  in terms of the variable  $E/\theta_2$  by,

$$L_j \left( \frac{E}{\theta_1} \right) = \sum_{k=0}^j \binom{j+1}{k+1} (R)^k (1-R)^{j-k} L_k \left( \frac{E}{\theta_2} \right) \quad (58)$$

$$\begin{aligned}
& a \left[ \frac{4}{3} \left(\frac{E}{\theta_1}\right)^{1/2} + \frac{2}{45} (4-11j) \left(\frac{E}{\theta_1}\right)^{3/2} + \dots \right] \\
& = a \left[ \frac{4}{3} R^{1/2} \left(\frac{E}{\theta_2}\right)^{1/2} + \frac{2}{45} (4-11j) R^{3/2} \left(\frac{E}{\theta_2}\right)^{3/2} \right. \\
& \quad \left. + \dots \right] \tag{59}
\end{aligned}$$

$$\begin{aligned}
& a^2 \left[ \frac{2}{3} \left(\frac{E}{\theta_1}\right) + \left(\frac{19}{135} - \frac{26}{135} j\right) \left(\frac{E}{\theta_1}\right)^2 \dots \right] \\
& = a^2 \left[ \frac{2}{3} R \left(\frac{E}{\theta_2}\right) + \left(\frac{19}{135} - \frac{26}{135} j\right) R^2 \left(\frac{E}{\theta_2}\right)^2 \dots \right] \tag{60}
\end{aligned}$$

Equation 58 is taken from Bateman compilations (17), therefore  $J_{mn}$  will assume the form

$$\begin{aligned}
J_{mn} = & \int_0^\infty w e^{-w} \left\{ L_n(w) + a \left[ \frac{4}{3} w^{1/2} + \frac{2}{45} (4-11n) w^{3/2} + \dots \right] \right. \\
& \left. + a^2 \left[ \frac{2}{3} w + \left(\frac{19}{135} - \frac{26}{135} j\right) w^2 + \dots \right] \right\} \\
& \left\{ \sum_{q=0}^m \binom{m+1}{q+1} R^q (1-R)^{m-q} L_q(w) + \right. \\
& \left. + a \left[ \frac{4}{3} R^{1/2} w^{1/2} + \frac{2}{45} (4-11m) w^{3/2} + \dots \right] \right. \\
& \left. + a^2 \left[ \frac{2}{3} R w + \left(\frac{19}{135} - \frac{26m}{135}\right) R^2 w^2 + \dots \right] \right\} dw \tag{61}
\end{aligned}$$

where  $w = E/\theta_2$

Equation 61 can be rearranged retaining terms up to order  $a^2$  as

$$J_{mn} = J_{mn}^1 + J_{mn}^2 + J_{mn}^3 + J_{mn}^4 + J_{mn}^5 + J_{mn}^6 \quad (62)$$

where

$$J_{mn}^1 = \int_0^{\infty} w e^{-w} L_n(w) \sum_{q=0}^m \binom{m+1}{q+1} R^q (1-R)^{m-q} L_q(w) \quad (63)$$

$$J_{mn}^2 = a^2 \int_0^{\infty} dw e^{-w} \left\{ \frac{16}{3} R^2 w + \frac{2}{135} \left[ (4-11n) R^{1/2} + (4-11m) R^{3/2} \right] w^2 + \frac{4}{2025} (4-11n)(4-11m) R^{3/2} w^3 + \dots \right\} \quad (64)$$

$$J_{mn}^3 = a \int_0^{\infty} dw w e^{-w} \left[ L_n(w) \right] \left[ \frac{4}{3} R^{1/2} w^{1/2} + \frac{2}{45} (4-11m) R^{3/2} w^{3/2} + \dots \right] \quad (65)$$

$$J_{mn}^4 = a^2 \int_0^{\infty} dw w e^{-w} L_n(w) \left[ \frac{2}{3} R w + \left( \frac{19}{135} - \frac{26}{135} n \right) R^2 w^2 + \dots \right] \quad (66)$$

$$J_{mn}^5 = a \int_0^{\infty} dw w e^{-w} L_m(w) \left[ \frac{4}{3} w^{1/2} + \frac{2}{45} (4-11n) w^{3/2} + \dots \right] \quad (67)$$

and

$$J_{mn}^6 = a^2 \int_0^{\infty} dw w e^{-w} L_m(w) \left[ \frac{2}{3} w + \left( \frac{19}{135} - \frac{26n}{135} \right) w^2 + \dots \right] \quad (68)$$

$J_{mn}^1$  when evaluated is

$$J_{mn}^1 = \sum_{q=0}^m \binom{m}{q} R^q (1-R)^{m-q} \quad (69)$$

The rest of the above integrals have one of the two forms.

$$\int_0^{\infty} dw w^n e^{-w} = \Gamma(n+1) \quad (70)$$

$$\int_0^{\infty} dw w^{\beta-1} e^{-w} L_n^{(\alpha)}(w) = \frac{\Gamma(\alpha-\beta+n+1)\Gamma(\beta)}{n! \Gamma(\alpha-\beta+1)} \quad \text{Re } \beta > 0 \quad (71)$$

The last integral has been taken from the Bateman compilations (18). The integrals are evaluated as

$$J_{mn}^2 = a^2 \left\{ R^{1/2} \left[ \frac{32}{9} + (4-11n) \frac{48}{135} \right] + R^{3/2} (4-11m) \left[ \frac{48}{135} + \frac{96}{2025} (4-11n) \right] \right\} \quad (72)$$

$$J_{mn}^3 = a \left[ R^{1/2} \frac{4}{3} \frac{\Gamma(n-1/2)\Gamma(2)}{n! \Gamma(-1/2)} + R^{3/2} \frac{(4-11m) \frac{2}{45} \Gamma(n-3/2)\Gamma(7/2)}{n! \Gamma(-3/2)} \right] \quad (73)$$

$$J_{mn}^4 = a^2 \left[ R \frac{2}{3} \frac{\Gamma(n-1)\Gamma(3)}{n! \Gamma(-1)} + R^2 \left( \frac{19}{135} - \frac{26}{135} m \right) \frac{\Gamma(n-2)\Gamma(4)}{n! \Gamma(-3/2)} \right] \quad (74)$$

$$J_{mn}^5 = a \left[ \frac{4}{3} \frac{\Gamma(m-1/2)\Gamma(3/2)}{m! \Gamma(-1/2)} + (4-11n) \frac{2}{45} \frac{\Gamma(m-3/2)\Gamma(5/2)}{m! \Gamma(-3/2)} \right] \quad (75)$$

$$J_{mn}^6 = a^2 \left[ \frac{2}{3} \frac{\Gamma(m-1)\Gamma(3)}{m! \Gamma(-1)} + \left( \frac{19}{135} - \frac{26}{135} n \right) \frac{\Gamma(m-2)\Gamma(4)}{m! \Gamma(-2)} \right] \quad (76)$$

It can be observed that Equations 74 and 76 contain  $\Gamma(+k)$

where  $k$  is a negative integer, for which gamma function behaves like  $\pm \infty$ . Hence they vanish for  $n > 0$ . However, for  $n = 0$  the value of the integral does exist, when evaluated directly, and can be found to be

$$J_{mn}^4 = a^2 \left[ \frac{2}{3} R + \left( \frac{19}{135} - \frac{26}{135} m \right) R^2 \right] \quad (77)$$

and

$$J_{mn}^6 = a^2 \left[ \frac{2}{3} + \left( \frac{19}{135} - \frac{26}{135} n \right) \right] \quad (78)$$

Summing up the individual  $J_{mn}^1$ 's from the above equations and simplifying results in

$$\begin{aligned} J_{mn} B_n = & \left[ \sum_{q=0}^m \binom{m}{q} R^q (1-R)^{m-q} B_q \right] + \left( R^{1/2} \left\{ a \frac{4}{3} \frac{\Gamma(n-1/2)\Gamma(5/2)}{n! \Gamma(-y_2)} \right. \right. \\ & + a^2 \left[ \frac{32}{9} + (4-11n) \frac{16}{45} \right] \left. \right\} + R a^2 \frac{2}{3} \\ & + R^{3/2} \left\{ a \frac{(4-11m) \frac{2}{45} \Gamma(n-3/2)\Gamma(7/2)}{n! \Gamma(-3/2)} + a^2 (4-11m) \right. \\ & \left. \left[ \frac{16}{45} + \frac{32}{675} (4-11n) \right] \right\} + R^2 a^2 \left( \frac{19}{135} - \frac{26m}{135} \right) \\ & + a \left[ \frac{4}{3} \frac{\Gamma(m-1/2)\Gamma(3/2)}{m! \Gamma(-1/2)} + (4-11n) \frac{2}{45} \frac{\Gamma(m-3/2)\Gamma(5/2)}{m! \Gamma(-3/2)} \right] \\ & \left. + a^2 \left[ \frac{2}{3} + \left( \frac{19}{135} - \frac{26m}{135} \right) \right] \right) B_n \quad (79) \end{aligned}$$

By means of Equations 79 and 55  $B_n$ 's can be evaluated,

although it is hard to find a simple closed expression for  $B_n$ . Similarly  $A_n$ 's can also be obtained.

It is useful to investigate the effect of 'a' on  $B_n$ 's as  $n \gg 1$ . To accomplish this the following method is adopted. Setting  $y = \sqrt{\frac{2\mu z^2}{D}}$  and  $\epsilon = \frac{E}{\theta}$  in Equation 2, and assuming a product solution of the form  $\psi(y, \epsilon) = f(\epsilon)h(y)$ , the following equations result by following the method of separation of variables.

$$h'' - nh = 0$$

and

$$\epsilon f'' + \epsilon f' + \left[ 1 - n - \frac{a}{\sqrt{\epsilon}} \right] f = 0 \quad (80)$$

It has been found that the WKB method developed for the solution of the eigen values of the one dimensional Schrödinger wave equation for bound particles, as given in Morse and Feshbach (14), can be applied to Equation 80.

Substituting

$$f = e^{-\epsilon/2} \psi(\epsilon)$$

transforms Equation 80 to

$$\psi'' + \frac{1}{\epsilon} \left[ l - \frac{\epsilon}{4} - \frac{a}{\sqrt{\epsilon}} \right] \psi = 0 \quad (81)$$

where  $l = n+1$ .

This form is not yet suitable. Setting

$$\epsilon = e^u$$

changes Equation 81 to

$$\psi'' - \psi' + e^u \left[ l - \frac{e^u}{4} - \frac{a}{e^{u/2}} \right] \psi = 0 \quad (82)$$

substituting

$$\psi(x) = e^{u/2} X(u)$$

Equation 82 assumes the form

$$X'' + e^u \left[ l - \left( \frac{e^u}{4} + \frac{e^{-u}}{4} - \frac{a}{e^{u/2}} \right) \right] X = 0 \quad (83)$$

Equation 83 has the same form as that of Morse and Feshbach where in their notation

$$q = e^{u/2} \sqrt{l - \left( \frac{e^u}{4} + \frac{e^{-u}}{4} - \frac{a}{e^{u/2}} \right)} \quad (84)$$

and

$$w = \int_{u_1}^{u_2} e^{u/2} \sqrt{l - \left( \frac{e^u}{4} + \frac{e^{-u}}{4} - \frac{a}{e^{u/2}} \right)} du = \left( n + \frac{1}{2} \right) \pi \quad (85)$$

Transforming back to the original variable leads to

$$w = \int_{\epsilon_1}^{\epsilon_2} \sqrt{l - \left( \frac{\epsilon^2}{16} + \frac{\epsilon^{-2}}{16} + \frac{a}{2\epsilon} \right)} d\epsilon = \left( n + \frac{1}{2} \right) \pi \quad (86)$$

It can be seen that for large values of  $l$ , the term  $\frac{a}{2\epsilon}$  can be ignored in comparison with other terms. Hence for large values of  $n$ , the problem essentially reduces to the

case of no absorption. Similar conclusions are drawn by Garelis (19) in a related problem. This suggests qualitatively that in evaluating the  $J_{mn}$ 's for large values of  $n$   $J_{mn}$  will be essentially  $J_{mn}'$  which will lead to the results obtained by Kottwitz (11). Before proceeding to obtain some numerical results the question of convergence of the series can be considered.

Since  $J_{mn}$  can not be easily expressed in a closed form convergence of the solution can not be discussed easily. However, as explained earlier, for large values of  $n$  the problem reduces to the case of non-absorption. For this problem Kottwitz has shown that the series converges if

$$\frac{1}{2} < \frac{\theta_2}{\theta_1} < 2$$

in both high and low temperature regions. Hence in the present problem also it is reasonable to expect the same type of convergence.

For the purpose of comparison with the work of Kottwitz and the approximate solutions obtained in this investigation  $\frac{\theta_2}{\theta_1}$  is chosen to be 2 and a value of 0.6 is chosen for 'a'. With these values  $J_{mn}$  and also the first four coefficients,  $B_0$ ,  $B_1$ ,  $B_2$  and  $B_3$ , are evaluated. The values of  $B_0$ ,  $B_1$ ,  $B_2$  and  $B_3$  are found to be

$$B_0 = 1$$

$$B_1 = 0.2888$$

$$B_2 = -0.1386$$

and

$$B_3 = 0.0324$$

A plot of  $\theta_1 F_2$  at the interface,  $y = 0$ , is shown in Figure 6 in the next section along with an approximate solution developed there.

## APPROXIMATE SOLUTIONS

In the previous section an attempt has been made to obtain a rigorous solution to the problem of the neutron flux spectrum in an absorbing medium with a temperature discontinuity. However if the temperature variation of the medium, with position was of a different nature, as, for example, a gradient, an analytical solution does not seem possible. In such cases, the problem can be solved, perhaps, by the use of computers. If an approximate solution to the problem is available it will be of great utility if not in itself at least in checking out such numerical methods developed for use in more complicated problems. Hence, a technique that will lead to an approximate solution to the same problem, considered in the previous section will be developed here. However, the method employed here is quite general so that it can be easily adapted to more complicated problems of similar nature.

An approximate solution to the problem will be developed by using Galerkin's method which has recently attained a wide application. The mathematical principles of this method have been presented by Kantorovich and Krylov (20). For convenience, the basic idea of Galerkin's method is presented here.

To illustrate the method of Galerkin, consider the problem of determining solutions to the equation

$$\hat{L}\psi = 0 \quad (87)$$

where  $\hat{L}$  is some differential operator, say, in two variables, the solution of which satisfies homogeneous boundary conditions. Approximate solution to Equation 87 can be sought in the form

$$\bar{\psi}(\xi, \eta) = \sum_{i=1}^n C_i X(\xi, \eta) \quad (88)$$

where the functions  $X(\xi, \eta)$  are chosen before hand so that they satisfy the boundary conditions. The coefficients  $C_i$  are to be determined. Further  $X_i$ 's can be considered to be linearly independent. Only the first  $n$  functions of the system of functions  $X_i(\xi, \eta)$  ( $i = 1, 2, \dots, n, \dots$ ) which is complete in the given region can be considered.  $\bar{\psi}(\xi, \eta)$  will be the exact solution to Equation 87 if and only if  $\hat{L}\bar{\psi}$  is identically equal to zero. If  $\hat{L}\bar{\psi}$  is continuous, this would mean that  $\hat{L}\bar{\psi}$  is orthogonal to all the functions of the system  $X_i$  ( $i = 1, 2, \dots, n, \dots$ ). However, due to the fact that only  $n$  constants  $C_1, C_2, \dots, C_n$  are considered, only  $n$  conditions of orthogonality can be satisfied. That is

$$\iint_D (\hat{L}\bar{\psi}) \cdot X_i(\xi, \eta) \, d\xi, \, d\eta = \iint_D L \left( \sum_{j=1}^n C_j X_j(\xi, \eta) \right) X_i(\xi, \eta) \, d\xi, \, d\eta = 0$$

$$(i = 1, 2, \dots, n, \dots) \quad (89)$$

From Equation 89 the coefficients  $C_i$  of the system can be determined and hence the approximate solution  $\bar{\Psi}(\xi, \eta)$ .

Before applying Galerkin's method to the problem of finding thermal neutron flux spectrum in an absorbing medium with a temperature discontinuity it will be worthwhile to use the method to solve a similar problem in a non-absorbing medium. Kottwitz (11) has been able to find an exact solution for the case of non-absorbing medium with a step type temperature distribution. Hence an approximate solution obtained by the application of Galerkin's method could be compared with the exact solution obtained by Kottwitz and the merit of the approximate method can be evaluated.

In the case of a non-absorbing medium and the temperature dependence given by

$$\theta(y) = \begin{cases} \theta_1 & \text{in region 1, } y \leq 0 \\ \theta_2 & \text{in region 2, } y \geq 0 \end{cases}$$

the equation to be considered will be

$$\frac{\partial^2 \phi_i(y, E)}{\partial y^2} + \phi_i + E \frac{\partial \phi_i(y, E)}{\partial E} + E \theta_i \frac{\partial^2 \phi_i(y, E)}{\partial E^2} = 0 \quad (90)$$

which is obtained from Equation 2 by setting  $y = \sqrt{\frac{2\mu\Sigma_s}{D}} \cdot z$  and  $a = 0$ . It has the same boundary conditions, given in the previous section by Equations 4 through 8. Since it is required that  $\phi(x, y)$  should tend to be a Maxwellian  $M(E)$

characterized by the local temperature of the medium far from the interface the boundary condition given in Equation 4 can be written as

$$\phi(y, E) \longrightarrow M(E) \text{ as } y \longrightarrow \infty \quad (91)$$

Galerkin's method requires homogeneous boundary conditions. Hence, the boundary conditions can be made homogeneous by constructing a new function.

$$F_1 = M_1(E) + \frac{e^y}{2} \left[ M_2(E) - M_1(E) \right] + G_1(y, E) \quad y \leq 0 \quad (92)$$

and

$$F_2 = M_2(E) + \frac{e^{-y}}{2} \left[ M_1(E) - M_2(E) \right] + G_2(y, E) \quad y \geq 0 \quad (93)$$

where

$$M_i(E) = \frac{E}{\theta_i^2} e^{-E/\theta_i} \quad (i = 1, 2) \quad (94)$$

$G_1$  and  $G_2$  are trial functions that will be chosen to satisfy the requirements. Substituting Equations 92 and 93 in Equation 90 leads to

$$H_1 G_{1n} + H_1 \left[ \frac{M_2 - M_1}{2} e^y \right] = 0 \quad y \leq 0 \quad (95)$$

and

$$H_2 G_{2n} + H_2 \left[ \frac{M_1 - M_2}{2} e^{-y} \right] = 0 \quad y \geq 0 \quad (96)$$

where 
$$H_i = \frac{\partial^2}{\partial y^2} + (1 + \epsilon \frac{\partial}{\partial \epsilon} + \epsilon \frac{\partial^2}{\partial \epsilon^2}) \quad (97)$$

Since

$$F_1 \longrightarrow M_1 \quad \text{as } y \longrightarrow -\infty$$

and

$$F_2 \longrightarrow M_2 \quad \text{as } y \longrightarrow \infty \quad (98)$$

Therefore

$$G_1 \longrightarrow 0 \quad \text{as } y \longrightarrow -\infty$$

and

$$G_2 \longrightarrow 0 \quad \text{as } y \longrightarrow \infty \quad (99)$$

Thus the boundary conditions are homogeneous while the differential equation is non-homogeneous. From the conditions at interface given by Equations 7 and 8 since

$$F_1(0, E) = F_2(0, E)$$

$$G_1(0, E) = G_2(0, E) \quad (100)$$

Again because

$$\left. \frac{\partial F_1}{\partial y} \right|_{y=0} = \left. \frac{\partial F_2}{\partial y} \right|_{y=0}$$

$$\left. \frac{\partial G_1}{\partial y} \right|_{y=0} = \left. \frac{\partial G_2}{\partial y} \right|_{y=0} \quad (101)$$

Further

$$F(y, 0) = 0$$

leads to

$$G_i(y, 0) = 0 \quad (102)$$

and

$$E^n F(y, E) \longrightarrow 0 \quad \text{as } E \longrightarrow \infty$$

leads to

$$E^n G_i(y, E) \longrightarrow 0 \quad \text{as } E \longrightarrow \infty \quad (103)$$

The rest of the terms  $F_i$  satisfy the conditions at the interface. Thus finally, the problem is reduced to finding solution to

$$H_1 G_1 + H_1 \left( \frac{M_2 - M_1}{2} e^y \right) = 0 \quad y \leq 0 \quad (104)$$

$$H_2 G_2 + H_2 \left( \frac{M_1 - M_2}{2} e^{-y} \right) = 0 \quad y \geq 0 \quad (105)$$

subject to the conditions

$$G_i(\pm \infty, E) = 0 \quad (106)$$

and at the interface  $y = 0$

$$G_1(0, E) = G_2(0, E) \quad (107)$$

and

$$\left. \frac{\partial G_1}{\partial y} \right|_{y=0} = \left. \frac{\partial G_2}{\partial y} \right|_{y=0} \quad (108)$$

The functions  $G_1$  and  $G_2$  are to be chosen such that they satisfy Equations 102 and 103.

The trial functions  $G_1$  and  $G_2$  considered are of the form

$$G_1 = Au_1 + Gv_1 \quad (109)$$

and

$$G_2 = Au_2 + Bv_2 \quad (110)$$

where  $u$  and  $v$  satisfy the boundary conditions and will be chosen later on.  $A$  and  $B$  are coefficients to be determined. To determine  $A$  and  $B$  the differential Equations 104 and 105 are multiplied by  $u$  and  $v$  and integrated over regions of  $y$  and  $E$ . This procedure yields,

$$\int_0^{\infty} \left[ \int_{-\infty}^0 u_1 \left( H_1 G_1 + H_1 \frac{M_2 - M_1}{2} e^y \right) dy + \int_0^{\infty} u_2 \left( H_2 G_2 + H_2 \frac{M_1 - M_2}{2} e^{-y} \right) dy \right] dx = 0 \quad (111)$$

and

$$\int_0^{\infty} \left[ \int_{-\infty}^0 v_1 \left( H_1 G_1 + H_1 \frac{M_2 - M_1}{2} e^y \right) dy + \int_0^{\infty} v_2 \left( H_2 G_2 + H_2 \frac{M_1 - M_2}{2} e^{-y} \right) dy \right] dx = 0 \quad (112)$$

Substituting for  $G_1$  and  $G_2$  from Equations 109 and 110 in Equations 111 and 112 gives

$$\int_0^{\infty} \left[ \int_{-\infty}^0 u_1 \left( H_1 Au_1 + H_1 Bv_1 + H_1 \frac{M_2 - M_1}{2} e^y \right) dy + \int_0^{\infty} u_2 \left( H_2 Au_2 + H_2 Bv_2 + H_2 \frac{M_1 - M_2}{2} e^{-y} \right) dy \right] dx = 0 \quad (113)$$

and

$$\int_0^{\infty} \left[ \int_{-\infty}^0 v_1 (H_1 A u_1 + H_1 B v_1 + H_1 \frac{M_2 - M_1}{2} e^y) dy + \int_0^{\infty} v_2 (H_2 A u_2 + H_2 B v_2 + H_2 \frac{M_1 - M_2}{2} e^{-y}) dy \right] dx = 0 \quad (114)$$

Equations 113 and 114 can be rearranged in the form

$$\begin{aligned} & A \int_0^{\infty} \left[ \int_{-\infty}^0 u_1 H_1 u_1 dy + \int_0^{\infty} u_2 H_2 u_2 dy \right] dE \\ & + B \int_0^{\infty} \left[ \int_{-\infty}^0 v_1 H_1 v_1 dy + \int_0^{\infty} v_2 H_2 v_2 dy \right] dE \\ & + \int_0^{\infty} \left[ \int_{-\infty}^0 u_1 H_1 \frac{M_2 - M_1}{2} e^y dy + \int_0^{\infty} u_2 H_2 \frac{M_1 - M_2}{2} e^{-y} dy \right] \\ & dE = 0 \quad (115) \end{aligned}$$

and

$$\begin{aligned} & A \int_0^{\infty} \left[ \int_{-\infty}^0 v_1 H_1 u_1 dy + \int_0^{\infty} v_2 H_2 u_2 dy \right] dE \\ & + B \int_0^{\infty} \left[ \int_{-\infty}^0 v_1 H_1 v_1 dy + \int_0^{\infty} v_2 H_2 v_2 dy \right] dE \\ & + \int_0^{\infty} \left[ \int_{-\infty}^0 v_1 H_1 \frac{M_2 - M_1}{2} e^y dy + \int_0^{\infty} v_2 H_2 \frac{M_1 - M_2}{2} e^{-y} dy \right] \\ & dE = 0 \quad (116) \end{aligned}$$

when the integrals are evaluated Equations 115 and 116 result in two simultaneous equations from which the coefficients A and B can be determined.

It has been found that the following trial functions for  $u_1$ ,  $u_2$ ,  $v_1$  and  $v_2$  satisfy the boundary conditions given in Equations 102 and 103 and 106 through 108

$$u_1 = y e^y \left(\frac{E}{\theta_1}\right)^3 e^{-pE} \quad (117)$$

$y < 0$

$$v_1 = (1-y) e^y \left(\frac{E}{\theta_2}\right)^2 e^{-pE} \quad (118)$$

and

$$u_2 = y e^{-y} \left(\frac{E}{\theta_1}\right)^3 e^{-pE} \quad (119)$$

$y > 0$

$$v_2 = (1-y) e^{-y} \left(\frac{E}{\theta_2}\right)^2 e^{-pE} \quad (120)$$

where  $p$  is an arbitrary constant, related to the temperature of the medium and can be so chosen as to suit the problem. In the present case where temperature of one medium can be expressed as a multiple of the other, it will be expedient to choose  $p$  as four times the harmonic mean of the temperatures of the two media. That is

$$p = \frac{2 (\theta_1 + \theta_2)}{\theta_1 \theta_2} \quad (121)$$

The evaluation of the integrals in Equations 115 and 116 is straightforward. After integrating and simplifying the two equations that result from 115 and 116 respectively are

$$\begin{aligned}
A \left[ \frac{85}{64} \frac{\theta_1 - \theta_2}{p^6} - \frac{45}{32} \frac{1}{p^7} \right] - B \frac{3}{16} \frac{\theta_2 - \theta_1}{p^5} \\
+ \left[ \frac{6\theta_1^3}{(p\theta_1+1)^5} \frac{2\theta_1 - \theta_2}{\theta_1} - \frac{6\theta_2^3}{(p\theta_2+1)^5} \frac{\theta_1}{\theta_2} \right. \\
\left. + \frac{15\theta_1^2}{(p\theta_1+1)^6} (\theta_2 - \theta_1) - \frac{15\theta_2^2}{(p\theta_2+1)^6} \frac{\theta_1^2 - \theta_2^2}{\theta_1} \right] = 0 \quad (122)
\end{aligned}$$

and

$$\begin{aligned}
A \frac{3(\theta_1 - \theta_2)}{2p^5} + B \left[ \frac{3}{2p^5} - \frac{5}{4p^4} (\theta_1 + \theta_2) \right] \\
+ \left[ \frac{12}{(p\theta_2+1)^4} (\theta_1\theta_2 - 2\theta_2^2) + \frac{24}{(p\theta_2+1)^5} (\theta_2^2 - \theta_1\theta_2) \right. \\
\left. + \frac{12}{(p\theta_1+1)^4} (2\theta_1^2 - \theta_1\theta_2) - \frac{24}{(p\theta_1+1)^5} (\theta_1^2 - \theta_1\theta_2) \right] \\
= 0 \quad (123)
\end{aligned}$$

A and B can be obtained explicitly provided  $\frac{\theta_2}{\theta_1}$  is specified.

The coefficients A and B have been calculated for  $\theta_2/\theta_1 = 2$ , which makes it possible for the approximate solution obtained by this method to be compared with the exact solution as obtained by Kottwitz (11).

Setting  $\theta_2/\theta_1 = 2$  would give

$$p = \frac{2(\theta_1 + \theta_2)}{\theta_1\theta_2} = \frac{3}{\theta_1}$$

$$(p\theta_1+1) = 4 \quad \text{and} \quad (p\theta_2+1) = 7$$

Inserting these values in Equations 122 and 123 and simplifying gives

$$387 \theta_1^4 - 61.7 \theta_1^3 B = -74$$

and

$$61.7 \theta_1^4 A + 401.2 \theta_1^3 B = -36.4$$

Solving for A and B from the above equations results in

$$A = - \frac{0.201}{\theta_1^4} \quad (124)$$

and

$$B = - \frac{0.065}{\theta_1^3} \quad (125)$$

Hence with the aid of Equations 92, 93, 94, 117 through 120, 124 and 125 the flux is given by

$$\begin{aligned} \theta_1 F_1(y, E) &= \frac{E}{\theta_1} e^{-x/\theta_1} + \frac{e^y}{2} \left( \frac{E}{4\theta_1} e^{-E/2\theta_1} - \frac{E}{\theta_1} e^{-E/\theta_1} \right) \\ &\quad - 0.201 y e^y \left( \frac{E}{\theta_1} \right)^3 e^{-3E/\theta_1} \\ &\quad - 0.0615 (1-y) e^y \left( \frac{E}{\theta_1} \right)^2 e^{-3E/\theta_1} \\ &\quad \text{for } y \leq 0 \end{aligned} \quad (126)$$

$$\theta_1 F_2(y, E) = \frac{E}{4\theta_1} e^{\theta E/2\theta_1} + \frac{e^{-y}}{2} \left( \frac{E}{\theta_1} e^{-E/\theta_1} - \frac{E}{4\theta_1} e^{-E/2\theta_1} \right)$$

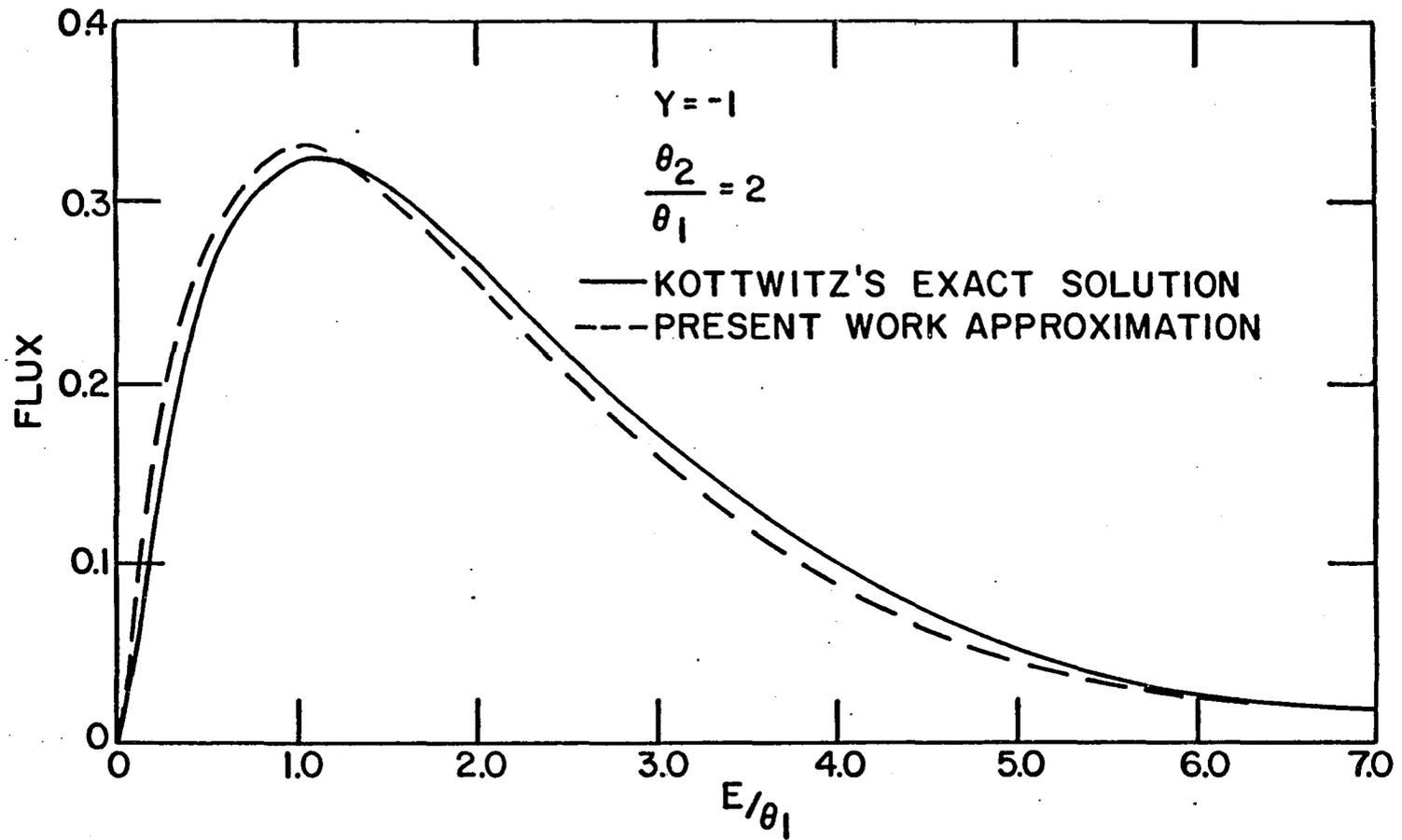


Figure 1. Flux spectrum at one relaxation length from interface in low temperature region and non-absorbing medium

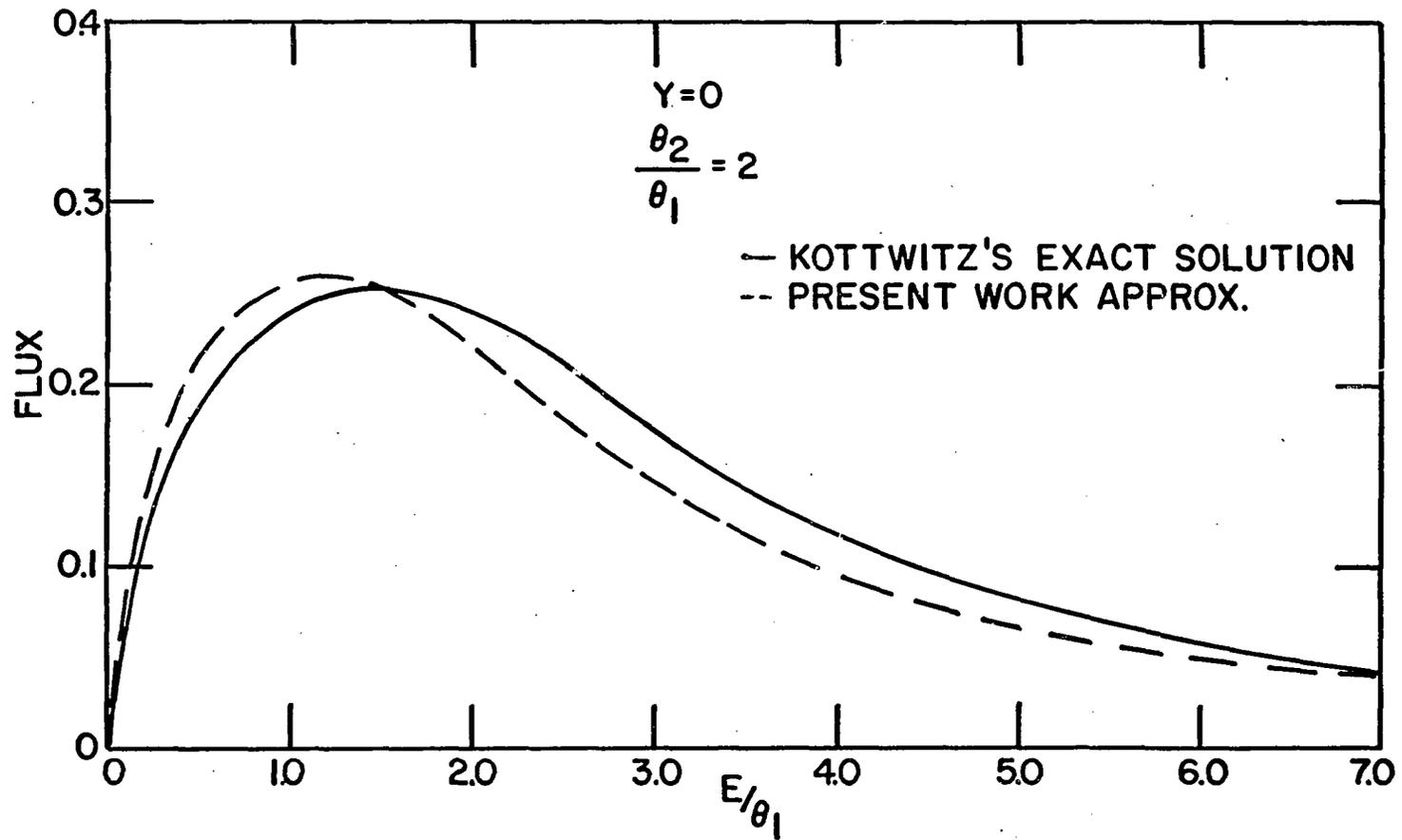


Figure 2. Flux spectrum at interface in non-absorbing medium

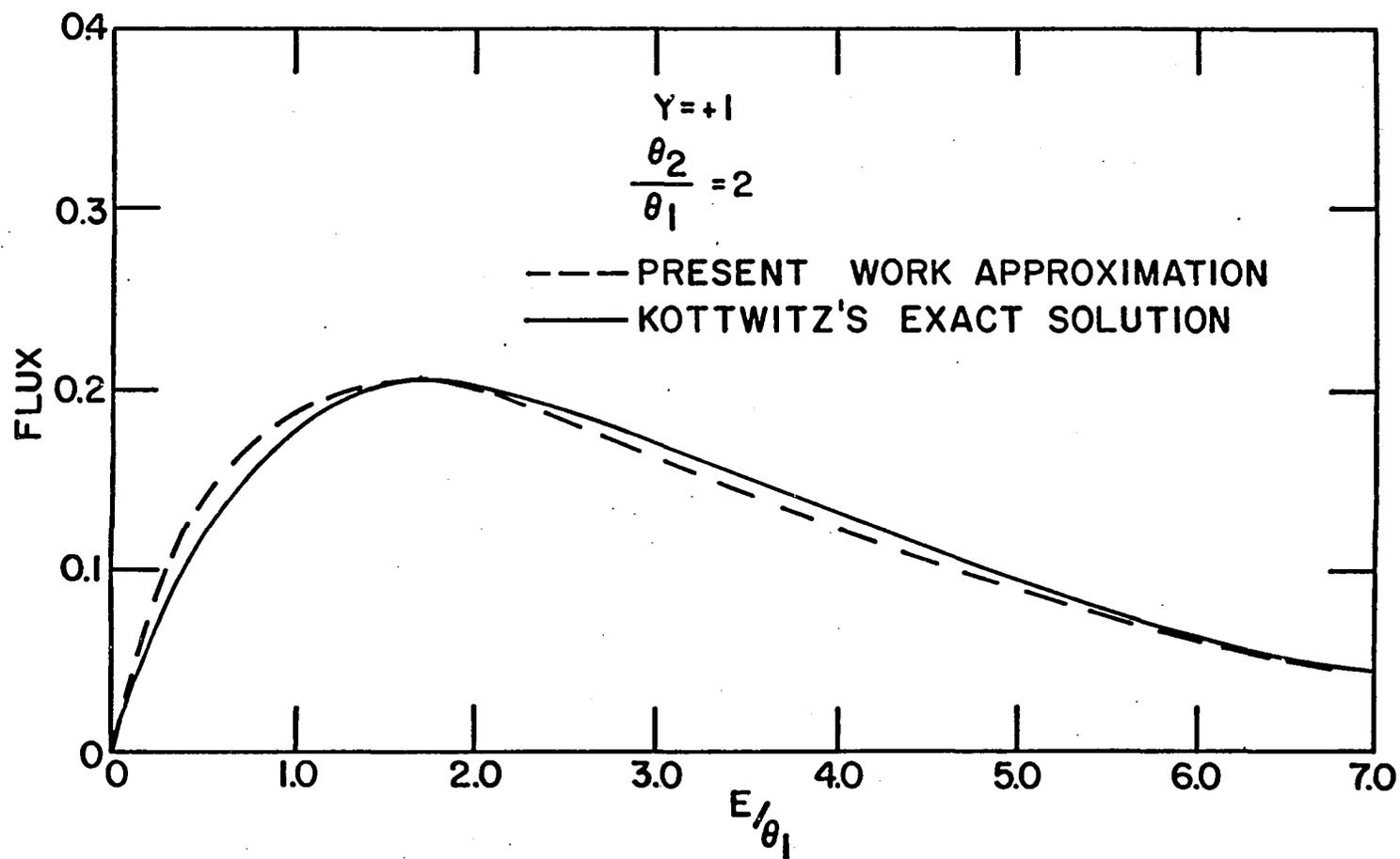


Figure 3. Flux spectrum at one relaxation length from interface in high temperature region and non-absorbing medium

$$- 0.201 y e^{-y} \left(\frac{E}{\theta_1}\right)^3 e^{-3E/\theta_1}$$

$$- 0.0615 (1+y) e^{-y} \left(\frac{E}{\theta_1}\right)^2 e^{-\frac{3E}{\theta_1}}$$

$$\text{for } y \geq 0 \quad (127)$$

These functions are shown plotted at  $y = -1$ ,  $y = 0$  and  $y = +1$  respectively in Figures 1, 2 and 3, together with the corresponding results obtained by Kottwitz. The values are calculated at intervals of  $\frac{E}{\theta_1} = 0.25$ , and the curves are normalized. The agreement between the exact solution and the approximate solutions is very good.

In the case of a medium with  $\frac{1}{V}$  absorption and with the same temperature distribution as before, the differential equation will be

$$H_1 \ddot{\phi}_1 = \frac{\partial^2 \phi_1}{\partial y^2} + \left[ 1 - \frac{a_1 \theta_1^{\frac{1}{2}}}{\sqrt{E}} + E \frac{\partial}{\partial E} + E \theta_1 \frac{\partial^2}{\partial E^2} \right] \phi_1 = 0 \quad (128)$$

and

$$H_2 \ddot{\phi}_2 = \frac{\partial^2 \phi_2}{\partial y^2} + \left[ 1 - \frac{a_2 \theta_2^{\frac{1}{2}}}{\sqrt{E}} + E \frac{\partial}{\partial E} + E \theta_2 \frac{\partial^2}{\partial E^2} \right] \phi_2 = 0 \quad (129)$$

In the present case

$$\phi_1(y, E) \longrightarrow \mathcal{L}_1(E) \quad \text{as } y \longrightarrow -\infty \quad (130)$$

and

$$\phi_2(y, E) \longrightarrow \mathcal{L}_2(E) \quad \text{as } y \longrightarrow +\infty \quad (131)$$

where  $\mathcal{L}_1$  and  $\mathcal{L}_2$  are the solutions to the space independent

problem,  $\alpha_1$  and  $\alpha_2$  can be obtained from Equations 35 and 36 respectively by setting  $n = 0$ . They are,

$$\alpha_1 = \frac{E}{\theta_1} e^{-E/\theta_1} \left\{ 1 + \frac{4}{3} a_1 \left[ \left(\frac{E}{\theta_1}\right)^{\frac{1}{2}} + \frac{2}{15} \left(\frac{E}{\theta_1}\right)^{\frac{3}{2}} + \frac{4}{175} \left(\frac{E}{\theta_1}\right)^{\frac{5}{2}} \dots \right] + \frac{2}{3} a_1^2 \left[ \left(\frac{E}{\theta_1}\right) + \frac{19}{90} \left(\frac{E}{\theta_1}\right)^2 + \dots \right] \right\} \quad (132)$$

and

$$\alpha_2 = \frac{E}{\theta_2} e^{-E/\theta_2} \left\{ 1 + \frac{4}{3} a_2 \left[ \left(\frac{E}{\theta_2}\right)^{\frac{1}{2}} + \frac{2}{15} \left(\frac{E}{\theta_2}\right)^{\frac{3}{2}} + \frac{4}{175} \left(\frac{E}{\theta_2}\right)^{\frac{5}{2}} \dots \right] + \frac{2}{3} a_2^2 \left[ \left(\frac{E}{\theta_2}\right) + \frac{19}{90} \left(\frac{E}{\theta_2}\right)^2 + \dots \right] \right\} \quad (133)$$

The other boundary conditions and the procedure to be adopted are essentially the same as in the case of non-absorbing medium. Thus the problem can be stated as

$$H_1 G_1 + H_1 \left( \frac{\alpha_2 - \alpha_1}{2} e^y \right) = 0 \quad y < 0 \quad (134)$$

$$H_2 G_2 + H_2 \left( \frac{\alpha_1 - \alpha_2}{2} e^{-y} \right) = 0 \quad y > 0 \quad (135)$$

with the following boundary conditions.

$$G_1 (-\infty, E) = 0 \quad (136)$$

$$G_2 (+\infty, E) = 0 \quad (137)$$

$$G_1 (0, E) = G_2 (0, E) \quad (138)$$

$$\left. \frac{\partial G_1}{\partial y} \right|_{y=0} = \left. \frac{\partial G_2}{\partial y} \right|_{y=0} \quad (139)$$

$$G_1(y,0) = 0 \quad (140)$$

$$G_2(y,0) = 0 \quad (141)$$

$$E^n G_1(y,E) \longrightarrow 0 \quad \text{as} \quad E \longrightarrow -\infty \quad (142)$$

$$E^n G_2(y,E) \longrightarrow 0 \quad \text{as} \quad E \longrightarrow +\infty \quad (143)$$

Once again trial functions which satisfy the Equations 136 through 143 of the form

$$G_1 = Au_1 + Bv_1 \quad (144)$$

$$G_2 = Au_2 + Bv_2 \quad (145)$$

can be considered. The functions  $u_1$ ,  $v_1$ ,  $u_2$  and  $v_2$  are chosen slightly differently. They are

$$u_1 = (1-y) e^y f_1\left(\frac{E}{\theta}\right) \quad y \leq 0 \quad (146)$$

$$v_1 = y e^y f_2\left(\frac{E}{\theta}\right) \quad y \leq 0 \quad (147)$$

$$u_2 = (1+y) e^{-y} f_1\left(\frac{E}{\theta}\right) \quad y \geq 0 \quad (148)$$

and

$$v_2 = y e^{-y} f_2\left(\frac{E}{\theta}\right) \quad y \geq 0 \quad (149)$$

where

$$f_1\left(\frac{E}{\theta}\right) = \frac{E}{\theta} e^{-E/\theta} \left\{ 1 - \frac{E}{2\theta} + a \left[ \frac{4}{3} \left(\frac{E}{\theta}\right)^{\frac{1}{2}} - \frac{14}{45} \left(\frac{E}{\theta}\right)^{\frac{3}{2}} - \frac{4}{175} \left(\frac{E}{\theta}\right)^{\frac{5}{2}} \right] + a^2 \left[ \frac{2}{3} \left(\frac{E}{\theta}\right) - \frac{7}{135} \left(\frac{E}{\theta}\right)^2 \right] \right\} \quad (150)$$

and

$$f_2\left(\frac{E}{\theta}\right) = \frac{E}{\theta} e^{-E/\theta} \left\{ 1 - \frac{E}{\theta} + \frac{1}{6} \left(\frac{E}{\theta}\right)^2 + a \left[ \frac{4}{3} \left(\frac{E}{\theta}\right)^{1/2} - \frac{4}{5} \left(\frac{E}{\theta}\right)^{3/2} + \frac{34}{525} \left(\frac{E}{\theta}\right)^{5/2} \right] + a^2 \left[ \frac{2}{3} \left(\frac{E}{\theta}\right) - \frac{11}{45} \left(\frac{E}{\theta}\right)^2 \right] \right\} \quad (151)$$

The functions  $f_1$  and  $f_2$  chosen are the two energy eigen functions of the problem, as given by Equations 37. This choice has been made since these energy eigen functions satisfy the conditions dictated by Equations 142 and 143. These form a subset of the complete set  $f_n(E)$ , ( $n = 0, 1, 2, \dots$ ) as explained earlier in this chapter. Only a few terms in the functions  $f_1$  and  $f_2$  will be sufficient for computational purposes as the coefficients of larger powers of  $E/\theta$  are rapidly decreasing. Using the procedure of orthogonalization, as before, will lead to

$$A \int_0^{\infty} \left[ \int_{-\infty}^0 u_1 H_1 u_1 dy + \int_0^{\infty} u_2 H_2 u_2 dy \right] dE + B \int_0^{\infty} \left[ \int_{-\infty}^0 u_1 H_1 v_1 dy + \int_0^{\infty} u_2 H_2 v_2 dy \right] dE$$

$$+ \int_0^{\infty} \left[ \int_{-\infty}^0 u_1 H_1 \frac{\alpha_2 - \alpha_1}{2} e^y dy + \int_0^{\infty} u_2 H_2 \frac{\alpha_1 - \alpha_2}{2} e^{-y} dy \right] dE = 0 \quad (152)$$

and,

$$\begin{aligned} & A \int_0^{\infty} \left[ \int_{-\infty}^0 v_1 H_1 u_1 dy + \int_0^{\infty} v_2 H_2 u_2 dy \right] dE \\ & + B \int_0^{\infty} \left[ \int_{-\infty}^0 v_1 H_1 v_1 dy + \int_0^{\infty} v_2 H_2 v_2 dy \right] dE \\ & + \int_0^{\infty} \left[ \int_{-\infty}^0 v_1 H_1 \frac{\alpha_2 - \alpha_1}{2} e^y dy + \int_0^{\infty} v_2 H_2 \frac{\alpha_1 - \alpha_2}{2} e^{-y} dy \right] dE = 0 \quad (153) \end{aligned}$$

Performing the indicated operations and simplifying results in

$$\begin{aligned} & A \left\{ -\frac{\theta}{2} (0.0625 + 0.677a + 0.53a^2) - \frac{5}{4} (\theta_1 + \theta_2 - 20)(0.094 \right. \\ & \quad \left. + 76.76a + 0.580a^2) + \frac{5}{4} \theta^{\frac{1}{2}} (2a\theta^{\frac{1}{2}} - [a_2\theta_2^{\frac{1}{2}} + a_1\theta_1^{\frac{1}{2}}]) \right. \\ & \quad \left. (5.54 + 0.17a - 0.986a^2) \right\} \\ & + B \left( \frac{\theta_1 - \theta_2}{2} \right) (0.406 + 316a - 1.33a^2) \\ & + \frac{3}{8} (\theta_1 - \theta_2) \left[ (a_2 - a_1) 11.84 + (a_2^2 - a_1^2) 0.55 - a(a_2 - a_1) 0.701 \right] \\ & \qquad \qquad \qquad = 0 \quad (154) \end{aligned}$$

and

$$\begin{aligned} & A(\theta_1 - \theta_2)(0.78 - 23.2a - 15.89a^2) \\ & + B \left\{ -\frac{\theta}{2}(0.0313 - 11.8a - 3.97a^2) + \frac{\theta^{\frac{1}{2}}}{4} (2a\theta^{\frac{1}{2}} - [a_1\theta_1^{\frac{1}{2}} + a_2\theta_2^{\frac{1}{2}}]) \right. \\ & \quad \left. (2.16 + 1.89a + 18.3a^2) + \frac{1}{4} (2\theta - [\theta_1 + \theta_2]) (0.781 + 5.02a - 81.94a^2) \right\} \\ & + \frac{\theta}{2} \left[ (a_2 - a_1) 1.46 + (a_2^2 - a_1^2) 0.206 - a(a_2 - a_1) 0.013 \right] \end{aligned}$$

$$\begin{aligned}
& + \frac{\theta^{\frac{1}{2}}}{4} \left[ 2a\theta^{\frac{1}{2}} - (a_1\theta_1^{\frac{1}{2}} + a_2\theta_2^{\frac{1}{2}}) \right] \left[ (a_2 - a_1)0.053 - (a_2^2 - a_1^2)156.7 \right. \\
& \quad \left. + a(a_2 - a_1)3.41 \right] + \frac{1}{4} \left[ 2\theta - \theta_1 - \theta_2 \right] \left[ (a_2 - a_1)2.24 \right. \\
& \quad \left. - (a_2^2 - a_1^2)0.044 - a(a_2 - a_1)0.576 \right] = 0 \quad (155)
\end{aligned}$$

From Equations 154 and 155 which are correct up to order  $a^2$ , A and B can be determined provided the ratio of  $\theta_2/\theta_1$  and the value of either  $a_1$  or  $a_2$  are specified.

In the above equations  $\theta$  is the mean temperature and  $a$  is the mean absorption parameter, which are arbitrary. The previous case considered, the case of zero absorption, suggests that  $\theta$  can be taken as the harmonic mean of the temperatures of the two regions. The absorption parameter can be regarded as the average of the two absorption values.

Once again a ratio of  $\theta_2/\theta_1 = 2$  is considered as an example so that comparisons with the preceding work can be made. Assigning a value of 0.5 for  $a_2$ , in the high temperature region the following results ensue:

$$a_1 = a_2 \sqrt{\frac{\theta_2}{\theta_1}} = a_2 \sqrt{2} = (0.5) (\sqrt{2}) = 0.707 \quad (156)$$

$$a = \frac{a_1 + a_2}{2} = \frac{0.5 + 0.707}{2} = 0.6035 \quad (157)$$

and

$$\theta = \frac{\theta_1 \theta_2}{2(\theta_1 + \theta_2)} = \frac{\theta_1}{3} \quad (158)$$

Substituting for  $a_1$ ,  $a_2$ ,  $a$  and  $\theta$  in Equations 154 and 155 and simplifying results in

$$(152.55)A + (95.41)B = 0.925 \quad (159)$$

and

$$(23.37)A - (16.73)B = 4.747 \quad (160)$$

Solving for A and B from the above equations gives,

$$A = 0.098 \quad (161)$$

and

$$B = -0.147 \quad (162)$$

Therefore, the solution can be written as

$$\begin{aligned} \theta_1 F_1 = & 1 + \frac{\mathcal{L}_2 - \mathcal{L}_1}{2} e^y + 0.092 (1-y) e^y f_1 \\ & - 0.147 y e^y f_2 \left(\frac{E}{\theta}\right) \quad y \leq 0 \end{aligned} \quad (163)$$

$$\begin{aligned} \theta_2 F_2 = & 2 + \left(\frac{\mathcal{L}_1 - \mathcal{L}_2}{2}\right) e^{-y} + 0.098 (1+y) e^{-y} f_1 \\ & - 0.147 y e^{-y} f_2 \quad y \geq 0 \end{aligned} \quad (164)$$

where  $\alpha_1, \alpha_2, f_1$  and  $f_2$  are given by Equations 132, 133, 150 and 151 respectively. The flux is shown plotted in Figures 4, 5, 6 and 7, at  $Y = -\infty$  and  $\infty, -1, 0$  and  $1$  respectively. The graphs at  $\pm\infty$  show the asymptotic distribution for comparative purposes the Maxwellian distribution in the low and high temperature regions are shown in Figure 8. In Figure 6 the exact values obtained in the previous section and the approximate values obtained in this section are plotted at

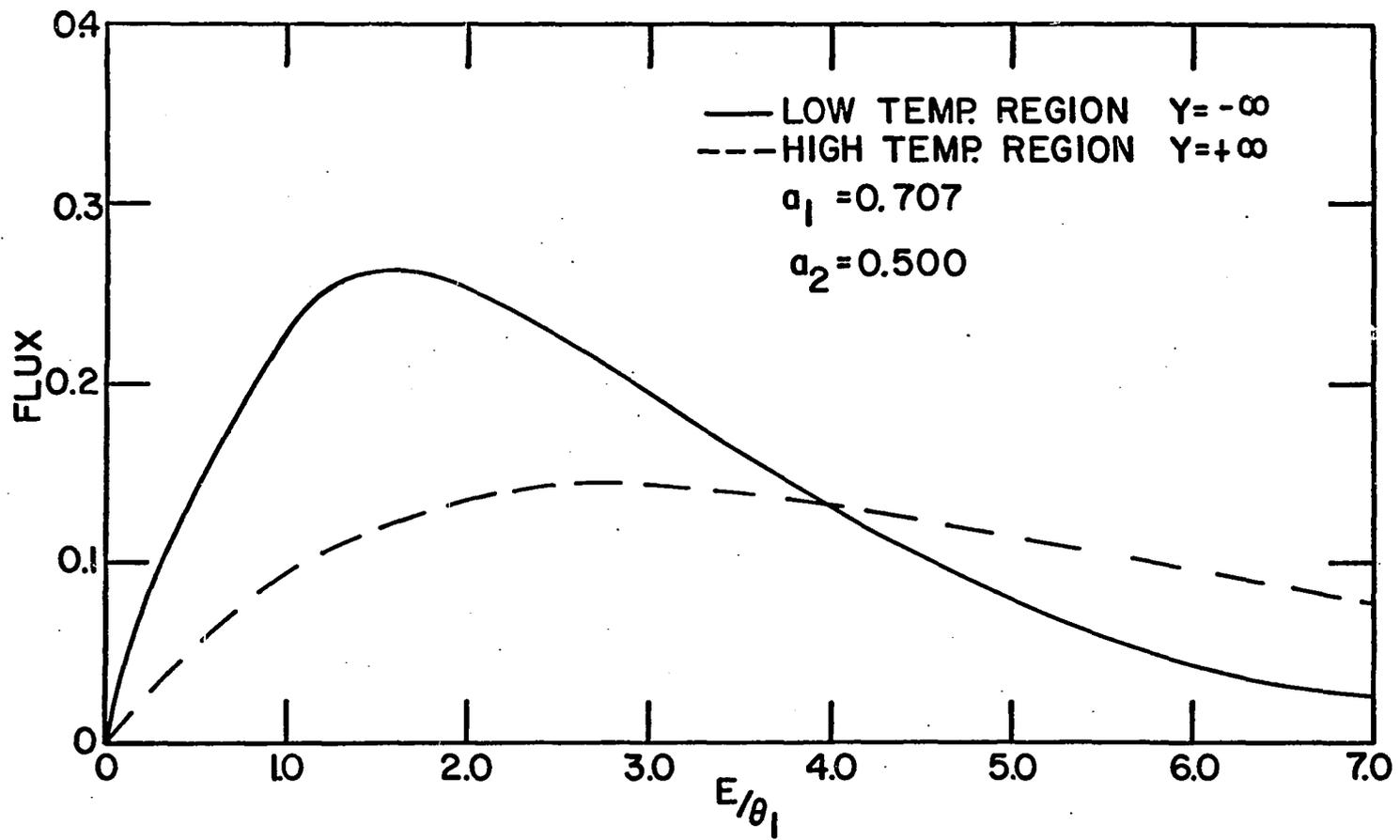


Figure 4. Asymptotic flux spectrum in a  $\frac{1}{V}$  absorbing medium

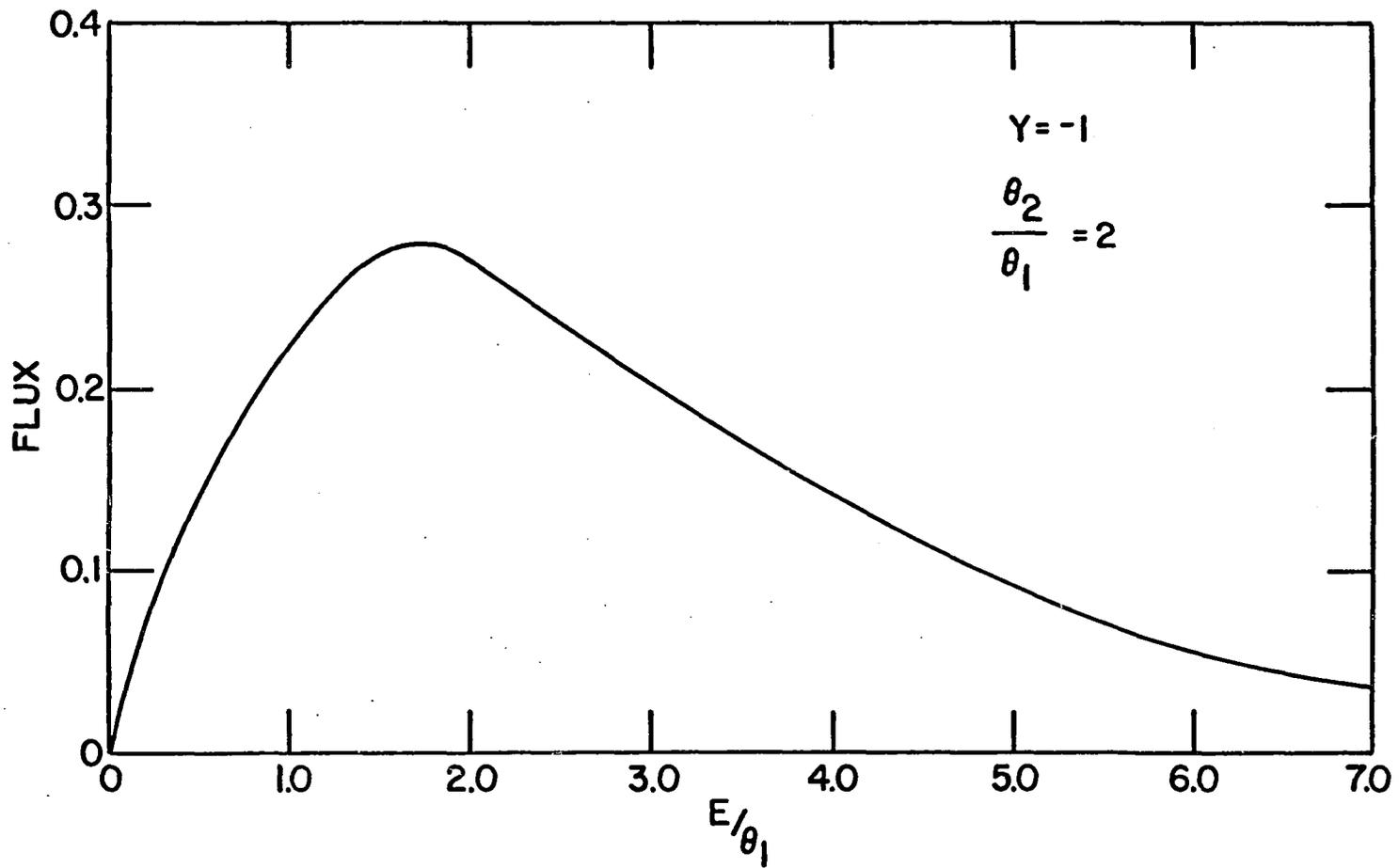


Figure 5. Flux spectrum at one relaxation length from interface in low temperature region and  $\frac{1}{V}$  absorbing medium

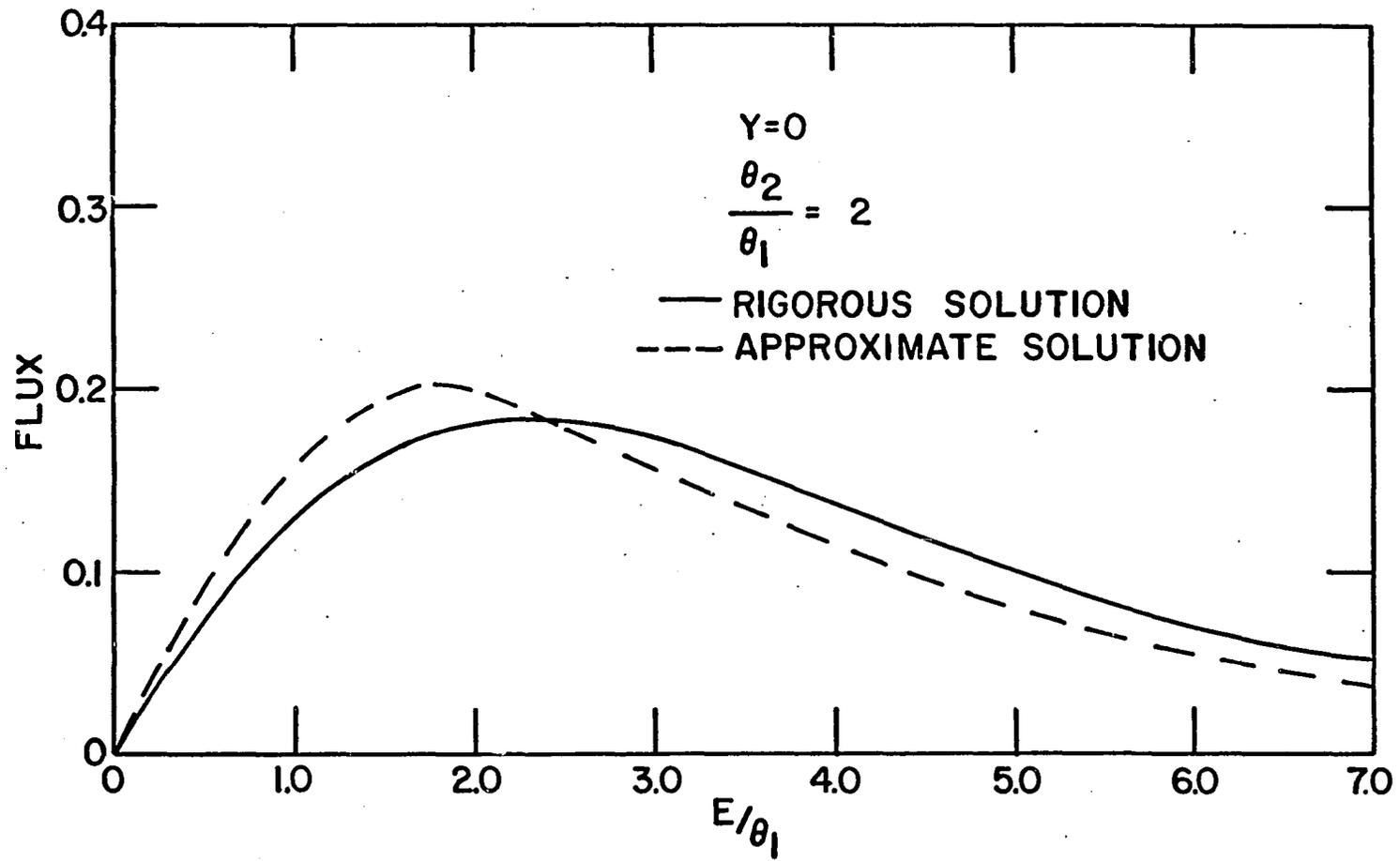


Figure 6. Flux spectrum at interface in a  $\frac{1}{V}$  absorbing medium

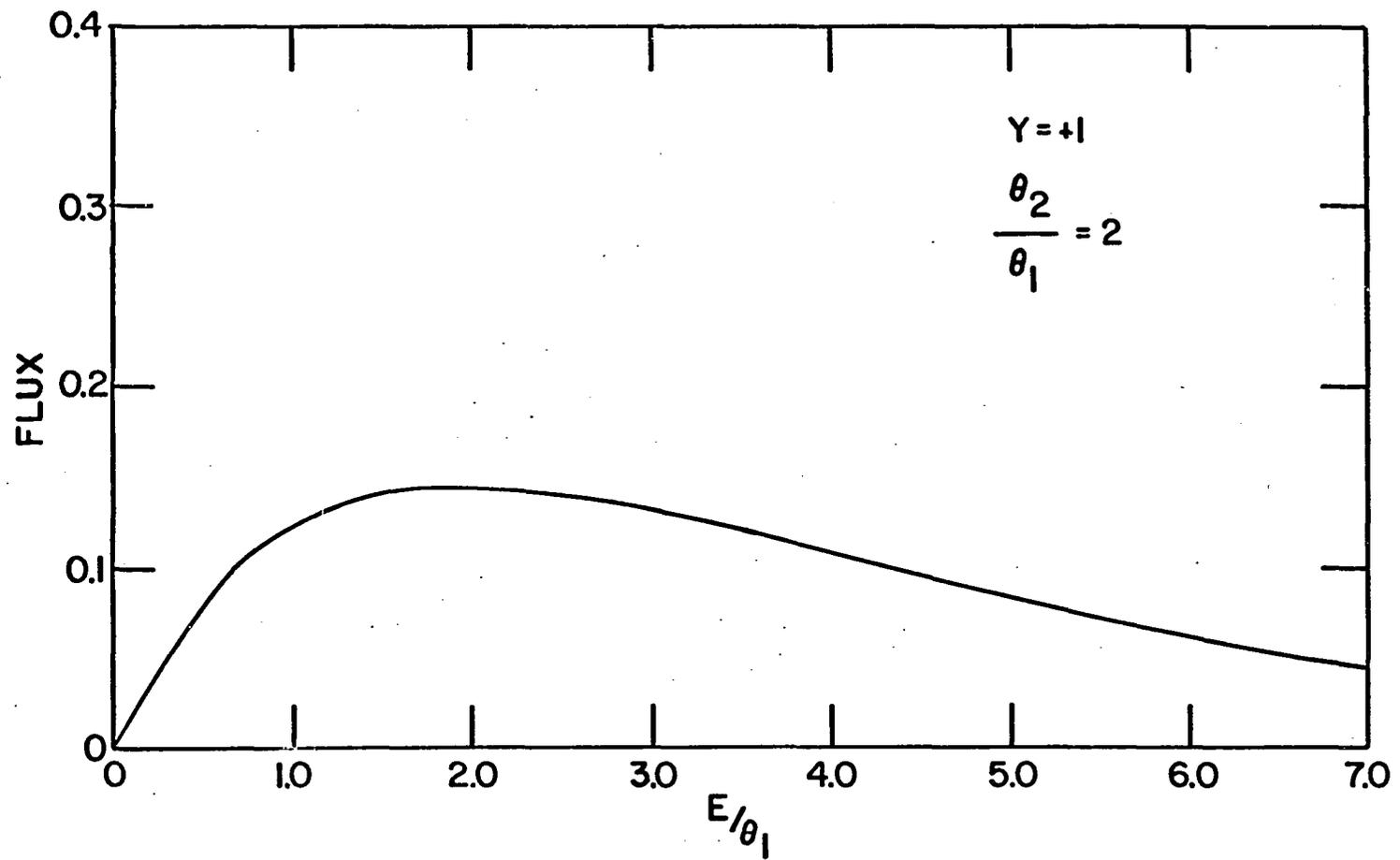


Figure 7. Flux spectrum at one relaxation length from interface in high temperature region and  $\frac{1}{V}$  absorbing medium

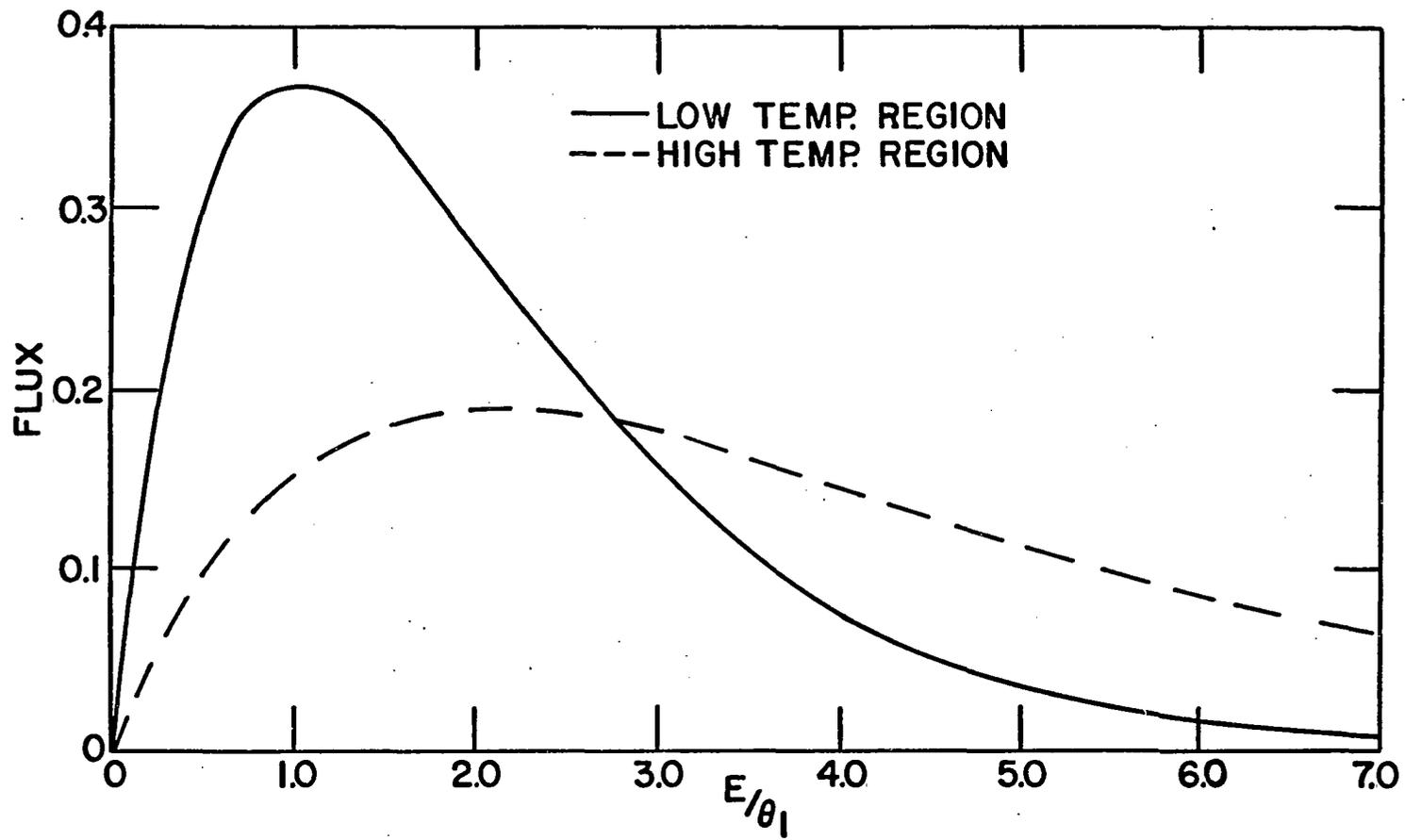


Figure 8. Maxwellian energy distribution

$Y = 0$ . All the curves are normalized so that

$$\int_0^{\infty} \phi(y, E) \frac{dE}{\theta_1} = 1.$$

## DISCUSSION

The present investigation has been carried out under the assumption that the diffusion theory is valid and that the medium can be treated as a heavy monoatomic gas. Besides, the type of temperature distribution chosen is not realistic and the medium is taken to be non-multiplying. This makes the problem idealistic. However, the diffusion theory is quite satisfactory at least as a first approximation. The heavy monoatomic gas model for the medium is valid in every case at sufficiently high temperatures so as to appreciably excite the lattice or molecular vibrations and rotations, as discussed in Weinberg and Wigner (1). Even otherwise the effect of chemical binding can be accounted for if it is possible to determine experimentally an effective nuclear mass and consider it as a parameter.

Thus far indications are that the crystalline and chemical binding effects seem to be secondary in nature, as explained by Nelkin and Cohen (3), especially in comparison with the effects considered in the present investigation.

The omission of sources and the multiplicative property of the medium help to isolate the desired effect from other related ones, especially as a first step in an investigation of this nature. With the absorption term included it has been possible to exhibit the spectral distortion due to the

combined effect of the temperature and absorption. Figure 9 gives a comparison of the spectral distortion from the Maxwellian arising from pure absorption, pure temperature variation and the combined effect of the two. Since the effect of temperature change is expected to be strong at the interface all the curves are plotted at the position  $Y = 0$ . It can be seen from Figure 9 that the effect of non-uniform temperature is not secondary as stated by de Ladonchamps and Grossman (13), especially when considered in conjunction with absorption. Many investigators have tried to describe this effect by means of effective neutron temperature, which enables one to express the low energy portion of the neutron spectrum empirically by means of Maxwellian distribution with a fictitious temperature. Cohen (8) has shown that such a description is quite ambiguous in the case of neutron spectrum in an absorbing medium with uniform temperature. However, for small values of 'a', the absorption parameter, the effective neutron temperature seems to be valid, according to the results of Coveyou et al. (5). But it is quite doubtful if such an empirical relation can be valid when both the effects are present.

In spite of the simplified model considered obtaining the analytical solution has been found to be complicated. Hence some simpler method that is not purely empirical in nature of determining the spectrum would be highly desirable. Kottwitz (11) has applied two simple schemes to the problem

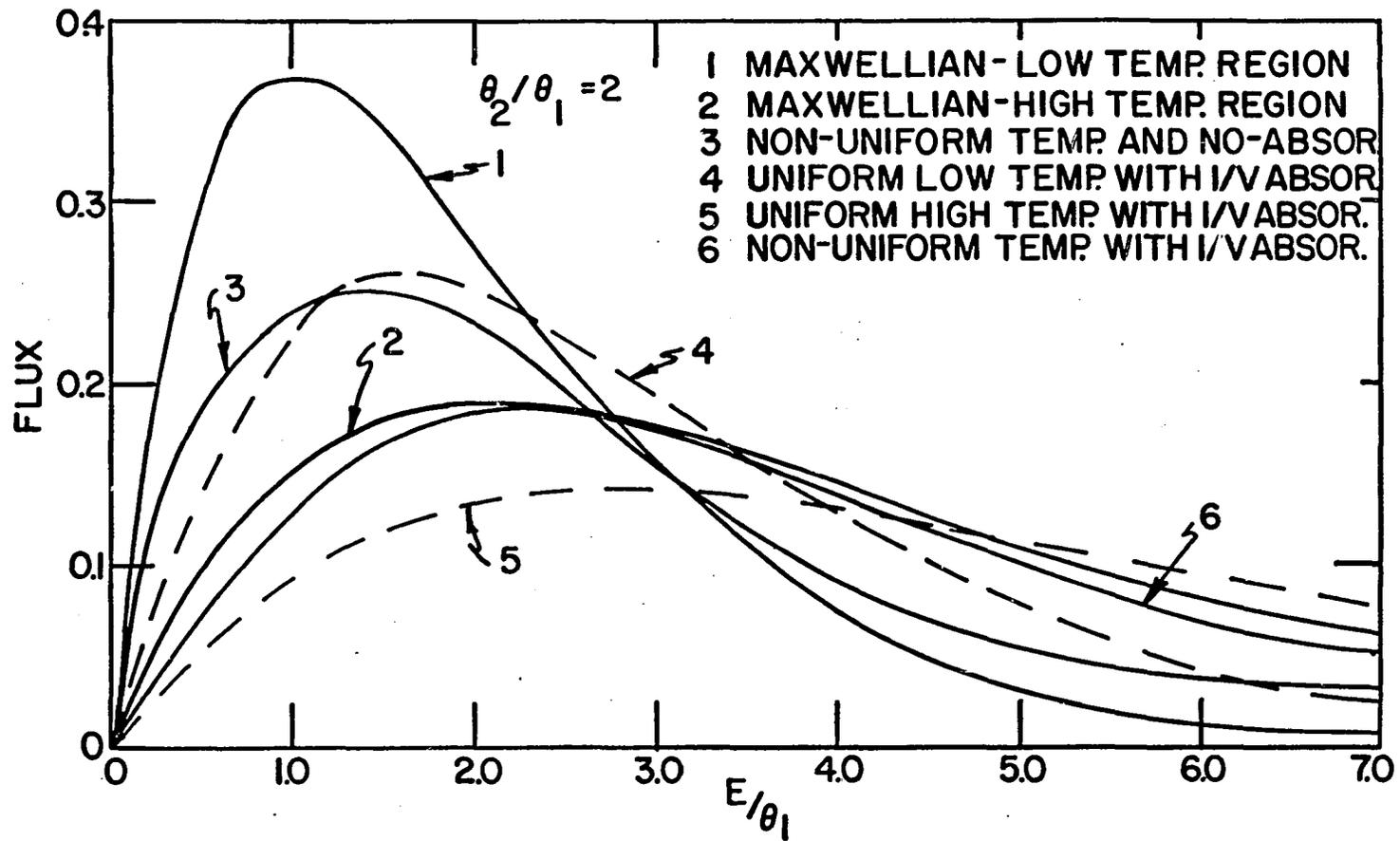


Figure 9. Deviation of flux spectrum from Maxwellian due to absorption only, due to non-uniform temperature only and due to both absorption and non-uniform temperature

in an non-absorption medium. Of these, the neutron temperature approximation which assumes that the thermal energy neutrons have a Maxwellian spectrum at every point in space has been shown to be less satisfactory than the other method due to Selengut (12). Recently, Pearce and Kennedy (21) have worked out the same problem as considered by Kottwitz by applying multigroup technique. They have used a G-20 computer to solve for flux spectrum by using 40-group diffusion equations. They have compared the two methods mentioned above and shown that Selenguts' method is by far more accurate than a single neutron temperature approximation.

In this investigation yet another method, the Galerkin's method, has been used to obtain a simple and yet quite accurate approximation for the thermal neutron spectrum. However, for this particular problem it has reduced to that of Selengut's scheme with a few correction terms added.

The comparative results obtained from all these methods when applied to the problem in a non-absorbing medium are shown in Figure 10. The curve designated as present work I is the one of the trials of the arbitrary constant  $p$ , taken as an arithmetic mean. The one called present work II is the one using a harmonic mean for the arbitrary constant  $p$ . This is shown to give closer values to the exact solution, hence this value for  $p$  is used throughout the rest of this work. The Galerkin's method has given values within an experimental accuracy, if an experiment can be performed

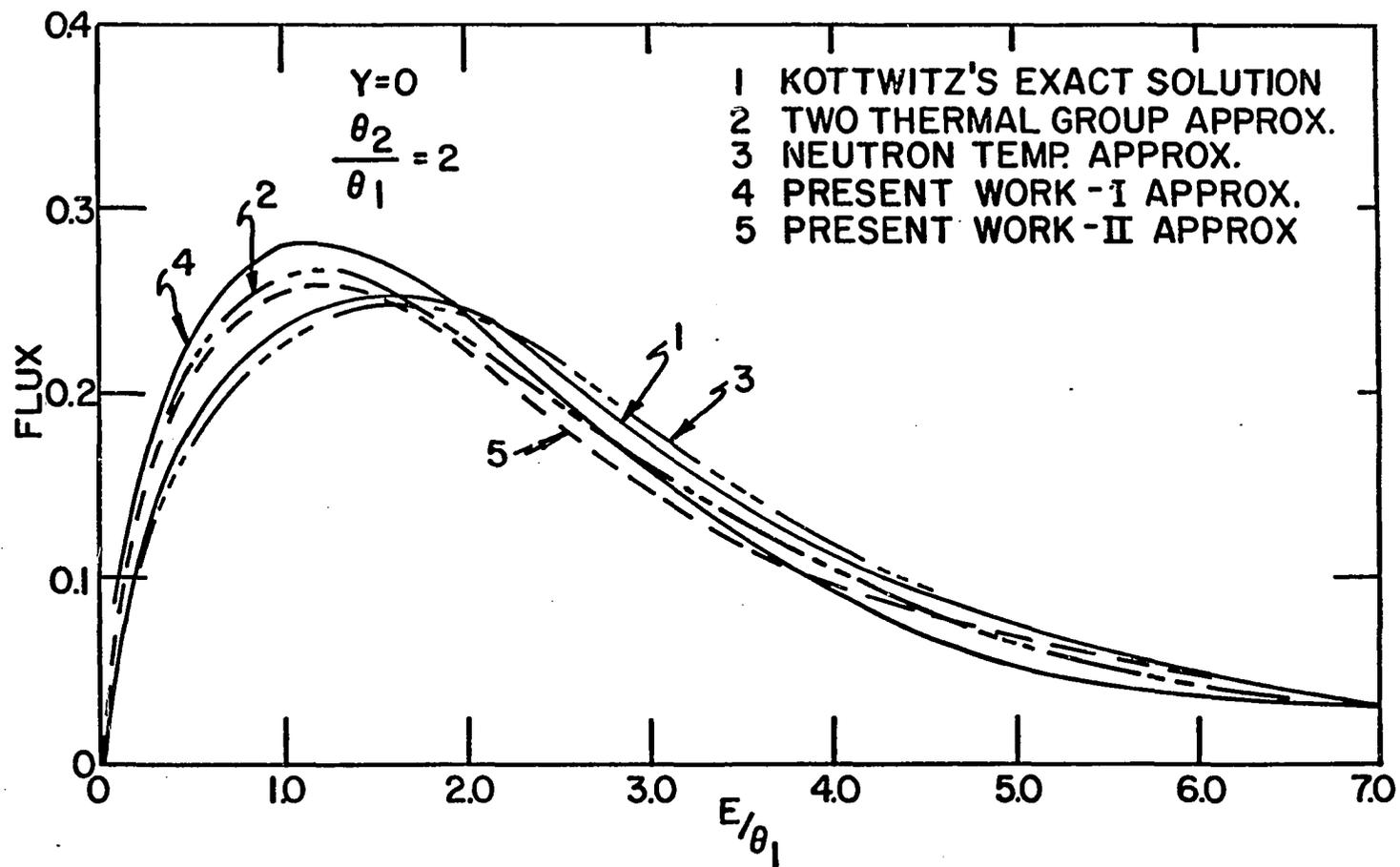


Figure 10. Comparison of exact and approximate solutions at interface in a non-absorbing medium

to verify the theoretical results.

In the case of the absorbing medium the functions obtained at every stage of the investigation have been checked to find that they reduce to the special cases when  $a = 0$  or  $\theta$  is uniform or when  $n = 0$ , i.e. space independent. This assures that the analytical expression is valid, although the questions of convergence and the number of eigenfunctions to be considered to assure accuracy in computation has not been discussed explicitly.

Galerkin's method can be applied successfully even when the temperature is not a simple function of position as chosen in the present investigation. Even with the same formulation of the problem, as given in the last section,  $\theta$  can be treated as  $\theta(y)$  in the operator  $H$ . The operations can then be carried on provided  $\theta(y)$  can be expressed explicitly.

Since the transport aspects of the problem are considered only in the  $P_1$  approximation the theory may be expected to be valid for a small temperature jump provided the transport properties do not change appreciably across the temperature discontinuity, although the range of validity is not yet known.

CONCLUSIONS AND RECOMMENDATIONS  
FOR FURTHER INVESTIGATION

Conclusions

Within the validity of assumptions made in this investigation, the following qualitative conclusions can be drawn.

1) The thermal neutron flux spectrum is considerably hardened due to the non-uniformity of temperature and the presence of absorbing media.

2) Neutrons tend to diffuse from the higher temperature region to the lower temperature region.

3) The shift in the peak of the spectrum from the Maxwellian distribution is not given by a simple empirical combination of the individual shifts due to the temperature and absorption effects.

4) In view of the complicated nature of the problem, analytical solutions can be obtained only in a few special cases such as the one considered. The approximation schemes used give results within an experimental accuracy. On the basis of this it can be extrapolated that solutions to more complicated problems can be successfully solved through approximate methods.

Scope for Further Research

Neither sources nor the multiplicative aspects of the medium have been considered in this investigation. Although

a similar procedure could be followed in seeking solutions it will be useful to consider these effects as well since they represent more realistic situations.

It will also be worthwhile to seek solutions to the partial differential equation by means of suitable analog methods or by computer techniques and estimate the accuracy of the approximation schemes.

The results obtained from this investigation could be compared by a suitably designed experimental method.

Since the heavy gas model is not expected to be satisfactory for all media, it is desirable to devise a new model that can encompass all materials.

## LITERATURE CITED

1. Weinberg, A. M. and Wigner, E. P. The physical theory of neutron chain reactors. Chicago, Illinois, The University of Chicago Press. 1959.
2. Poole, M. J., Nelkin, M. S. and Stone, R. S. The measurement and theory of reactor spectra. In Hughes, D. J., Sanders, J. E. and Horowitz, J., eds. Progress in nuclear energy. Series 1. Vol. 2. pp. 91-164. New York, New York, Pergamon Press, Ltd. 1958.
3. Nelkin, M. S. and Cohen, E. R. Recent work in neutron thermalization. In Hughes, D. J., Sanders, J. E. and Horowitz, J., eds. Progress in nuclear energy. Series 1. Vol. 3. pp. 179-193. New York, New York, Pergamon Press, Ltd. 1959.
4. Wigner, E. P. and Wilkins, J. E., Jr. Effect of the temperature of the moderator on the velocity distribution of neutrons with numerical calculations for H as moderator. U. S. Atomic Energy Commission Report AECD-2275. Technical Information Service Extension, AEC. 1948.
5. Coveyou, R. R., Bate, R. R. and Osborne, R. K. Effect of moderator temperature upon neutron flux in infinite, capturing medium. Journal of Nuclear Energy 2: 153-167. 1956.
6. Wilkins, J. E., Jr. Effect of the temperature of the moderator on the velocity distribution of neutrons for a heavy moderator. U. S. Atomic Energy Commission Report CP-2481 Chicago. University. Metallurgical Lab. 1944.
7. Hurwitz, H., Jr., Nelkin, M. S. and Habetler, G. J. Neutron thermalization. 1. Heavy gaseous moderator. Nuclear Science and Engineering 1: 280-312. 1956.
8. Cohen, E. R. The neutron velocity spectrum in a heavy moderator. Nuclear Science and Engineering 2: 227-245. 1957.
9. Kazarnovsky, M. V., Stepanov, A. V. and Shapiro, F. L. Neutron thermalization and diffusion in heavy media. In Hughes, D. J., Sanders, J. E. and Horowitz, J., eds. Progress in nuclear energy. Series 1. Vol. 3. pp. 227-246. New York, New York, Pergamon Press, Ltd. 1959.

10. Michael, P. Thermal neutron flux distribution in space and energy. Nuclear Science and Engineering 8: 426-431. 1960.
11. Kottwitz, D. A. Thermal neutron flux spectrum in a medium with a temperature discontinuity. Nuclear Science and Engineering 7: 345-354. 1960.
12. Selengut, D. S. Thermal neutron flux in a cell with temperature discontinuities. Nuclear Science and Engineering 9: 94-96. 1961.
13. Ladonchamps, J. R. L. de. and Grossman, L. M. Neutron diffusion in a temperature gradient. Nuclear Science and Engineering 12: 238-242. 1962.
14. Morse, P. M. and Feshbach, H. Methods of theoretical physics. New York, N. Y., McGraw-Hill Book Co., Inc. 1953.
15. Ince, E. L. Ordinary differential equations. New York, N. Y., Dover Publications, Inc. 1956.
16. Erdelyi, A. Asymptotic expansions. New York, N. Y., Dover Publications, Inc. 1956.
17. Bateman, H. Higher transcendental functions. Vol. 2. Compiled by the staff of Bateman Manuscript Project. Erdelyi, A. Director. New York, N. Y., McGraw-Hill Book Co., Inc. 1953.
18. \_\_\_\_\_. Tables of integral transforms. Vol. 1. Compiled by the staff of Bateman Manuscript Project, Erdelyi, A. Director. New York, N. Y. McGraw-Hill Book Co., Inc. 1953.
19. Garelis, E. Eigen values for Wilkin's equation. Nuclear Science and Engineering 13: 197-199. 1962.
20. Kantorovich, L. V. and Krylov, V. I. Approximate methods of higher analysis. (Translated by Benster, C. D.) New York, N. Y., Inter Science Publishers, Inc. 1958.
21. Pearce, R. M. and Kennedy, J. M. Thermal neutron spectrum in a moderator with a temperature discontinuity. Nuclear Science and Engineering 19: 102-107. 1964.

## ACKNOWLEDGMENTS

The author wishes to express his deep and sincere gratitude to his major professor Dr. Glenn Murphy, Anson Marston Distinguished Professor and the head of the Department of Nuclear Engineering, for all the encouragement and advice received during the course of the present investigation.

Thanks are also due to Dr. G. A. Nariboli, visiting Associate Professor in the Department of Mathematics for valuable suggestions and to Dr. C. G. Maple, Director, Iowa State Computation Center, for informative discussions.