Numerical Solutions of the One-Speed Neutron Transport Equation in Two-Medium Slabs and Spheres

by

Ninos Garis
NUMERICAL SOLUTIONS OF THE ONE-SPEED NEUTRON TRANSPORT EQUATION IN TWO-MEDIUM SLABS AND SPHERES

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ABSTRACT

The monoenergetic neutron transport equation with isotropic scattering has been applied to two-medium spherical and plane critical systems. The plane system has been considered both with vacuum boundary conditions and with repeated multiplying and non-multiplying material. The mean-free-path is assumed to be the same even though the multiplication factors are different in both media. The two coupled integral equations that are obtained are numerically solved using the spatial Legendre polynomial method (Carlvik's method).

Benchmark values of the fundamental and higher eigenvalues are given for various dimensions of the bodies. The total flux is calculated from the eigenvector and the first 4 or 5 flux modes are plotted for some typical cases.

The time-eigenvalue spectrum in subcritical two-medium systems has also been studied for vacuum boundary conditions. Using the close relation between the eigenvalues arising from the time-dependent and stationary transport equation the results for the stationary, critical case have been transformed to those for the time-dependent one. Further, the decay constants have been calculated by an iterative process when some parameter is varied.

In addition, simple approximate formulae for very high-order eigenvalues have been derived for both monoenergetic and two-medium systems. The formulae were tested against available and new numerical results.

Keywords: Neutron transport equation, two-medium systems, Carlvik's method, eigenvalue spectrum, criticality factor, time-decay constant.
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TO MY PARENTS
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In addition, simple approximation formulae for very high-order eigenvalues have been derived for both homogeneous and two-medium systems. The formulae were tested against available and new numerical results.
This thesis consists of the present paper and the following articles which are published or under printing.


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1. Introduction

The neutron transport equation is a linearized version of the equation originally developed by Boltzmann for the kinetic theory of gases. The equation can be applied to many problems pertaining to the transport of neutrons, gamma quanta or electrons, etc., see Duderstadt and Martin (1978). A very important practical application is the energy-dependent transport of neutrons in nuclear reactors, where the processes of neutron scattering, fission and absorption events with no self-interactions are modeled. An approximation of this form of the transport equation is usually made by introducing a set of coupled one-speed equations. In assessing the accuracy of such approximating techniques it is desirable that accurate solutions of the one-speed neutron transport equation are available. Studying the one-speed neutron transport equation also gives some information about the structure of the more general neutron transport equation and the nature of its solutions for more complicated problems.

Throughout the years, the properties of the solutions of the one-speed neutron transport equation have been studied from both theoretical and computational angles. The results of theoretical studies which e.g. deal with the nature of the eigenvalue spectrum are summarized in books by Kaper et al. (1982) and Greenberg et al. (1987). From computational point of view, Sahni and Sjöstrand (1990) have recently given a review of the criticality and time-eigenvalues for one-speed neutrons in simple systems with vacuum boundary conditions.

As noted by the latter authors, there are not so many detailed results on two-medium systems. To increase the knowledge about these systems, the one-speed neutron transport equation with isotropic scattering and vacuum boundary conditions has been applied to two-medium spherical and plane systems in the present work. The equation has also been applied to the closely related system of an infinite, two-medium slab of alternating multiplying and non-multiplying material. The fundamental and higher eigenvalues for both the stationary and the time-dependent case are calculated as functions of various dimensions of the bodies. For some cases the total neutron scalar flux for the first 4 or 5 modes are plotted. The results are compared with those given by so called asymptotic reactor theory, i.e. the buckling approximation.

Thus, the aim of the present work is to clarify the picture of the eigenvalue spectrum and to give highly accurate results of benchmark quality for these
The calculation method used here was first developed by Carlvik (1968). The principle of the method is to expand the scalar neutron flux in terms of Legendre polynomials of spatial coordinates. Generally, the method gives better results for eigenvalues, flux ratios, and average fluxes than most other methods, see Stepanek (1981).

In Chapter 2 the different forms of the one-speed neutron transport equation are presented. Applying the appropriate form of the transport equation to the cases studied in the present work, the integral equations used for numerical calculations are then deduced. After a short description of some useful calculation methods in Chapter 3, Carlvik's method is then applied to the critical systems considered here and the results are presented in Chapter 4. Chapter 5 deals with the time-dependent problem in reflected slabs and spheres while Chapter 6 gives some conclusions.
2. The One-Speed Neutron Transport Equation

The transport equation for neutrons of one-speed with isotropic scattering can be written (see e.g. Duderstadt and Martin 1979) as

\[
\frac{1}{v} \frac{\partial \phi(r, \Omega, t)}{\partial t} + \Omega \cdot \nabla \phi(r, \Omega, t) + \Sigma_t \phi(r, \Omega, t) = \left( \frac{c \Sigma_t}{4\pi} \right) \int \phi(r, \Omega', t) \, d\Omega'
\]  

(2.1)

where

- \(\phi(r, \Omega, t)\) is the neutron angular flux as a function of position, direction and time,
- \(v\) the neutron speed,
- \(\Sigma_t\) the total cross section,
- \(c\) the number of secondary neutrons per collision.

It has been assumed that \(\Sigma_t\) and \(c\) do not vary in space or direction, and that there are no external sources.

First, we apply Eq. (2.1) to a stationary, critical system, i.e. when \(\frac{\partial \phi}{\partial t}\) is zero and obtain

\[\Omega \cdot \nabla \phi(r, \Omega) + \Sigma_t \phi(r, \Omega) = \left( \frac{c \Sigma_t}{4\pi} \right) \int \phi(r, \Omega') \, d\Omega' \]  

(2.2)

The multiplicity \(c\) is related to the material cross sections by the equation

\[c = \frac{v \Sigma_f + \Sigma_s}{\Sigma_t} \]  

(2.3)

where \(\Sigma_f\) is the fission cross section, \(\Sigma_s\) the scattering cross section and \(v\) the number of neutrons per fission.

Secondly, we apply Eq. (2.1) to a time-decaying neutron population in a non-multiplying system. Instead of the factor \(c \Sigma_t\) in front of the integral we then have the scattering cross section \(\Sigma_s^\ast\). To distinguish from the critical case we denote the parameters of the time-dependent system with an asterisk. If we assume that the whole neutron population decays exponentially with the decay constant \(\lambda\), i.e.
\[
\phi(r, \Omega, t) = \Psi(r, \Omega) \cdot \exp(-\lambda t) ; \lambda > 0
\]  

(2.4)

then Eq. (2.1) becomes

\[
\Omega \cdot \nabla \Psi(r, \Omega) + (\Sigma_i^* - \lambda/v) \cdot \Psi(r, \Omega) = \Sigma^*_i \int \Psi(r, \Omega') \, d\Omega
\]  

(2.5)

Through the ansatz in Eq. (2.4) we may obtain both the fundamental and higher order time-eigenvalues and corresponding flux distributions.

Eq. (2.2) is a linear first order partial integro-differential equation which can be converted into an integral equation by a standard procedure known as the method of characteristics. Assuming that we are considering the transport problem in a bounded region V and that no neutrons enter V from the outside (vacuum boundary conditions), Eq. (2.2) can be written as

\[
\phi(r) = \frac{c \Sigma_i}{4 \pi} \int \frac{\exp(-\Sigma_i^* |r - r'|)}{|r - r'|^2} \phi(r') \, dV'
\]  

(2.6)

which is the integral form of the one-speed neutron transport equation. Converting Eq. (2.5) in a similar way gives

\[
\Psi(r) = \frac{\Sigma^*_i}{4 \pi} \int \frac{\exp(-(\Sigma_i^* - \lambda/v) |r - r'|)}{|r - r'|^2} \Psi(r') \, dV'
\]  

(2.7)

which is the integral form for the time-dependent case. It can be seen that the integro-differential form of the neutron transport equation gives angular fluxes while the integral form only contains scalar fluxes.

2.1 Analogy Between the Critical and Time-Decay eigenvalues

Comparing Eqs. (2.2) and (2.5) or (2.6) and (2.7) we can see that they are identical if we put

\[
\Sigma_i = \Sigma_i^* - \lambda/v = \Sigma^*_i + \Sigma^*_s - \lambda/v
\]  

(2.8)
and

\[ c \cdot \Sigma_i = \Sigma_i^* \]  \hspace{1cm} (2.9)

By introducing the dimensionless decay constant

\[ \Lambda = \frac{\lambda}{\nu \Sigma_s^0} \] \hspace{1cm} (2.10)

we obtain the following relation between \( c \) and \( \Lambda \)

\[ \Lambda = 1 - 1/c \] \hspace{1cm} (2.11)

From Eq. (2.9) it can be seen that if a characteristic dimension (radius or half-thickness) of the system is denoted \( a \), then the size of the system is conveniently expressed as \( a \Sigma_s^* \) for the time-dependent and as \( a \Sigma_i \) for the stationary case. Then we have obviously the relation

\[ a \Sigma_i^* = c \cdot a \Sigma_i \] \hspace{1cm} (2.12)

Thus, if we have a plot of the \( c \)-eigenvalues as a function of \( a \Sigma_i \), then the time eigenvalues \( \Lambda \) can be obtained from the intersection points with the hyperbola defined by Eq. (2.12) for a certain value of \( a \Sigma_i^* \). Similarly, in a plot of \( \Lambda \) versus \( a \Sigma_i^* \) the points corresponding to a certain value of \( a \Sigma_i \) will fall on the curve

\[ \Lambda = 1 - \frac{a \Sigma_i}{a \Sigma_i^*} \] \hspace{1cm} (2.13)

The transformation from the dimension \( a \Sigma_i \) to the dimension \( a \Sigma_i^* \) is straightforward if the quantity \( c \) is real. However, to obtain all possible \( \Lambda \) values, \( \Sigma_i \) must be allowed to take all complex values.

2.2 The Integral Equations for a Two-Medium Plane System

For plane geometry, we start from the integro-differential form of the neutron
transport equation. The neutron angular flux, $\phi(r,\Omega)$, is a function only of the position $x$ and the direction $\theta$. If we set $\mu = \cos \theta$, then Eq. (2.2) can be written as

$$\mu \frac{d}{dx} \phi(x,\mu) + \Sigma_1 \phi(x,\mu) = \frac{c_1 \Sigma_1}{2} \int_{-1}^{+1} \phi(x,\mu') \, d\mu' = \frac{c_1 \Sigma_1}{2} \phi_0(x)$$

(2.14)

We consider a two-region plane system (as shown in Fig. 1) with an inner medium of multiplication factor $c_1$ and thickness $2a$ and an outer medium with multiplication factor $c_2$ and thickness $d (= b - a)$. Subscripts 1 and 2 are used for the inner and outer medium, respectively. To simplify the notation, we assume that the mean-free-path is the same in both media and that all the lengths are measured in mean-free-paths. Before applying Eq. (2.14) to the two-medium plane system we use the integration factor $\exp(x\Sigma_1/\mu)$ to rewrite the equation as

$$\frac{d}{dx} \left[ \exp(x\Sigma_1/\mu) \cdot \phi(x,\mu) \right] = \frac{c_1 \Sigma_1}{2} \phi_0(x) \cdot \exp(x\Sigma_1/\mu)$$

(2.15)

Then this can be integrated over $x$. Following the same procedure as done by Sjöstrand (1986a) we start the integration at $-b$ for $\mu > 0$ and at $x = b$ for $\mu < 0$ where $\phi(x,\mu) = 0$ (i.e. vacuum boundary conditions). In this way we obtain expressions for $\phi(x,\mu)$ over all $\mu$ and $x$. Integrating these over $\mu$ we obtain an integral equation for the flux $\phi_0(x)$ in $-a \leq x \leq a$ and another integral equation for the flux $\phi_2(x)$ in $a \leq x \leq b$, i.e.
\[ \phi_{01}(x) = \frac{c_1}{2} \int_{-a}^{+a} \phi_{01}(x') \cdot E_1(\mid x - x' \mid) \, dx' \]
\[ + \frac{c_2}{2} \left[ \int_{a}^{b} \phi_{02}(x') \cdot E_1(x - x') \, dx' - \int_{-b}^{-a} \phi_{02}(x') \cdot E_1(x - x') \, dx' \right]; \]
\[ -a \leq x \leq a \quad (2.16) \]

\[ \phi_{02}(x) = \frac{c_1}{2} \int_{-a}^{+a} \phi_{01}(x') \cdot E_1(x - x') \, dx' \]
\[ + \frac{c_2}{2} \left[ \int_{a}^{b} \phi_{02}(x') \cdot E_1(\mid x - x' \mid) \, dx' + \int_{-b}^{-a} \phi_{02}(x') \cdot E_1(x - x') \, dx' \right]; \]
\[ a \leq x \leq b \quad (2.17) \]

where

\[ E_n(z) \text{ denotes the exponential integral of order } n: \]
\[ E_n(z) = \int_1^\infty \exp(-zt)t^n \, dt \quad (2.18) \]

If we transform the integrals with the integration limits from \(-b\) to \(-a\) using \(\phi_{02}(-x) = (-1)^q \cdot \phi_{02}(x)\) where

\[ q = \begin{cases} 0 & \text{for even modes} \\ 1 & \text{for odd modes} \end{cases} \quad (2.19) \]

we obtain

\[ \phi_{01}(x) = \frac{c_1}{2} \int_{-a}^{+a} \phi_{01}(x') \cdot E_1(\mid x - x' \mid) \, dx' \]
\[ + \frac{c_2}{2} \int_{a}^{b} \phi_{02}(x') \cdot \left[ E_1(x - x') + (-1)^q \cdot E_1(x + x') \right] \, dx' ; \]
\[ -a \leq x \leq a \quad (2.20) \]
2.3 Integral Equations for a Two-Medium Spherical System

With the same assumptions as for the plane system we now consider a spherical system with inner radius $a$ and outer radius $b$, see Fig. 2. According to Sjöstrand (1986b), it is convenient to start from the integral form of the transport equation (2.6). Then, the neutron scalar flux $\phi_1(r)$ of the inner medium can be obtained by looking at the contribution in the point $r$ from neutrons interacting in a volume element $dV$ at a point $r'$, i.e.

$$
\phi_1(r) = \frac{c_1\Sigma_i}{4\pi} \int_{V_1} \frac{\exp(-\Sigma_i|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|^2} \phi_1(r') dV_1
$$

$$
\quad + \frac{c_2\Sigma_i}{4\pi} \int_{V_2} \frac{\exp(-\Sigma_i|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|^2} \phi_2(r') dV_2
$$

(2.22)
The equation for the scalar flux $\phi_2(r)$ in the outer medium is similar. The substitutions

$$dV = 2\pi \sin \theta \, d\theta \, r^2 dr$$

(2.23)

and

$$R^2 = |r - r'|^2 = r^2 + r'^2 + 2rr'\cos \theta$$

(2.24)

and an integration over $\theta$ give

$$r \cdot \phi_1(r) = \frac{c_1}{2} \int_0^a r' \phi_1(r') \cdot \left[ E_1(|r-r'|) - E_1(r+r') \right] \, dr'$$

$$+ \frac{c_2}{2} \int_a^b r' \phi_2(r') \cdot \left[ E_1(|r-r'|) - E_1(r+r') \right] \, dr'; \quad 0 \leq r \leq a$$

(2.25)

$$r \cdot \phi_2(r) = \frac{c_1}{2} \int_0^a r' \phi_1(r') \cdot \left[ E_1(|r-r'|) - E_1(r+r') \right] \, dr'$$

$$+ \frac{c_2}{2} \int_a^b r' \phi_2(r') \cdot \left[ E_1(|r-r'|) - E_1(r+r') \right] \, dr'; \quad a \leq r \leq b$$

(2.26)

Now, for a spherical system we use the fact that the neutron scalar flux, $\phi(r)$, is equal everywhere on a spherical shell centred on the origin. This implies that $r \cdot \phi(r)$ is always an odd function for a sphere. If we make use of this relation to transform all the terms with $E_1(r+r')$ in the interval $0 \leq r \leq a$ and combine these with the term $E_1(|r-r'|)$ in the same equation, we obtain

$$r \cdot \phi_1(r) = \frac{c_1}{2} \int_0^a r' \phi_1(r') \cdot E_1(|r-r'|) \, dr'$$

$$+ \frac{c_2}{2} \int_a^b r' \phi_2(r') \cdot \left[ E_1(r'-r) - E_1(r+r') \right] \, dr'; \quad 0 \leq r \leq a$$

(2.27)
Comparing with Eqs. (2.20) and (2.21), it can be seen that Eqs. (2.27) - (2.28) for a sphere are identical to those for a slab with odd modes ($a$ and $b$ measured in mfp).

### 2.4 The Integral Equations for an Infinite, Two-Medium Slab Lattice

The derivation of the integral equations for a two-region slab lattice is very similar to that of a two-medium slab with vacuum boundary conditions, see Sec. 2.2. Therefore, only those parts of the derivation procedure which are different will be considered here. We now consider a two-region plane lattice as shown in Fig. 3 with the same notation as for the system with vacuum boundary conditions.

![Fig. 3 A two-region slab lattice](image)

Starting from Eq. (2.15) we make an integration over $x$. For $\mu > 0$ we start the integration at $x = -a$ and for $\mu < 0$ we start at $x = b$. In this way we obtain expressions for $\phi(x,\mu)$ over all $\mu$ and $x$. Integrating these over $\mu$ we obtain an integral equation for the scalar flux $\phi_0(x)$ in $-a \leq x \leq a$ and another integral equation for the scalar flux $\phi_2(x)$ in $a \leq x \leq b$, i.e.
\[
\phi_1(x) = \frac{c_1}{2} \int_{-a}^{a} \phi_1(x') \cdot E_1(|x-x'|) \, dx' + \int_{0}^{1} \phi_1(-a\mu) \cdot \exp(-(x+a\mu)) \, d\mu \\
+ \frac{c_2}{2} \int_{a}^{b} \phi_2(x') \cdot E_1(x'-x) \, dx' + \int_{-1}^{0} \phi_2(b\mu) \cdot \exp((b-x)\mu) \, d\mu ; \\
\ -a \leq x \leq a 
\]

\[
\phi_2(x) = \frac{c_1}{2} \int_{-a}^{a} \phi_1(x') \cdot E_1(x-x') \, dx' + \int_{0}^{1} \phi_1(-a\mu) \cdot \exp(-(x+a\mu)) \, d\mu \\
+ \frac{c_2}{2} \int_{a}^{b} \phi_2(x') \cdot E_1(|x-x'|) \, dx' + \int_{-1}^{0} \phi_2(b\mu) \cdot \exp((b-x)\mu) \, d\mu ; \\
\ a \leq x \leq b 
\]

Using the continuity and periodicity conditions we obtain the following equations:

\[
\phi_1(x) = \frac{c_1}{2} \int_{-a}^{a} \phi_1(x') \cdot \left[ E_1(|x-x'|) + Q(a+b+x-x',a+b) + Q(a+b-x-x',a+b) \right] \, dx' \\
+ \frac{c_2}{2} \int_{a}^{b} \phi_2(x') \cdot \left[ E_1(x-x') + Q(a+b+x-x',a+b) + Q(a+b-x-x',a+b) \right] \, dx' ; \\
\ -a \leq x \leq a 
\]

\[
\phi_2(x) = \frac{c_1}{2} \int_{-a}^{a} \phi_1(x') \cdot \left[ E_1(x-x') + Q(a+b+x-x',a+b) + Q(a+b-x-x',a+b) \right] \, dx' \\
+ \frac{c_2}{2} \int_{a}^{b} \phi_2(x') \cdot \left[ E_1(|x-x'|) + Q(a+b+x-x',a+b) + Q(a+b-x-x',a+b) \right] \, dx' ; \\
\ a \leq x \leq b 
\]

where

\[
Q(\alpha,\beta) = \int_{0}^{1} \frac{\exp(-\alpha/\mu)}{\mu \left[ 1 - \exp(-\beta/\mu) \right]} \, d\mu 
\]
2.5 The Integral Equation for Homogeneous Systems

We consider a homogeneous system with isotropic scattering and vacuum boundary conditions. For a slab or a sphere with the half-thickness or radius \( a \), the integral equation describing the neutron flux distribution, \( \phi(r) \), can be simply obtained by setting \( b = a \) in Eq. (2.20) or Eq. (2.27), i.e.

\[
\phi(r) = \frac{c}{2} \int_{-a}^{+a} \phi(r') \cdot E_{1}(|r-r'|) \, dr' \quad ; \quad 0 \leq r \leq a
\]  

(2.34)

2.6 The Buckling Approximation

It is sometimes interesting to compare the eigenvalues obtained from the systems with vacuum boundary conditions with those from the so called buckling approximation. In the latter case the spatial variation of the neutron flux is assumed to be proportional to \( \exp(iB \cdot r) \) where \( r \) is the spatial variable and \( B \) (or \( B^2 \)) is the buckling parameter. This means that the flux satisfies the equation

\[
\nabla^2 \phi(r) + B^2 \phi(r) = 0
\]  

(2.35)

By insertion of \( \exp(iB \cdot r) \) into the transport equation (2.2) we obtain the equation

\[
\tan \left( \frac{B \ell}{c} \right) = B \ell
\]  

(2.36)

where \( \ell (=1/\Sigma_a) \) is the mean-free-path. This gives us a relation between the criticality factor \( c \) and the buckling \( B^2 \). When \( c < 1 \) the buckling \( B^2 \) becomes negative and \( B \) will be replaced by the diffusion length \( L \) through the relation

\[
B^2 = - \frac{1}{L^2}
\]  

(2.37)

Solving the time-independent transport equation we obtain various criticality
eigenvalues $c_n$ as function of the dimensions of the system. From these criticality values the corresponding $B_n$ values can be obtained from the relation in Eq. (2.36). This means that we can obtain $B_n$ as a function of the dimension.

In the buckling approximation the neutron flux is assumed to be zero at a distance $z_n$ outside the boundary. Now, if $B_n$ and the dimension $a$ of a system are known, then the extrapolation distance $z_n$ can be determined through the relations

\[ B_n(a + z_n) = n \cdot \pi/2 \quad ; \text{for a sphere} \]  
\[ B_n(a + z_n) = n \cdot \pi \quad ; \text{for a slab} \]

where $n = 1,2,3,...$
3. Calculation Methods

Over the years, much work has been done pertaining to the numerical solutions of the neutron transport equation. Sanchez and McCormick (1982) have given a thorough review of the basic methods for solving the general transport equation where the relative advantages and limitations of the methods are pointed out. For the one-speed neutron transport equation, Sahni and Sjöstrand (1990) have reviewed the methods which can give criticality and time-eigenvalues of benchmark quality in simple systems with vacuum boundary conditions.

In the present Chapter we give a short description of some calculation methods which may be used to study monoenergetic neutron transport in simple systems and which give accurate results of benchmark quality.

3.1 The Spatial Spherical Harmonics Method (Carlvik's Method)

The spatial Legendre expansion method which originally was developed by Carlvik (1968) for homogeneous slabs and spheres is based on the integral equation. The principle of the method is to expand the scalar neutron flux in terms of Legendre polynomials of the spatial coordinate. Truncating the expansion at some order reduces the integral equation to a matrix eigenvalue problem.

The accuracy of the results increases when more terms in the expansion are used. But the cumulation of round-off errors due to repeated use of recursion relations reduces the accuracy. For small geometries the method gives very good results especially for the fundamental mode. For larger geometries, on the other hand, other methods are recommended. The method also gives less accurate results for the boundary flux. More details about the method will be given in Chapter 4.

3.2 The Integral Transform Method

The integral transform method, which is based on the integral form of the transport equation, utilizes a Fourier transform with respect to the space variable. The kernel in the transformed equation is then expanded in spherical Bessel functions. A truncation of the expansion at some order reduces the integral equation
to a matrix eigenvalue problem. For more details see e.g. Sahni (1972).

3.3 **The Singular Expansion Method (Case's Method)**

The singular expansion method was originally derived by Case (1960) for a plane geometry with isotropic scattering. The method is based on the integro-differential form of the transport equation and utilizes an expansion of the flux in each region in a complete set of eigenfunctions of the Boltzmann equation. Except for very simple systems the method is complicated to use.

3.4 **The Discrete Ordinates Method**

The discrete ordinates method - also called the $S_n$ method - is perhaps the simplest method of finding fundamental eigenvalues and is also well documented in the literature, see e.g. Bell and Glasstone (1970). The method is based on the integro-differential form of the Boltzmann equation. By choosing a sufficient number of directions and integrating over the scattering kernel by a numerical quadrature formula, the Boltzmann equation turns into a set of coupled differential equations. This set can then be solved by finite difference techniques once the boundary conditions and the character of the problem are specified. The accuracy of the method is largely dependent on making a good choice of the set of directions.
4. Critical Systems

4.1 Numerical Method for Reflected Systems

In Sec. 2.3 it was shown that the integral equations for a sphere are identical to those for a slab with odd modes. Applying the numerical method to only one case is therefore sufficient. Now, we consider the integral equations (2.20) and (2.21). Before applying Carlvik's method we substitute

\[ x = ay, \quad x = \frac{b+a}{2} + \frac{b-a}{2} y \]  

in Eq. (2.20) and Eq. (2.21), respectively. The substitutions

\[ x' = ay', \quad x' = \frac{b+a}{2} + \frac{b-a}{2} y' \]  

are then made in the first and second integral, respectively, in both equations to obtain integration limits from -1 to +1. We get the following system of equations for both the plane and spherical case

\[ \phi_1(y) = \frac{c_1}{a} \int_{-1}^{+1} \phi_1(y') \cdot E_1(ay-y') \, dy' \]

\[ + \frac{c_2(b-a)}{4} \int_{-1}^{+1} \phi_2(y') \cdot \left[ E_1\left(\frac{b+a}{2} - \frac{b-a}{2} y'y' \right) \right] dy' \]  

\[ \phi_2(y) = \frac{c_1}{a} \int_{-1}^{+1} \phi_1(y') \cdot E_1\left(\frac{b+a}{2} + \frac{b-a}{2} y - ay' \right) \, dy' \]

\[ + \frac{c_2(b-a)}{4} \int_{-1}^{+1} \phi_2(y') \cdot \left[ E_1\left(\frac{b-a}{2} |y-y'| \right) \right] dy' \]  

where
\[ \phi(y) = \begin{cases} \Psi(y), & \text{for a slab} \\ y \cdot \Psi(y), & \text{for a sphere} \end{cases} \]  

(4.5)

To solve Eqs. (4.3) and (4.4), the functions \( \phi_1(y) \) and \( \phi_2(y) \) are expanded into series of Legendre polynomials

\[ \phi_1(y) = \sum_{l^* = 0,2,4,\ldots}^{\infty} \frac{2l^*+1}{2} u_{l^*} P_{l^*}(y) \]  

(4.6)

\[ \phi_2(y) = \sum_{l=0,1,2,\ldots}^{\infty} \frac{2l+1}{2} v_l P_l(y) \]  

(4.7)

By inserting the series into Eqs. (4.3) and (4.4), multiplying by \( P_m(x) \) and integrating from \(-1\) to \(+1\), we obtain

\[ u_m = \frac{a c}{2} \sum_{l^* = 0,2,4,\ldots}^{\infty} \frac{2l^*+1}{2} A_{m,l^*} u_{l^*} + \frac{c_2(b-a)}{4} \sum_{l=0,1,2,\ldots}^{\infty} \frac{2l+1}{2} (B_{m,l} (-1)^q C_{m,l}) v_l \]  

(4.8)

\[ v_m = \frac{a c}{2} \sum_{l^* = 0,2,4,\ldots}^{\infty} \frac{2l^*+1}{2} D_{m,l^*} u_{l^*} + \frac{c_2(b-a)}{4} \sum_{l=0,1,2,\ldots}^{\infty} \frac{2l+1}{2} (E_{m,l} (-1)^q F_{m,l}) v_l \]  

(4.9)

where

\[ A_{m,l^*} = \int_{-1}^{+1} P_m(x) \, dx \int_{-1}^{+1} P_{l^*}(y) E_1(a|x-y|) \, dy \]  

(4.10)

\[ B_{m,l} = \int_{-1}^{+1} P_m(x) \, dx \int_{-1}^{+1} P_l(y) E_1(\frac{b+a}{2} y - ax + \frac{b-a}{2} y - ax) \, dy \]  

(4.11)
\[ C_{m,l} = \int_{-1}^{+1} P_m(x) \, dx \int_{-1}^{+1} P_l(y) \, E_1\left( \frac{b+a}{2} + \frac{b-a}{2} y + ax \right) \, dy \quad (4.12) \]

\[ D_{m,l} = \int_{-1}^{+1} P_m(x) \, dx \int_{-1}^{+1} P_l(y) \, E_1\left( \frac{b+a}{2} + \frac{b-a}{2} x - ay \right) \, dy \quad (4.13) \]

\[ E_{m,l} = \int_{-1}^{+1} P_m(x) \, dx \int_{-1}^{+1} P_l(y) \, E_1\left( \frac{b-a}{2} |x-y| \right) \, dy \quad (4.14) \]

and

\[ F_{m,l} = \int_{-1}^{+1} P_m(x) \, dx \int_{-1}^{+1} P_l(y) \, E_1\left( b+a + \frac{b-a}{2} (x+y) \right) \, dy \quad (4.15) \]

Now we introduce

\[ \lambda_1 = \frac{ac_1}{2} \quad (4.16) \]

and

\[ \lambda_2 = \frac{(b-a)c_2}{4}. \quad (4.17) \]

Eqs. (4.8) and (4.9) can then be expressed more conveniently by using block matrices

\[ \begin{bmatrix} A & 0 \\ D & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \lambda_2 \begin{bmatrix} 0 & B(-1)^q \cdot C \\ 0 & E(-1)^q \cdot F \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \quad (4.18) \]

where
0 = the zero matrix
1 = the unit matrix
\[ A = \left\{ \frac{2l+1}{2} A_{m,l} \right\}, \text{etc.} \]

This equation is a generalized eigenvalue problem which can be solved by standard methods. If \( \lambda_1 \) (or \( \lambda_2 \)) is known, then all the eigenvalues \( \lambda_{2n} \) (or \( \lambda_{1n} \)) can be obtained solving the eigenvalue problem. Further, the total neutron fluxes in both media can be calculated if the corresponding eigenvectors for the eigenvalues in both media are known.

The size of the matrices \( A, B, C, D, E \) and \( F \) depends on where the expansion series in Eqs. (4.6) and (4.7) are truncated. If we assume that this is done after \( L \) terms, then the effective number of Legendre polynomials is

\[ j = \frac{L}{2} + i \quad (4.19) \]

where

\[
i = \begin{cases} 
1 & \text{for a slab with even modes; } L \text{ even} \\
1/2 & \text{for } L \text{ odd} \\
0 & \text{for a sphere and a slab with odd modes; } L \text{ even}
\end{cases}
\]

### 4.2 Calculation of the Matrix Elements

Finding the matrix elements \( A_{m,l}, B_{m,l}, C_{m,l}, D_{m,l}, E_{m,l}, \) and \( F_{m,l} \) is what remains of our problem. Initially it can be observed that all the matrix elements can be divided into the following two types of integrals, i.e.

\[
S_{m,l}(\alpha) = \int_{-1}^{+1} P_m(x) \, dx \int_{-1}^{+1} P_l(y) \, E_l(\alpha \, |x-y|) \, dy \quad (4.20)
\]

and
\[ T_{m,l} (\alpha, \beta, \gamma) = \int_{-1}^{+1} P_m(x) \, dx \int_{-1}^{+1} P_l(y) \, E_1(\alpha + \beta x + \gamma y) \, dy \]  

(4.21)

We note that \( A_{m,l} \) and \( E_{m,l} \) are of the first type while the others are of the second type. Writing these in terms of \( S_{m,l} (\alpha) \) and \( T_{m,l} (\alpha, \beta, \gamma) \) we obtain:

\[ A_{m,l} = S_{m,l} (\alpha) \]  

(4.22)

\[ B_{m,l} = T_{m,l} \left( \frac{b+a}{2}, -a, \frac{b-a}{2} \right) \]  

(4.23)

\[ C_{m,l} = (-1)^m \cdot B_{m,l} \]  

(4.24)

\[ D_{m,l} = B_{l,m} \]  

(4.25)

\[ E_{m,l} = S_{m,l} \left( \frac{b-a}{2} \right) \]  

(4.26)

\[ F_{m,l} = T_{m,l} \left( b+a, \frac{b-a}{2}, \frac{b-a}{2} \right) \]  

(4.27)

The calculation of the matrix elements \( S_{m,l} \) has already been considered by e.g. Carlvik (1963) and Stepanek (1972). The principle is that certain low order elements must be calculated from the explicit expression and the rest by means of recurrence formulae. In this work we use the relevant formulae from these papers. For the elements \( T_{m,l} \), two methods have been used: One method utilizes recursion while the other one uses series expansion. For more details we refer to paper I.
4.3 Numerical Method for an Infinite, Two-Region Slab Lattice

First we use the substitution $\mu = 1/z$ in Eq. (2.33) and expand the obtained factor $1/(1-\exp(-(a+b)z))$ in an infinite series. The integral $Q(\alpha, \beta)$ can then be expressed in terms of the exponential integral function as

$$Q(\alpha) = \sum_{n=0}^{\infty} E_1(\alpha + n \cdot (a+b))$$  \hspace{1cm} (4.28)

Before applying the Legendre expansion method we substitute

$$x = ay \quad \text{and} \quad x = \frac{b+a}{2} + \frac{b-a}{2} y$$  \hspace{1cm} (4.29)

in Eq. (2.31) and Eq. (2.32), respectively. The substitutions

$$x' = ay' \quad \text{and} \quad x' = \frac{b+a}{2} + \frac{b-a}{2} y'$$  \hspace{1cm} (4.30)

are then made in the first and second integral, respectively, in both equations to change the integration limits to $-1$ and $+1$. We obtain the following system of equations:

$$\phi_{01}(y) = \sum_{n=1}^{\infty} \left[ \frac{ac}{2} \int_{-1}^{1} \phi_{01}(y') \cdot \left[ E_1(a | y-y' |) + E_1(n(a+b) + ay - ay') ight. ight.$$

$$\left. + E_1(n(a+b) - ay + ay') \right] dy'$$

$$+ \frac{(b-a)c_2}{4} \int_{-1}^{1} \phi_{02}(y') \cdot \left[ E_1\left(\frac{b+a}{2} - ay + \frac{b-a}{2} y\right)' + E_1\left((n-\frac{1}{2})(a+b) + ay - \frac{b-a}{2} y\right) ight.$$

$$\left. + E_1\left((n+\frac{1}{2})(a+b) + \frac{b-a}{2} y - ay\right) \right] dy' ;$$

$$-1 \leq y \leq 1$$  \hspace{1cm} (4.31)
\[ \phi_{02}(y) = \sum_{n=1}^{\infty} \left[ \frac{ac_1}{2} \int_{-1}^{+1} \phi_{01}(y') \cdot \left[ E_1 \left( \frac{b-a}{2} y + ay' \right) + E_1 \left( (n-\frac{1}{2})(a+b) + \frac{b-a}{2} y - ay' \right) \right. \right. \]
\[ \left. \left. + E_1 \left( (n-\frac{1}{2})(a+b) - \frac{b-a}{2} y + ay' \right) \right] \, dy' \right] \right] dy' \]
\[ + \frac{(b-a)c_2}{4} \int_{-1}^{+1} \phi_{02}(y') \cdot \left[ E_1 \left( \frac{b-a}{2} |y-y'| \right) + E_1 \left( (n(a+b) + \frac{b-a}{2} (y-y')) + \right. \right. \]
\[ \left. \left. E_1 \left( (n(a+b) + \frac{b-a}{2} (y'-y)) \right) \right] \, dy' \right] \right] dy' ; \]
\[ \frac{a}{b} \leq y \leq 1 \quad (4.32) \]

To solve Eqs. (4.31) and (4.32), the functions \( \phi_{01}(y) \) and \( \phi_{02}(y) \) are expanded into series of Legendre polynomials

\[ \phi_{01}(y) = \sum_{l=1}^{\infty} \frac{2l+1}{2} u_l P_l(y) \quad (4.33) \]
\[ \phi_{02}(y) = \sum_{l=1}^{\infty} \frac{2l+1}{2} v_l P_l(y) \quad (4.34) \]

where

\[ l = \begin{cases} 1, 3, 5, \ldots \text{ for a slab with odd modes} \\ 0, 2, 4, \ldots \text{ for a slab with even modes} \end{cases} \quad (4.35) \]

By inserting the series into Eqs. (4.31) and (4.32), multiplying by \( P_n(x) \) and integrating from \(-1\) to \(+1\), we obtain

\[ u_m = \frac{ac}{2} \sum_l \frac{2l+1}{2} \left[ A_{m,l}^1 + B_{m,l}^1 + C_{m,l}^1 \right] u_l P_l(y) + \]
\[ \frac{c_2(b-a)}{4} \sum_l \frac{2l+1}{2} \left[ A_{m,l}^2 + B_{m,l}^2 + C_{m,l}^2 \right] v_l P_l(y) \quad (4.36) \]
\[
\nu_m = \frac{ac_1}{2} \sum_l \frac{2l+1}{2} \left[ A_{m,l}^3 + B_{m,l}^3 + C_{m,l}^3 \right] u_l P_l(y) + c_2(b-a) \sum_l \frac{2l+1}{2} \left[ A_{m,l}^4 + B_{m,l}^4 + C_{m,l}^4 \right] v_l P_l(y) \tag{4.37}
\]

where the matrix elements can be written in terms of \( S_{m,l}(\alpha) \) (see Eq. (4.20)) and \( T_{m,l}(\alpha,\beta,\gamma) \) (see Eq. (4.21)) as

\[
A_{m,l}^1 = S_{m,l}(a) \tag{4.38}
\]

\[
B_{m,l}^1 = \sum_{n=1}^{\infty} T_{m,l}(n(a+b), a, -a) \tag{4.39}
\]

\[
C_{m,l}^1 = \sum_{n=1}^{\infty} T_{m,l}(n(a+b), -a, a) \tag{4.40}
\]

\[
A_{m,l}^2 = T_{m,l}(\frac{b+a}{2}, -a, \frac{b-a}{2}) \tag{4.41}
\]

\[
B_{m,l}^2 = \sum_{n=1}^{\infty} T_{m,l}(n - \frac{1}{2}(a+b), a, -\frac{b-a}{2}) \tag{4.42}
\]

\[
C_{m,l}^2 = \sum_{n=1}^{\infty} T_{m,l}(n + \frac{1}{2}(a+b), a, \frac{b-a}{2}) \tag{4.43}
\]

\[
A_{m,l}^3 = T_{m,l}(\frac{b+a}{2}, \frac{b-a}{2}, -a) \tag{4.44}
\]

\[
B_{m,l}^3 = \sum_{n=1}^{\infty} T_{m,l}(n + \frac{1}{2}(a+b), \frac{b-a}{2}, -a) \tag{4.45}
\]
Eqs. (4.36) and (4.37) can then be expressed more conveniently by using block matrices

\[
C_m^3 = \sum_{n=1}^{\infty} T_m(n \cdot (n - \frac{1}{2})(a+b), - \frac{b-a}{2}, a)
\]  \hspace{1cm} (4.46)

\[
A_m^4 = S_m \left( \frac{b-a}{2} \right)
\]  \hspace{1cm} (4.47)

\[
B_m^4 = \sum_{n=1}^{\infty} T_m(n(a+b), \frac{b-a}{2}, - \frac{b-a}{2})
\]  \hspace{1cm} (4.48)

\[
C_m^4 = \sum_{n=1}^{\infty} T_m(n(a+b), - \frac{b-a}{2}, - \frac{b-a}{2})
\]  \hspace{1cm} (4.49)

where

\[
0 = \text{the zero matrix}
\]

\[
I = \text{the unit matrix}
\]

\[
A^1 = \left\{ \frac{2l+1}{2} A_m^1 \right\}, \text{etc.}
\]

If \( \lambda_1 \) (i.e. \( c_1 \)) is known, then \( \lambda_2 \) can be obtained from

\[
\begin{bmatrix}
1 - \lambda_1(A^1 + B^1 + C^1) & 0 & u \\
-\lambda_1(A^3 + B^3 + C^3) & I & v
\end{bmatrix} = \lambda_2
\begin{bmatrix}
0 & A^2 + B^2 + C^2 & u \\
0 & A^4 + B^4 + C^4 & v
\end{bmatrix}
\]  \hspace{1cm} (4.51)

which is a generalized eigenvalue problem. Similarly, if \( \lambda_2 \) is known then \( \lambda_1 \) can be evaluated from

\[
\begin{bmatrix}
1 & -\lambda_2(A^2 + B^2 + C^2) & u \\
0 & 1 - \lambda_2(A^4 + B^4 + C^4) & v
\end{bmatrix} = \lambda_1
\begin{bmatrix}
A^1 + B^1 + C^1 & 0 & u \\
A^3 + B^3 + C^3 & 0 & v
\end{bmatrix}
\]  \hspace{1cm} (4.52)
The sizes of the matrices $A^1$, $B^1$, ..., $C^4$ depend on where the expansion series in Eqs. (4.33) and (4.34) are truncated. If we assume that this is done after $L$ terms, then the effective number of Legendre polynomials is

$$ j = \begin{cases} \frac{L}{2} + 1 & \text{for a slab with even modes} \\ \frac{L+1}{2} & \text{for a slab with odd modes} \end{cases} \quad (4.53) $$

4.4 Accuracy and Test

The accuracy of the matrix elements has been analyzed by performing a maximum error calculation in parallel to the calculation of the matrix elements, see also Dahl (1985).

For $S_{m,l}$ the accuracy was relatively good for elements up to a certain number. The accuracy of the matrix elements $T_{m,l}$ is almost the same as $S_{m,l}$ because of similar recursion formulae. When the integral of $T_{m,l}$ has an end-point singularity, which occurs for the elements $B_{m,l}$, the recursion formula has been used. For other cases, a quite fast method using series expansion has been developed, see paper I.

By assuming that both the regions have the same properties, we determined the value of $c$ for different thicknesses. The results were compared with those given by Dahl and Sjöstrand (1979). The agreement, which is very good, is not surprising because the methods are similar.

To test the method on two different media with vacuum boundary conditions we have compared the results for the fundamental mode for spheres and slabs with those given by Sjöstrand (1986a) and Sjöstrand (1986b), respectively. The same accuracy for the first eigenvalue was obtained with only eight effective terms in the expansion of Legendre polynomials. Rather good agreement for inner radius up to 10 mfp was also obtained when the results were compared with those by Aronson (1984).

From the results given by Kschwendt (1970) and by Premuda and Trombetti (1976) we conclude that our method converges as the number of polynomials increases. As regards these works, Dahl (1985) used a calculation scheme for
determining the accuracy of the obtained eigenvalues. We also use this scheme which has the following principle:

For every dimension we first calculate all the matrix elements for a certain number of Legendre polynomials and at the same time note the maximum error in each matrix. Using the routine for eigenvalue calculations, we calculate the lowest eigenvalue for this particular number of Legendre polynomials. The routine solves a generalized matrix eigenvalue problem with double precision based on the method developed by Moler and Stewart (1973). Now, for various lower numbers of polynomials, we calculate the lowest eigenvalue and compare it with the one we obtained first. When the difference between these eigenvalues (=truncation error) becomes greater than the maximum error in our matrices we choose the number of polynomials at which this occurs.

The sensitivity of the eigenvalues of the generalized matrix eigenvalue problem $Ax = \lambda Bx$ to perturbations of $A$ and $B$ has also been investigated. Using results of the first order perturbation theory according to Stewart (1978), the condition number which measures how a perturbation of a certain size in the matrices $A$ and $B$ affects $\lambda$ has been calculated in parallel with the calculation of the eigenvalues. Obtaining a condition number around unity we conclude that our eigenvalues are well-conditioned.

All the computations in this work were made on a VAX/VMS V4.5 computer in double precision.

4.5 Calculation of the Spectrum of $c$

Although the fundamental $c$-value for homogeneous spheres and slabs is known with great accuracy, the higher $c$-eigenvalues are known only up to a limited order. The most extensive data are given by Dahl and Sjöstrand (1979) and Dahl (1985), where the higher $c$-eigenvalues up to at least the sixth order have been calculated. In order to calculate higher $c$-eigenvalues the accumulated errors from the recursion formula have to be minimized. This has been achieved by calculating the matrix elements with quadruple precision. In paper I the following results have been obtained:
i) For homogeneous slabs with thicknesses \( d = 0.2, 2 \) and 20 the 23 first \( c \) -eigenvalues have been calculated.

ii) For homogeneous spheres with diameters \( d = 0.2, 2 \) and 20 the first 23 \( c \) -eigenvalues have been calculated.

From these results it could be seen that for higher \( c \)-eigenvalues the difference between two adjacent eigenvalues tends to converge towards a certain value.

For two-medium slabs and spheres only the fundamental eigenvalues were known earlier. In paper I the following results were obtained:

i) For reflected slabs with \( c_2 = 0.5 \) or 0.9, \( a = 1, 2 \) and 3, \( d = 1, 2, 3, 4 \) and 5 the first 8 \( c_1 \)-eigenvalues were calculated. Also the corresponding \( c_2 \)-eigenvalues when \( c_1 = 0 \) and 1.

ii) For reflected spheres with \( c_2 = 0.5 \) or 0.9, \( a = 1, 2 \) and 3, \( d = 1, 2, 3, 4 \) and 5 the first 8 \( c_1 \)-eigenvalues were calculated. Also the corresponding \( c_2 \)-eigenvalues when \( c_1 = 0 \) and 1.

As for the homogeneous case, similar regularities in the spectrum of \( c \) could be observed.

For an infinite, periodic slab lattice neither the fundamental nor the higher \( c \)-eigenvalues were known earlier. In paper II, the following results were obtained:

i) With \( c_2 = 0.2, 0.5 \) and 0.9 and for 5 different combinations of thicknesses the first 7 \( c_1 \)-eigenvalues were calculated.

ii) With \( c_1 = 1.0 \) and for 5 different combinations of thicknesses the first 8 \( c_2 \)-eigenvalue were calculated.

As for the homogeneous case, similar regularities in the spectrum of \( c \) could be observed.
4.6 Calculation of the Flux

The total neutron scalar fluxes, $\phi_1(x)$ in the core and $\phi_2(x)$ in the reflector, can be calculated if the corresponding eigenvectors for the eigenvalues $c_1$ and $c_2$ are known. Thus, the fundamental modes are given by the eigenvalues belonging to the eigenvalues $c_{10}$ and $c_{20}$, the next modes by eigenvectors belonging to $c_{11}$ and $c_{21}$, and so on.

The normalized total scalar flux $\phi(x)$ can be expressed as

$$\phi(x) = \frac{1}{K} \sum_{l} \frac{?1}{2} w_l P_l(x)$$

where $K$ is the normalization constant. For a slab with odd modes the odd terms in the expansion of $\phi(x)$ will be used and analogously for a sphere and for a slab with even modes. Further, the flux for a slab with odd modes will be normalized at a point where the flux is maximum while the flux for other cases will be normalized at the origin. For the infinite, two-medium slab lattice only two cases are considered: Either the flux in both core and reflector is symmetric or antisymmetric. This limitation is a consequence of the continuity and periodicity conditions.

For two-medium slabs and spheres the spatial flux distribution for the first 5 modes has been plotted in paper I while for the two-medium slab lattice the neutron scalar flux for the first 4 modes has been plotted, see paper II.

4.7 Comparison with Buckling Approximation

The numerical results for the homogeneous systems in Sec. 4.5 revealed that for higher eigenvalues the difference between two adjacent eigenvalues tended to converge towards a certain value. These regularities were then discussed in detail in paper IV and simple formulae for the high-order eigenvalues were derived. The derivation was based on the buckling approximation. Some assumptions had to be made on the limiting values of the extrapolation distance. The formulae were tested against numerical results and the agreement was good.

When the numerical results for reflected slabs and spheres indicated similar regularities, Sjöstrand (1989) extended the study to also include these systems and
cylinders. Here, a larger discrepancy could be noted. This was expected because an additional assumption of interface conditions from the diffusion theory had to be used.

All the approximate formulae for the cases mentioned above can be written as

\[ c_n \rightarrow 4 \cdot \frac{\pi^2}{\lambda^2} + \frac{2n - q}{a l} \]  

(4.54)

where \( n = 1, 2, 3, \ldots \) and the value of \( q \) for different systems is tabulated in Table 1.

<table>
<thead>
<tr>
<th></th>
<th>Homogeneous systems</th>
<th>Two-medium systems with multiplying core</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>3/4</td>
<td>1</td>
</tr>
<tr>
<td>Cylinder</td>
<td>5/4</td>
<td>3/2</td>
</tr>
<tr>
<td>Slab with even modes</td>
<td>3/4</td>
<td>2</td>
</tr>
<tr>
<td>Slab with odd modes</td>
<td>7/4</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 1. The value of the quantity \( q \) (see Eq. (4.54)) for different systems.

For two-medium systems with multiplying reflector the quantity \( q \) is equal to 7/4 for all cases and \( a \) in the denominator is replaced by the thickness of the reflector \( d \). This means that the formulae are identical for all the three systems with multiplying reflector.

From the numerical results for the two-medium periodic problem, i.e. an infinite, two-medium slab lattice, regularities in the spectrum of \( c \)-eigenvalues could also be pointed out, see paper II. Following the same procedure approximate formulae for the high-order eigenvalues were derived. Comparing with the relations for the corresponding two-medium problem with vacuum boundary conditions it could be noted that the relations were identical.
5. **Time-Dependent Reflected Systems**

The analogy between the critical and time-decay eigenvalues was discussed in Chapter 2. There, it was stated that if the total cross section $\Sigma_t$ was allowed to take all complex values then all the $\lambda$- or $\Lambda$-eigenvalues for a given system can be determined from the $c$-eigenvalues for the corresponding critical system.

For homogeneous systems with vacuum boundary conditions and linearly anisotropic scattering real time-eigenvalues have been studied by Dahl and Sjöstrand (1989). For a sphere with isotropic scattering complex time-eigenvalues have been calculated by Dahl and Sahni (1990) in the region $\Lambda > 1$. For reflected spheres or infinite slabs on the other hand it seems difficult to transfer results from criticality calculations to time eigenvalues, even for the fundamental mode. The reason is that the effective dimension changes as the decay constant changes.

However, by making some assumptions the problem becomes somewhat simpler. For the case when the mean-free-path is the same in both media and the decay constant $\lambda = v\Sigma_{a1}$, where $\Sigma_{a1}$ is the absorption cross section of the core, Sjöstrand (1986a,b) has calculated the fundamental decay constant as a function of the core and reflector thickness for infinite slabs and spheres.

In Chapter 2 we applied Eq. (2.1) to a whole neutron population decaying exponentially with the decay constant $\lambda$ and obtained the integral form of the time-dependent transport equation (2.7). In the present chapter we first apply this equation to two-medium systems with vacuum boundary conditions. The obtained two coupled integral equations are then numerically solved using the spatial Legendre expansion method (Carlvik's method).

### 5.1 Theory

We consider a two-medium spherical system (similarly for a plane system) with an inner medium $V_1$ and outer medium $V_2$. The scattering is assumed to be isotropic and no neutrons enter the system from the outside. We also assume the same macroscopic total cross section $\Sigma_t^* = \Sigma_s^* + \Sigma_a^*$, where $\Sigma_s^*$ and $\Sigma_a^*$ denote the absorption and scattering cross sections, respectively. The time-dependent integral transport equation for the total flux of the inner medium can according to Eq. (2.7)
be written as

\[ \Psi_1(r) = \frac{\Sigma^*_1}{4\pi} \int \frac{\Psi_1(r') \exp(-(\Sigma^*_1 - \lambda/\nu) \cdot |r - r'|)}{|r - r'|^2} \, dr' + \]

\[ \frac{\Sigma^*_2}{4\pi} \int \frac{\Psi_2(r') \exp(-(\Sigma^*_1 - \lambda/\nu) \cdot |r - r'|)}{|r - r'|^2} \, dr' ; \]  

(5.1)

where subscripts 1 and 2 are used for the inner and outer medium, respectively. The equation for the total flux of the outer medium is similar. Applying this to a sphere and an infinite slab we obtain

\[ \Psi_1(x) = \frac{\Sigma^*_1}{2} \int_{-a}^{a} \Psi_1(x') \cdot E_1((\Sigma^*_1 - \lambda/\nu) \cdot |x - x'|) \, dx' + \]

\[ \frac{\Sigma^*_2}{2} \int_{a}^{b} \Psi_2(x') \cdot \left[ E_1((\Sigma^*_1 - \lambda/\nu) \cdot (x - x')) + (-1)^q \cdot E_1((\Sigma^*_1 - \lambda/\nu) \cdot (x + x')) \right] \, dx' ; \]  

(5.2)

\[ \Psi_2(x) = \frac{\Sigma^*_1}{2} \int_{-a}^{a} \Psi_1(x') \cdot E_1((\Sigma^*_1 - \lambda/\nu) \cdot (x - x')) \, dx' + \]

\[ \frac{\Sigma^*_2}{2} \int_{a}^{b} \Psi_2(x') \cdot \left[ E_1((\Sigma^*_1 - \lambda/\nu) \cdot |x - x'|) + (-1)^q \cdot E_1((\Sigma^*_1 - \lambda/\nu) \cdot (x + x')) \right] \, dx' ; \]  

(5.3)

where

\[ q = \begin{cases} 
0 & \text{for even modes} \\
1 & \text{for odd modes} 
\end{cases} \]  

(5.4)

and

\[ \Psi(y) = \begin{cases} 
\Psi(y), & \text{for a slab} \\
y \cdot \Psi(y), & \text{for a sphere} 
\end{cases} \]  

(5.5)
Comparing these equations with those valid for the critical case, see Eq. (2.20) and (2.21), it is seen that the equations are identical if

\[ \Sigma_{s1} = c_1 \cdot \Sigma_i \]  \hspace{1cm} (5.6)

\[ \Sigma_{s2} = c_2 \cdot \Sigma_i \]  \hspace{1cm} (5.7)

\[ \Sigma_i = \Sigma_i^* - \lambda/\nu \]  \hspace{1cm} (5.8)

These relations could also be obtained directly from the analogy between the critical and time-decay eigenvalues, see Sec. 2.1.

5.2 Numerical method

The system of equations for the critical case has been considered in paper I, where the criticality factors \( c_{1n} \) and \( c_{2n} \) have been calculated for different dimensions of the bodies. From these calculations \( \Lambda_{1n} \) (or \( \Lambda_{2n} \)) can be obtained through Eq. (2.8) for the corresponding thickness of the time-dependent system, which in its turn is obtained using Eq. (5.6) or (5.7). As long as the criticality factor is real the transformation from the critical case to the time-dependent is straightforward.

A direct method to solve the decay constant \( \lambda \) in Eqs. (5.2) and (5.3) where \( \lambda \) appears as an implicit parameter in \( E_1 \), requires that the parameters \( a, d, \Sigma^*_1, \Sigma^*_2, \Sigma^*_1 \) and \( \Sigma^*_2 \) are given. Then the values of \( \lambda \) can be calculated by an iterative process described later. Now, we multiply Eqs. (5.2) and (5.3) with a constant \( \mu \) on the left side and make substitutions to change the integration limits to -1 and +1. Further, if we apply Carlvik's method, i.e. expand the scalar neutron flux in terms of Legendre polynomials of spatial coordinates, and express the system of equations by using block matrices according to the same procedure as before we obtain

\[
\begin{bmatrix}
\varepsilon_1 A & \varepsilon_2 (B + (-1)^q \cdot C) \\
\varepsilon_1 D & \varepsilon_2 (E + (-1)^q \cdot F)
\end{bmatrix}
\begin{bmatrix}
u \\
v
\end{bmatrix} = \mu \cdot
\begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}
\begin{bmatrix}
u \\
v
\end{bmatrix}
\]  \hspace{1cm} (5.9)
where

\[
\begin{align*}
\varepsilon_1 &= \frac{a \cdot \Sigma_1^*}{2} \\
\varepsilon_2 &= \frac{(b-a) \cdot \Sigma_2^*}{4}
\end{align*}
\] (5.10)

\[
A_{m,l} = S_{m,l}(a \Sigma_1)
\] (5.12)

\[
B_{m,l} = T_{m,l}(\Sigma_1 \cdot \left(\frac{b+a}{2}, -a, +\frac{b-a}{2}\right))
\] (5.13)

\[
C_{m,l} = T_{m,l}(\Sigma_1 \cdot \left(\frac{b+a}{2}, a, +\frac{b-a}{2}\right))
\] (5.14)

\[
D_{m,l} = T_{m,l}(\Sigma_1 \cdot \left(\frac{b+a}{2}, -a, -\frac{b-a}{2}\right))
\] (5.15)

\[
E_{m,l} = S_{m,l}(\Sigma_1 \cdot \frac{b-a}{2})
\] (5.16)

\[
F_{m,l} = T_{m,l}(\Sigma_1 \cdot (b+a \cdot \frac{b-a}{2}, b-a \cdot \frac{b-a}{2}))
\] (5.17)

\[0 = \text{the zero matrix} \] (5.18)

and

\[I = \text{the unit matrix} \] (5.19)

5.3. Accuracy and Test

The calculation of the matrix elements and the accuracy has already been considered in Sec. 4.5. To test the direct method described above we have considered the case where both regions have the same properties. This means that
the results can be compared with those given by Dahl et al. (1983) for homogeneous systems. From the value of the decay constant $\lambda$ for a certain dimension, the corresponding criticality factor $c$ and dimension for the stationary case have been calculated via

$$c = \frac{1}{1 - \lambda \nu \Sigma^*}$$  \hspace{1cm} (5.20)

and

$$a \Sigma_t = \frac{a \Sigma^*_t}{c}$$  \hspace{1cm} (5.21)

where $a$ is the radius or half-thickness of the homogeneous system. Using these values as input and setting $\Sigma_t$ equal to unity, which corresponds to the value of the decay constant, we obtained an eigenvalue $\mu$ equal to unity within the limits of uncertainty.

For determining the accuracy of the obtained time eigenvalues a calculation scheme with the following principle has been used: We assume that the six parameters of the system are given. For a certain number of Legendre polynomials we vary $\Sigma_t$ (i.e. $\lambda$) and solve Eq. (5.9) each time until $\mu_1 = 1.0$ which, according to the definition of $\Sigma_t$, gives the fundamental time-eigenvalue. At the same time we note the maximum error in the matrix. Then, for various lower numbers of polynomials we repeat the same procedure and compare the time-eigenvalue with the one we obtained first. When the difference between these time eigenvalues (= truncation error) becomes greater than the maximum error in our matrix we choose the number of polynomials at which this occurs. Similarly, for higher time eigenvalues.

The eigenvalue problem was solved by a routine from EISPACK and all the computations were made on a SUN Sparcserver 330 in double precision.

5.4 Results

Using Eqs. (5.6), (5.7) and (2.8) we have in paper III made a transformation of the results for the critical case to decay constants $\Lambda_{1n}$ (or $\Lambda_{2n}$) and to dimensions
\( d \Sigma_1^+ \) (or \( d \Sigma_2^+ \)) for the time-dependent system. The decay constants \( \Lambda_{in} \) are then plotted as functions of the radius or half-thickness of a sphere or slab with reflector thickness \( d \Sigma_s^+ = 0.9 \). Compared to those given by Dahl and Sjöstrand (1989) for homogeneous systems we could note that the eigenvalue curves were similar.

Furthermore, using the direct method where six parameters of the time-dependent system were given all the real \( \lambda \)-eigenvalues for a reflected slab and the first four \( \lambda \)-eigenvalues for a reflected sphere were calculated. The results are given in paper III.
6. Conclusions

In this work the one-speed neutron transport equation with isotropic scattering has been solved in two-medium slabs and spheres, and results with high accuracy have been given. Both stationary and time-dependent cases have been considered.

For homogeneous slabs and spheres more accurate and higher eigenvalues than those known so far have been calculated. From the results it could be noted that the difference between two adjacent eigenvalues tended to converge towards a certain value. Thus, regularities in the spectrum of the criticality eigenvalues could be pointed out which in turn stimulated us to derive approximate formulae for very high-order eigenvalues, see paper IV. The derivation was based on the buckling approximation and the obtained simple formulae were tested against new numerical results. The agreement was good. For completeness, also the linearly anisotropic scattering case and cylinders were considered and the agreement between the approximate formulae and numerical results was good.

When the numerical results for two-medium systems were calculated, see paper I, similar regularities as for homogeneous systems could be indicated. Regarding this, Sjöstrand (1989) derived approximate formulae for the high-order eigenvalues of two-medium infinite slabs, spheres and cylinders. The derivation was based on the buckling approximation and interface conditions from diffusion theory. The discrepancies were somewhat larger than those for homogeneous systems.

The eigenvalue spectrum for an infinite, two-medium slab lattice seems to be very similar to that for a two-medium slab system with vacuum boundary conditions, see paper II. The approximate formulae were identical and the results could be rather well described by the buckling approximation.

As is well known there exists a close analogy between the criticality eigenvalues and time-eigenvalues, see Davison (1957), Case and Zweifel (1968) and Carlvik (1968). Applying this to the reflected slabs and spheres a rather good picture of the fundamental and higher time-eigenvalues has been obtained, see paper III. Deriving approximate formulae for high-order time-eigenvalues at the so called Corngold limit, i.e. \( \Lambda = 1 \), in homogeneous systems the agreement became remarkably good.
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Appendix A  Buckling approximation

The calculation of the fundamental eigenvalue and the derivation of approximate formulae for high-order eigenvalues by the buckling approximation are straightforward. However, the procedure applied to the periodic two-medium slab lattice will be included here for completeness.

Let us consider the even flux modes in a system with multiplying core \( c_1 > 1 \) and non-multiplying reflector \( c_2 < 1 \). The core half-thickness is \( a \) and reflector thickness \( d = b - a \). The neutron flux in the two media is then given by

\[
\phi_1(x) = A_1 \cdot \cos(Bx) \quad ; \quad 0 \leq x \leq a
\]

\[
\phi_2(x) = A_2 \cdot \cosh\left(\frac{x-(a+d/2)}{L}\right) \quad ; \quad a \leq x \leq b
\]

where

\[ B^2 \quad \text{the buckling of the core} \]
\[ L \quad \text{the diffusion length of the reflector} \]

For odd modes we will have \( \sin \) and \( \sinh \) functions instead. Now, using the boundary conditions of equal flux and current at the interface we obtain

\[
A_1 \cdot \cos(Ba) = A_2 \cdot \cosh\left(-\frac{d}{2L}\right) \quad (A.3)
\]

\[
-D_1 A_1 B \cdot \sin(Ba) = \frac{D_2 A_2}{L} \cdot \sinh\left(-\frac{d}{2L}\right) \quad (A.4)
\]

where \( D_1 \) and \( D_2 \) are the diffusion constants of the media. Since the numerical comparison will be made on media having the same mean free path, we assume already here that \( D_1 = D_2 \). By division we obtain

\[
B \cdot \tan(Ba) = \frac{1}{L} \cdot \tanh\left(\frac{d}{2L}\right) \quad (A.5)
\]
1. Calculation of the fundamental eigenvalue

If now $c_2$ is known, the calculation procedure to calculate $c_1$ will be

\[ c_2 \text{ known } \Rightarrow L \Rightarrow B \Rightarrow c_1 \]

At 1, we use the relation between the criticality factor and the buckling $B^2$, i.e.

\[ \tan \left( \frac{B\ell}{c} \right) = B\ell \]  \hspace{1cm} (A.6)

where $\ell$ is the mean-free-path. Now, because $c_2 < 1$, $B$ in Eq. (A.6) will be replaced by $i/L$. This gives the value of $L$ from Eq. (A.6) via iteration. Inserting the value of $L$ into Eq. (A.5) we calculate the value of $B$ via iteration. Using Eq. (A.6) again we obtain the multiplicity factor of the core, $c_1$.

2. Approximate formulae for high-order eigenvalues

For homogeneous systems we have in paper IV given simple formulae for the high-order eigenvalues. The derivation was based on the buckling approximation. Sjöstrand (1989) extended this to two-medium systems with vacuum boundary conditions. Here, the same procedure will be followed.

First, we note that Eq. (A.5) has a set of different solutions $B_n$. The right hand side is a limited quantity which we denote by $f$. Since $B_n$ increases with increasing $n$, the expression $\tan(Ba)$ must go to zero. For large $n$ we therefore have

\[ B_n a \cdot \tan \delta = af = (n-1)\pi + \delta + \frac{\delta^3}{3} + ... \]  \hspace{1cm} (A.7)

where $\delta$ is small. Insertion into Eq. (A.5) gives

\[ B_n a \cdot \tan \delta = af = (n-1)\pi + \delta + \frac{\delta^3}{3} + ... \]  \hspace{1cm} (A.8)
In the first approximation we have

\[ \delta \equiv \frac{af}{(n-1)\pi} \quad (A.9) \]

Eq. (A.6) can be re-written as

\[ c_n = \frac{B_n l}{\tan^{-1}(B_n t)} \quad (A.10) \]

By insertion of the approximate value of \( B_n a \) and the approximation of \( \tan^{-1}(B_n t) \)

\[ \tan^{-1}(B_n t) \approx \frac{\pi}{2} - \frac{1}{B_n t} \quad (A.11) \]

into Eq. (A.10) we finally obtain

\[ c_n \rightarrow \frac{2(n-1)}{a/l} + \frac{4}{\pi^2} \quad (A.12) \]

i.e. \( c_n \) is independent of the size and diffusion properties of the reflector. If the same procedure is applied to the case of odd flux modes, the results can be combined and written as

\[ c_n \rightarrow \frac{n-1}{a/l} + \frac{4}{\pi^2} \quad ; \quad n = 1, 2, 3, ... \quad (A.13) \]

Comparing with the relation for the corresponding two-medium problem with vacuum boundary conditions we note that the relations are identical.