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A New Method for the Solution of the Transport Equation in Slab Geometry*

P. ERDÖS AND S. B. HALEY

Department of Physics, The Florida State University, Tallahassee, Florida, 32306

J. T. MARTI

Department of Mathematics, University of Illinois, Urbana, Illinois, 61801

AND

J. MENNIG

Eidgenössisches Institut für Reaktorforschung, Switzerland

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A new method, called the method of analytic angles, is developed for the solution of the transport equation (Boltzmann integro-differential equation) in slab geometry.

The essence of the method is the discretization of the spatial variable accompanied by an analytic solution for the resulting difference equation with respect to the angular variable.

This contrasts to other procedures, such as to the spherical harmonic, Wick–Chandrasekhar and Carlson's S_N-method, which are restricted to a finite number of values of the angular variable.

Two examples have been worked out. One is the phonon transport in solids with randomly distributed scattering centers. Here the numerical solution agrees very well with the asymptotic analytical solutions.

The other example, a neutron transport problem, allows comparison with the S_N-method, and indicates the excellence of the solution.

I. INTRODUCTION

Let us consider a very large number of particles (e.g., neutrons, phonons, photons, etc.) in a homogeneous medium characterized by the following properties: it can scatter, absorb, and create particles. If, in addition the boundaries of the

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medium are planes parallel to the (y, z) coordinate plane, then the density distribution of particles will only depend on the x coordinate due to the translational symmetry in the (y, z) plane.

The momentum or velocity distribution of the particles will also be independent of the (azimuthal) angle between the projection of the momentum or velocity upon the (y, z)-plane and y-axis.

Consequently, the distribution function of the particles, i.e., the density of particles at the point $\mathbf{x}$ with momentum $\mathbf{p}$ may be written as $\psi(x, p, \mu)$. Here

$$\mu = \cos(\mathbf{p}, \hat{\mathbf{x}}).$$

As is well-known, in thermodynamic equilibrium the distribution function is a Bose- or Fermi-function, depending on the spin of the particles [1]. It is independent of the coordinate $\mathbf{x}$, but depends on the energy ϵ, hence, on the momentum through the dispersion relation $\epsilon = \epsilon(\mathbf{p})$. It depends, furthermore, on the temperature T, chemical potential ϵ_F, the drift velocity $\mathbf{v}_D$, and the total angular momentum $\mathbf{J}$ of the system of particles.

We are interested in nonequilibrium steady state situations, created by the imposition of certain boundary conditions on $\psi(x, p, \mu)$. For instance, a certain influx of particles through a boundary may be given, or the temperature at the boundaries may be specified.

The distribution function in these cases may be obtained as the solution of the Boltzmann transport equation.

Even with many simplifications the transport equation can rarely be solved analytically; consequently, one must rely upon approximate methods leading to a numerical solution.

Several methods have been developed and tested, all using finite difference schemes. Such methods are, e.g., the spherical harmonic approximations (Wick–Chandrasekhar-method [2]) and the S_N-method (Carlson [3]).

In this paper we present a new method of solving the non-equilibrium steady state transport problem in the slab geometry with isotropic elastic *energy dependent* scattering of particles on randomly positioned scatterers.

We include the case, when the number of particles is not conserved in the collisions,[1] such as one has in the neutron multiplication in fission, and we also include a source or sink term in the transport equation, such as one has in the case of spontaneous fission, or absorption of neutrons.

The transport equation is transformed into a finite difference equation by discretizing the spatial variable x. The dependence on the angular variable μ is treated analytically.

[1] In this case the energy of the particles is not conserved in the collisions either; hence, strictly speaking, the collision is not elastic. We assume, that each emerging particle has the same energy as the incident particle.

Attention is called to the fact that the solution presented here does not linearize the transport equation with respect to the temperature gradient. Hence, arbitrarily large derivations from the equilibrium are encompassed by this treatment.

Our method is compared in a specific example with the S_N-method to demonstrate the advantages of the former. The S_N-method cannot be easily extended to the case of directional sources, such as the ones encountered in Section VI. There, the phonon sources $S^{\pm}(\pm a, \mu)$ describe the emission of phonons with different intensities in different directions.

Note that due to the discretization of the angular variable, the S_N-method yields only a linear approximation to the distribution function (angular flux) between discretization points of the angle. In contrast to this, the method of analytic angles does not use angular discretization, and gives therefore the analytic dependence of the distribution function on the angle. The reader will also note, that the spherical harmonic approximation is not well suited to the boundary conditions used in the phonon transport problem treated in a later section. These boundary conditions are easily handled in the method presented here. Furthermore, the method of analytic angles can be extended to include spherical and cylindrical geometries.[2]

II. Formulation of the Problem

The steady state (time independent) transport equation in plane slab geometry with isotropic, elastic scattering in the laboratory system may be reduced to

$$\mu \frac{\partial \psi(x, \mu)}{\partial x} + \Sigma(x)\, \psi(x, \mu) = \tfrac{1}{2}\lambda c(x)\, \Sigma(x) \int_{-1}^{1} \psi(x, \mu')\, d\mu' + S(x, \mu). \tag{II.1}$$

Since in this paper we are concerned with the mathematical problem of the solution of the transport equation, we do not elaborate on the physical significance of the different terms. It suffices to remark, that $\Sigma(x)$ is the total scattering cross section, $c(x)$ is the multiplication factor (proportional to the net number of particles produced in one scattering event). The real number λ is introduced for mathematical convenience. In the homogeneous problem, defined by $S(x, \mu) \equiv 0$, λ represents the eigenvalue. As is well-known, the inhomogeneous problem has only solutions if λ is *not* an eigenvalue. $S(x, \mu)$ represents the production or absorption of particles by sources or sinks in the bulk of the medium or at the boundary planes.

Because the scattering is elastic, p does not occur in Eq. (II.1) as a variable, with respect to which $\psi(x, p, \mu)$ is differentiated or integrated. Thus p may be treated as a parameter, and will not be denoted explicitly in the sequel.

In general, the functions $\Sigma(x)$, $c(x)$, $S(x, \mu)$, all depend parametrically on p. Consequently, $\psi(x, \mu)$ will also depend on p.

[2] Work in this direction is being carried out at the Institute for Reactor Technology, Swiss Federal Institute of Technology by Hälg, Halin and Mennig (private communication).

We have to keep in mind, that there is an equation of the type (II.1) for every group of particles, whose momentum has a modulus in the range $(p, p + dp)$.

Discretization of Eq. (II.1) is achieved by assuming that the value of $\psi(x_{i-1/2})$ at a space point $x_{i-1/2}$ can be replaced by its average value $\frac{1}{2}(\psi_i + \psi_{i-1})$ in the interval (x_i, x_{i-1}).[3] Thus Eq. (II.1) becomes

$$\mu(\psi_i - \psi_{i-1}) + \alpha_i(\psi_i + \psi_{i-1}) = \lambda\beta_i(\Phi_i + \Phi_{i-1}) + X_i(\mu), \quad \text{for } i = 1,..., n, \quad \text{(II.2)}$$

where we define

$$\begin{aligned} \alpha_i &= \tfrac{1}{2}\Sigma(x_{i-1/2})(x_i - x_{i-1}), \\ \beta_i &= \tfrac{1}{2}\alpha_i c(x_{i-1/2}), \\ \Phi_i &= \int_{-1}^{1} \psi_i(\mu')\, d\mu' \end{aligned} \quad \text{(II.3)}$$

and

$$X_i(\mu) = S(x_{i-1/2}, \mu)(x_i - x_{i-1}), \qquad \text{for } i = 1,..., n.$$

The quantities Φ_i will be called the *fluxes*.

Defining ψ_i^+ and ψ_i^- by

$$\begin{aligned} \psi_i^+(\mu) &\equiv \psi_i(\mu), \qquad \text{for } \mu > 0, \\ \psi_i^-(\mu) &\equiv \psi_i(-\mu), \qquad \text{for } \mu > 0, \end{aligned} \quad \text{(II.4)}$$

and X_i^+ and X_i^- by

$$\begin{aligned} X_i^+(\mu) &= X_i(\mu), \qquad \text{for } \mu > 0 \\ X_i^-(\mu) &= X_i(-\mu), \qquad \text{for } \mu > 0 \end{aligned} \quad \text{(II.5)}$$

and solving Eq. (II.2) for ψ_i^+ and ψ_{i-1}^- results in the following set of two coupled integro-difference equations for $\mu > 0$:

$$\psi_i^+(\mu) = \eta_i(\mu)\, \psi_{i-1}^+(\mu) + (\mu + \alpha_i)^{-1}[\lambda\beta_i(\Phi_i + \Phi_{i-1}) + X_i^+(\mu)], \quad \text{for } i = 1,..., n, \quad \text{(II.6)}$$

$$\psi_{i-1}^-(\mu) = \eta_i(\mu)\, \psi_i^-(\mu) + (\mu + \alpha_i)^{-1}[\lambda\beta_i(\Phi_i + \Phi_{i-1}) + X_i^-(\mu)], \quad \text{for } i = 1,..., n, \quad \text{(II.7)}$$

where

$$\eta_i(\mu) = (\mu - \alpha_i)/(\mu + \alpha_i)\,. \quad \text{(II.8)}$$

The boundary conditions, including the cases mentioned in the introduction, can be expressed in the form,

$$\psi_0^+(\mu) = \gamma_{11}\psi_0^-(\mu) + \gamma_{12}\,, \qquad \text{for } \mu > 0, \quad \text{(II.9)}$$

[3] Once the solution has been obtained, one has to verify, that this assumption is justified. This will be the case, if the intervals are chosen so small, that, $|\psi_i - \psi_{i-1}| \ll \frac{1}{2}|\psi_i + \psi_{i-}|$ or $\psi(x)$ is a linear function of x.

and

$$\psi_n^-(\mu) = \gamma_{21}\psi_n^+(\mu) + \gamma_{22}, \qquad \text{for} \quad \mu > 0. \tag{II.10}$$

The quantities γ_{ik} will be regarded as constants. It is possible to generalize to the case, where the γ_{ik} are functions of μ; however, the analytic integrations of Section IV have to be replaced by numerical integrations.

III. Evaluation of $\psi_i^{\pm}(\mu)$

Equations (II.6), (II.7), (II.9), and (II.10) constitute a set of $2n + 2$ linear integro-difference equations in the $2n + 2$ unknown functions $\psi_0^{\pm}(\mu),..., \psi_n^{\pm}(\mu)$. In order to determine $\psi_i^+(\mu)$, one substitutes successively $\psi_j^+(\mu)$ for $j = 1, 2,..., i-1$ into Eq. (II.6) and eliminates $\psi_{j-1}^+(\mu)$ at each step by use of the previous substitution. The result is

$$\psi_i^+(\mu) = \xi_{1,i}\psi_0^+(\mu) + \sum_{l=1}^{i} \frac{\xi_{l+1,i}}{\mu + \alpha_l}[\lambda\beta_l(\Phi_{l-1} + \Phi_l) + X_l^+(\mu)], \qquad \text{for} \quad i = 1,..., n, \tag{III.1}$$

where we defined

$$\xi_{l,i} = \prod_{\nu=l}^{i} \eta_\nu(\mu), \qquad \text{for} \quad l \leqslant i, \qquad \text{with} \quad \xi_{i+1,i} = 1, \qquad \text{and} \quad i = 1,..., n. \tag{III.2}$$

Note that $\xi_{l,i}$ are functions of μ; for typographical simplicity this will not be explicitly shown in the sequel. Similarly, to find ψ_i^- one substitutes successively ψ_j^- for $j = n, n-1,..., i+1$ into Eq. (II.7). This yields

$$\psi_i^-(\mu) = \xi_{i+1,n}\psi_n^-(\mu) + \sum_{l=1}^{n-i} \frac{\xi_{i+1,n-l}}{\mu + \alpha_{n+1-l}}[\lambda\beta_{n+1-l}(\Phi_{n-l} + \Phi_{n+1-l}) + X_{n+1-l}^-(\mu)], \qquad \text{for} \quad i = 0,..., n-1. \tag{III.3}$$

Evaluating Eq. (III.1) for $i = n$ and Eq. (III.3) for $i = 0$ gives,

$$\psi_n^+(\mu) - \xi_{1,n}\psi_0^+(\mu) = h^+(\mu),$$

and (III.4)

$$\psi_0^-(\mu) - \xi_{1,n}\psi_n^-(\mu) = h^-(\mu),$$

where

$$h^+(\mu) = \sum_{l=1}^{n} \frac{\xi_{l+1,n}}{\mu + \alpha_l}[\lambda\beta_l(\Phi_{l-1} + \Phi_l) + X_l^+(\mu)],$$

and (III.5)

$$h^-(\mu) = \sum_{l=1}^{n} \frac{\xi_{1,n-l}}{\mu + \alpha_{n+1-l}}[\lambda\beta_{n+1-l}(\Phi_{n-l} + \Phi_{n+1-l}) + X_{n+1-l}^-(\mu)].$$

The boundary conditions (II.9) and (II.10) are used now to eliminate ψ_n^+ and ψ_0^- from (III.4). This enables one to express ψ_0^+ and ψ_n^- entirely in terms of the fluxes Φ_i and the functions $X^+(\mu)$ and $X^-(\mu)$:

$$\psi_0^+(\mu) = \frac{\gamma_{11}(h^- + \gamma_{21}\xi_{1,n}h^+ + \gamma_{22}\xi_{1,n}) + \gamma_{12}}{1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2}, \tag{III.6}$$

and

$$\psi_n^-(\mu) = \frac{\gamma_{21}(h^+ + \gamma_{11}\xi_{1,n}h^- + \gamma_{12}\xi_{1,n}) + \gamma_{22}}{1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2}. \tag{III.7}$$

When these expressions are substituted back into Eqs. (III.1) and (III.3) the results can be written in the form

$$\psi_i^+(\mu) = \lambda \sum_{l=0}^{n} [(1 - \delta_{n,l})\,\beta_{l+1}F_{i,l+1}^+(\mu) + (1 - \delta_{0,l})\,\beta_l F_{i,l}^+(\mu)]\,\Phi_l + Z_i^+(\mu) \tag{III.8}$$

and

$$\psi_i^-(\mu) = \lambda \sum_{l=0}^{n} [(1 - \delta_{n,l})\,\beta_{l+1}F_{i,l+1}^-(\mu) + (1 - \delta_{0,l})\,\beta_l F_{i,l}^-(\mu)]\,\Phi_l + Z_i^-(\mu),$$

where the new symbols are defined by

$$\begin{aligned} F_{i,l}^+(\mu) &= \frac{\gamma_{11}\xi_{1,i}(\xi_{1,l-1} + \gamma_{21}\xi_{1,n}\xi_{l+1,n})}{(1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2)(\mu + \alpha_l)} + \frac{\theta_{i,l}\xi_{l+1,i}}{\mu + \alpha_l}, \\ F_{i,l}^-(\mu) &= \frac{\gamma_{21}\xi_{i+1,n}(\xi_{l+1,n} + \gamma_{11}\xi_{1,n}\xi_{1,l-1})}{(1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2)(\mu + \alpha_l)} + \frac{\theta_{l-1,i}\xi_{i+1,l-1}}{\mu + \alpha_l}, \end{aligned} \tag{III.9}$$

$$\begin{aligned} Z_i^+(\mu) = \sum_{l=1}^{n} (\mu + \alpha_l)^{-1} \Big\{ & X_l^+(\mu) \left[\theta_{i,l}\xi_{l+1,i} + \frac{\gamma_{11}\gamma_{21}\xi_{1,i}\xi_{1,n}\xi_{l+1,n}}{1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2}\right] \\ & + X_l^-(\mu)\,\frac{\gamma_{11}\xi_{1,i}\xi_{1,l-1}}{1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2}\Big\} + G_i^+(\mu) \end{aligned} \tag{III.10}$$

$$\begin{aligned} Z_i^-(\mu) = \sum_{l=1}^{n} (\mu + \alpha_l)^{-1} \Big\{ & X_l^-(\mu) \left[\theta_{l-1,i}\xi_{i+1,l-1} + \frac{\gamma_{21}\gamma_{11}\xi_{i+1,n}\xi_{1,n}\xi_{1,l-1}}{1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2}\right] \\ & + X_l^+(\mu)\,\frac{\gamma_{21}\xi_{i+1,n}\xi_{l+1,n}}{1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2}\Big\} + G_i^-(\mu) \end{aligned}$$

$$\theta_{i,l} = \begin{cases} 1, & \text{for } l \leqslant i \\ 0, & \text{for } l > i \end{cases} \tag{III.11}$$

and

$$G_i^+(\mu) = \frac{\xi_{1,i}(\gamma_{11}\gamma_{22}\xi_{1,n} + \gamma_{12})}{1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2},$$
$$G_i^-(\mu) = \frac{\xi_{i+1,n}(\gamma_{12}\gamma_{21}\xi_{1,n} + \gamma_{22})}{1 - \gamma_{11}\gamma_{21}\xi_{1,n}^2}. \tag{III.12}$$

The symbol $\delta_{i,j}$ is the Kronecker delta.

Equations (III.8) are analytical expressions for $\psi_i^{\pm}$ written entirely in terms of μ and the unknown fluxes Φ_l. As will be seen presently, simple linear equations can be formulated for the fluxes Φ_l. Thereby, the problem of the calculation of $\psi_i^{\pm}$ is reduced to the solution of a set of linear equations for Φ_i followed by a substitution of the Φ_i into the equation (III.8) which expresses $\psi_i^{\pm}$ in terms of the fluxes Φ_i. In order to determine Φ_i at each point x_i, we write

$$\Phi_i = \int_{-1}^{1} \psi_i(\mu)\, d\mu = \int_0^1 [\psi_i^+(\mu) + \psi_i^-(\mu)]\, d\mu, \qquad \text{for} \quad i = 0,..., n. \tag{III.13}$$

Substitution of $\psi_i^{\pm}$ from Eqs. (III.8) into (III.13) leads to a set of simultaneous linear algebraic equations for Φ_i which can be written in concise form as

$$\sum_{l=0}^{n} (\delta_{i,l} - \lambda M_{i,l})\, \Phi_l = Z_i, \qquad \text{for} \quad i = 0,..., n. \tag{III.14}$$

The matrix elements occurring in this equation are

$$M_{i,l} = \int_0^1 \{(1 - \delta_{n,l})\, \beta_{l+1}[F_{i,l+1}^+(\mu) + F_{i,l+1}^-(\mu)] + (1 - \delta_{0,l})\, \beta_l[F_{i,l}^+(\mu) + F_{i,l}^-(\mu)]\}\, d\mu, \qquad \text{for} \quad i, l = 0,..., n, \tag{III.15}$$

and the inhomogeneous terms are

$$Z_i = \int_0^1 [Z_i^+(\mu) + Z_i^-(\mu)]\, d\mu, \qquad \text{for} \quad i = 0,..., n. \tag{III.16}$$

The solutions of these equations are

$$\Phi_l = \sum_{i=0}^{n} G_{l,i} Z_i \qquad \text{for} \quad l = 0,..., n, \tag{III.17}$$

with

$$G_{l,i} = (I - \lambda M)_{l,i}^{-1}, \tag{III.18}$$

where I is the $(n + 1) \times (n + 1)$ unit matrix, and M is the matrix with elements $M_{i,l}$.

Equations (III.8), together with Eq. (III.17), represent the complete solution of the transport Eq. (II. 1) with the boundary conditions included. These equations give the intregrated flux Φ_l as well as the distribution function (angular flux)$\Psi_i^{\pm}(\mu)$.

In summary, then, the numerical solution of the transport equation in slab geometry is reduced to a set of quadratures, followed by the solution of a set of linear algebraic equations, and a number of substitutions. The next sections will deal with these operations in detail.

IV. Evaluation of the Matrix Elements $M_{i,l}$ and of the Inhomogeneous Terms Z_i

So far no approximations have been introduced except for choosing discrete values of the spatial coordinate x. The determination of $M_{i,l}$ and Z_i is now reduced to the evaluation of integrals involving only rational functions of μ, the cosine of the angular coordinate.

While it is always possible to perform the integrations numerically, we notice that they can be done analytically, thereby eliminating some of the computational inaccuracies.

Analytical integration becomes easy, if α_i are chosen to be independent of i, i.e.,

$$\alpha_i = \alpha = \text{const}, \qquad \text{for} \quad i = 1,..., n. \tag{IV.1}$$

This condition can be satisfied to any degree of accuracy by a suitable choice of the intervals $\Delta x_i = x_i - x_{i-1}$ (see Eq. II.3).

Letting

$$\eta = (\mu - \alpha)/(\mu + \alpha), \tag{IV.2}$$

one has from (III.2)

$$\xi_{l,i}(\mu) = \eta^{i+1-l}, \qquad \text{for} \quad l \leqslant i, \quad \text{and} \quad i = 1,..., n. \tag{IV.3}$$

Using (IV.3) and changing the integration variable to η, Eqs. (III.15) and (III1.16) written out in detail become,

$$\begin{aligned} M_{i,l} = \int_{-1}^{u} \{&[(1 - \delta_{n,l})\,\beta_{l+1}(\gamma_{11}\eta^{i+l} + \gamma_{11}\gamma_{21}\eta^{2n+i-l-1} + \gamma_{21}\eta^{2n-i-l-1} \\ &+ \gamma_{11}\gamma_{21}\eta^{2n-i+l}) + (1 - \delta_{0,l})(\gamma_{11}\eta^{i+l-1} + \gamma_{11}\gamma_{21}\eta^{2n+i-l} + \gamma_{11}\gamma_{21}\eta^{2n+l-i-1} \\ &+ \gamma_{21}\eta^{2n-i-l})]/[(1 - \gamma_{11}\gamma_{21}\eta^{2n})(1 - \eta)] \\ &+ [(1 - \delta_{n,l})\,\beta_{l+1}(\theta_{i-1,i}\eta^{i-1-l} + \theta_{l,i}\eta^{l-i}) \\ &+ (1 - \delta_{0,l})\,\beta_i(\theta_{i,l}\eta^{i-l} + \theta_{l-1,i}\eta^{l-1-i})]/(1 - \eta)\}\, d\eta, \qquad \text{for} \quad i, l = 0,...,n, \end{aligned} \tag{IV.4}$$

and with $X_l(\eta) \equiv X(\mu(\eta))$, as defined in Eq. (II.3),

$$Z_i = \sum_{l=1}^{n} \int_{-1}^{u} \left\{ \frac{X_l(\eta)}{1-\eta} \left[\frac{\gamma_{21}\eta^{2n-l-i}(\gamma_{11}\eta^{2i}+1)}{1-\gamma_{11}\gamma_{21}\eta^{2n}} + \theta_{i,i}\eta^{i-l} \right] + \frac{X_l(\eta)}{1-\eta} \left[\frac{\gamma_{11}\eta^{l+i-1}(\gamma_{21}\eta^{2n-2i}+1)}{1-\gamma_{11}\gamma_{21}\eta^{2n}} + \theta_{l-1,i}\eta^{l-1-i} \right] \right\} d\eta + 2\alpha \int_{-1}^{u} \frac{\gamma_{12}\eta^{i} + \gamma_{11}\gamma_{22}\eta^{n+i} + \gamma_{12}\gamma_{21}\eta^{2n-i} + \gamma_{22}\eta^{n-i}}{(1-\gamma_{11}\gamma_{21}\eta^{2n})(1-\eta)^2} d\eta, \quad \text{for } i = 0,\ldots,n. \tag{IV.5}$$

In these expressions, the upper limit of the integration is given by

$$u = (1-\alpha)/(1+\alpha). \tag{IV.6}$$

We shall treat the special case when X_l is independent of η. This case is the most important for reactor applications. Physically it means that the sources are non-directional, i.e., $S(x_{i-\frac{1}{2}}, \mu)$ does not depend on the angular variable μ. (See (II. 3), last Equation). It should be pointed out, that the independence of X_l of η is not essential for the following analytic integration. The method can be used equally well in the more general case, e.g. by using a series expansion of X_l in powers of μ. Section VI gives an example for directional sources.

The integrations in the above expressions are still difficult to carry out unless either $\gamma_{11} = \gamma_{21} = 1$ and $\gamma_{12} = \gamma_{22} = 0$, or $\gamma_{11}\gamma_{21} = 0$. Fortunately, these conditions comprise the most important applications of the theory to reactors, i.e.,

(a) $\gamma_{11} = \gamma_{12} = \gamma_{21} = \gamma_{22} = 0$: unsymmetric finite system,
(b) $\gamma_{11} = 1, \gamma_{12} = \gamma_{21} = \gamma_{22} = 0$: symmetric finite system,
(c) $\gamma_{12} = 1, \gamma_{11} = \gamma_{21} = \gamma_{22} = 0$: shielding problem with isotropic incident flux,
(d) $\gamma_{11} = \gamma_{21} = 1, \gamma_{12} = \gamma_{22} = 0$: cell problem.

The first three cases can be treated together by setting $\gamma_{11}\gamma_{21} = 0$ in Eqs. (IV.4) and (IV.5), while the fourth case has to be treated separately. Hence, the four cases fall into two categories, which will be discussed in the sequel.

A. *Matrix Elements and Inhomogeneous Terms in the Cases* a, b, *and* c

Substitution of $\gamma_{11}\gamma_{21} = 0$ into Eqs. (IV.4) and (IV.5) leads to

$$M_{i,l} = (1-\delta_{n,l})\,\beta_{l+1}(\gamma_{11}P_{1,i+l} + \gamma_{21}P_{1,2n-i-l-1} + \theta_{i-1,l}P_{1,i-1-l} + \theta_{l,i}P_{1,l-i}) + (1-\delta_{0,l})\,\beta_l(\gamma_{11}P_{1,i+l-1} + \gamma_{21}P_{1,2n-i-l} + \theta_{i,l}P_{1,i-l} + \theta_{l-1,i}P_{1,l-1-i}), \tag{IV.7}$$

and

$$Z_i = \sum_{l=1}^{n} X_l(\gamma_{11}P_{1,l+i-1} + \gamma_{21}P_{1,2n-i-l} + \theta_{i,l}P_{1,i-l} + \theta_{l-1,i}P_{1,l-1-i}) + 2\alpha(\gamma_{12}P_{2,i} + \gamma_{22}P_{2,n-i}),$$

where

$$P_{j,\nu} = \int_{-1}^{u} \eta^{\nu}(1-\eta)^{-j}\, d\eta, \qquad \text{for } j = 0, 1, 2. \tag{IV.8}$$

The integrals $P_{1,\nu}$ and $P_{2,\nu}$ may be calculated recursively from the standard integrals $P_{0,\nu}$, $P_{1,0}$, and $P_{2,0}$ by the use of the relations

$$P_{j,\nu} = P_{j,\nu-1} - P_{j-1,\nu-1}, \qquad \text{for } j = 1, 2, \text{ and } \nu = 1, 2, \ldots, n. \tag{IV.9}$$

B. *Matrix Elements and the Inhomogeneous Terms in the Case* d

Setting $\gamma_{11} = \gamma_{21} = 1$ and $\gamma_{12} = \gamma_{22} = 0$ in (IV.4) and (IV.5), one obtains

$$M_{i,l} = (1-\delta_{n,l})\,\beta_{l+1}(R_{i+1} + Q_{i-l} + \theta_{i-1,l}P_{1,i-l-1} + \theta_{l,i}P_{1,-i-l}) + (1-\delta_{0,l})\,\beta_l(R_{i+l-1} + Q_{i-l+1} + \theta_{i,l}P_{1,i-l} + \theta_{l-1,i}P_{1,-i+l-1}), \tag{IV.10}$$

and

$$Z_i = \sum_{l=1}^{n} X_l(R_{i+l-1} + Q_{i-l+1} + \theta_{i,l}P_{1,i-l} + \theta_{l-1,i}P_{1,l-1-i}).$$

Here, R_ν and Q_ν are defined by the following relations:

$$R_\nu = \int_{-1}^{u} (\eta^{\nu} + \eta^{2n-1-\nu})(1 - \eta - \eta^{2n} + \eta^{2n+1})^{-1}\, d\eta = \frac{1}{2n\alpha} + \frac{1}{n}\sum_{l=1}^{n} \frac{\cos\left[\frac{\pi}{2}\frac{(2\nu+1)l}{n}\right]}{\sin\frac{\pi l}{2n}} \arctan\left(\frac{1}{\alpha}\tan\frac{\pi l}{n}\right), \quad \text{for } \nu = 0, \ldots, n-1,$$

$$R_{2n-\nu-1} = R_\nu, \qquad \text{for } \nu = 0, \ldots, n-1, \tag{IV.11}$$

$$Q_\nu = \int_{-1}^{u} (\eta^{2n-1-\nu} + \eta^{2n-\nu})(1 - \eta - \eta^{2n} + \eta^{2n+1})^{-1}\, d\eta = P_{\nu-1} - P_{1,\nu-1}, \qquad \text{for } \nu = 1, \ldots, n, \tag{IV.12}$$

and

$$Q_{-\nu+1} = Q_\nu \qquad \text{for } \nu = 1, \ldots, n.$$

V. Neutron Transport. Comparison with the S_N-Method

As a first example we apply the theory outlined in the first four sections to the transport equation of neutrons in slab geometry.

Simultaneously, we solve the same problem by means of the well-known S_N-method [3]. This was done using the DTF-IV code [4]. This allows comparison of the two methods with respect to their accuracy and with regard to the time needed for computation.

For the sake of a meaningful comparison of the method of analytic angles with other methods, such as the spherical harmonic method, the Wick–Chandrasekhar method, or the S_N-method of Carlson, the following remarks are in order.

In the last-mentioned methods, the angular variable $\mu = \cos \alpha$ is discretized in addition to the coordinate x. In these methods the distribution function is not obtained as an analytic function of μ, as in our case, but for a discrete set of values μ_i $(i = 1,..., N)$. Hence, only for $N = \infty$ would these methods yield the same amount of information as ours—the number n of mesh points used for the variable x being equal. Since for $N = \infty$ these methods would require an infinite computation time, this comparison would clearly be unfair. We compare the S_N-method and the method of analytic angles using the same number n of spatial mesh points, varying the number N of angular mesh points in the former.

The methods which utilize angular discretization first invert an $N \times N$ band matrix, generated by the angular discretization, and then solve the spatially discretized equation in n points through an iterative procedure which expresses $\Psi(x_i, \mu_l)$ linearly in terms of $\Psi(x_0, \mu_j)$.

One should note that due to the nature of the N boundary conditions (see (II.9) and (II.10)) an $N \times N$ dense matrix equation has to be solved to find the distribution $\Psi(x_0, \mu_j)$ at the boundary for all μ_j. In contrast to this, the present method requires the solution of an one $n \times n$ dense matrix equation.

It follows from this that the method of analytic angles is more suitable than the S_N-method if the angular variation of the distribution function is very pronounced.

Let us turn now to the neutron transport problem. We consider a homogeneous critical slab; consequently, the inhomogeneous term in Eq. (II.1) is absent

$$S(x, \mu) = 0. \tag{V.1}$$

Furthermore, the scattering cross-section is taken to be isotropic in the laboratory system as well as independent of x, hence,

$$\Sigma(x) = \Sigma. \tag{V.2}$$

We formulate the transport equation for a monoenergetic group of neutrons; consequently the distribution function $\Psi(x, \mu)$ refers to this group of neutrons only.

The equation to be solved is now

$$\mu \frac{\partial \Psi(x, \mu)}{\partial x} + \Sigma \Psi(x, \mu) = \frac{1}{2} \lambda c \Sigma \int_{-1}^{1} \Psi(x, \mu')\, d\mu'. \tag{V.3}$$

Note that the solutions of this equation will depend on Σ and the slab thickness $2a$ only in the combination $2a\Sigma$.

The neutron multiplication factor λc is independent of x due to the homogeneity of the medium. Its value is yet unknown, and will be found as the eigenvalue of the equation for the fluxes.

The neutron flux $\Phi(x)$ will be calculated at the point $x = 0$ (center of the slab) as well as at the boundary $x = a$. The neutron flux is defined by the formula

$$\Phi(x) = \int_0^1 [\Psi^+(x, \mu) + \Psi^-(x, \mu)]\, d\mu. \tag{V.4}$$

Noting that c is included in the matrix elements $M_{i,l}$, Eq. (III.14) in the homogeneous case becomes

$$\sum_{l=0}^{n} (\delta_{i,l} - \lambda M_{i,l})\, \Phi_l = 0, \qquad \text{for} \quad i = 0,..., n. \tag{V.5}$$

The solution of these equations will yield the flux

$$\Phi(0) = \Phi_{n/2} \qquad \text{and} \qquad \Phi(a) = \Phi_0 = \Phi_n\,.$$

First, the eigenvalue λc of (V.5) was determined numerically using an iterative procedure. This quantity represents the mean number of secondary neutrons per collision, which will make the slab critical.

Table I gives $c\lambda$ (smallest eigenvalue) as obtained with different numbers n of mesh points (discretization intervals) used.

TABLE I

Eigenvalue λc and Ratio of Flux at the Boundary to that at the Center of the Slab for Eq. (V.3)[a]

	Method of Analytic Angles (this work)				Bennet[b]
n	2	10	50	150	
λc	1.654	1.6169	1.61544	1.615386	1.615379
$\Phi(a)/\Phi(0)$	0.5705	0.5521	0.5554	0.55553	

[a] For $2a\Sigma = 1.0$, the results are obtained for various mesh sizes n. For comparison, the result of Bennet is also given.

[b] See [5].

The computing time for the complete solution of the problem [i.e. to find the distribution function (angular fluxes) and the integrated fluxes] on a CDC-1604 computer was found to be given by

$$t \simeq 0.04\, n \text{ sec for } 2 \leqslant n \leqslant 20,$$

$$t \simeq 0.0013\, n^2 \text{ sec for } 50 \leqslant n \leqslant 150.$$

TABLE II

Comparison of the Results Obtained by the S_N-Method and the Method Described Here[a]

N	S_N-Method DTF-IV Code[b]					Present Method (S_∞)
	2	4	6	12	16	
$\Phi(a)/\Phi(0)$	0.8184	0.7492	0.7251	0.6900	0.6791	0.652

[a] The parameter $2a\Sigma = 0.5$.
[b] See [4].

For $n = 150$ the calculations were also performed by the S_N-method, using the same computer and the DTF-IV code. It was found that for $N > 6$ the computing time for the S_N-method exceeds the computing time for the method of analytic angles, and increases rapidly with N.

Table II and Fig. 1 will make it clear, what values of N are needed in the S_N-method to achieve an accuracy comparable to that of the method of analytic angles.

In Table II we list the ratio of the fluxes $\Phi(a)$ and $\Phi(0)$ obtained both by the S_N-method with different values of N as well as by the method outlined in this paper. The number of mesh points used was $n = 20$.

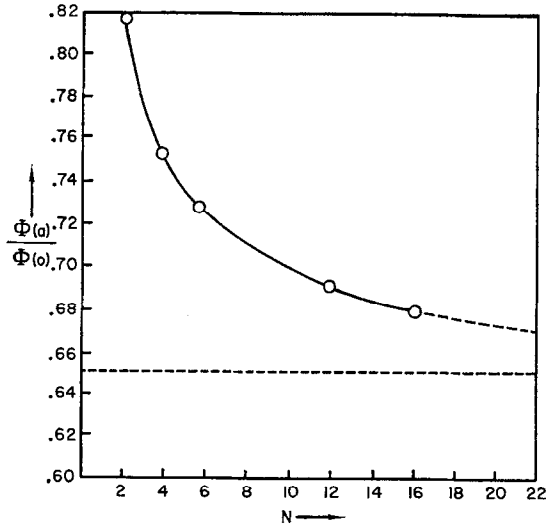

FIG. 1. Ratio of the fluxes $\Phi(a)$ at the boundary and $\Phi(0)$ at the center of the slab vs. the parameter N of the S-method. The dashed straight line represents the result obtained by the method of analytic angles.

In this table, the method of analytic angles is denoted with the symbol S_∞, to emphasize the fact that the number of mesh points N of the angular variable, which characterizes the S_N-method, is infinite.

In Fig. 1. the values listed in Table II are plotted, to indicate the rather uniform convergence of the flux ratios obtained by the S_N-method towards our value. Figure 1 shows that a large number N would be needed to obtain a good approximation to our value.

The high accuracy obtained as well as the short computing time used in the [illegible] power of the method, the solution of a phonon transport problem is developed.

VI. Application to the Problem of Energy Transport by Phonons in a Solid

A. *Exposition of the problem and discretization of the transport equation*

The problem of heat (energy) conduction through an electrically insulating crystal at low temperatures leads to the formulation of the Boltzmann transport equation for quantized elastic waves known as phonons. In Ref. [6] the authors formulate the transport equation for the phonon distribution function in a plane slab of thickness $2a$ with point scattering of the phonons. The two boundary planes of the slab are at temperatures T_1 and T_2, respectively (see Fig. 2). This equation is formulated here for the *change* f^1 of the distribution function due to the scattering—the distribution function f^0 in the absence of scattering being the Bose distribution. The equation for $f^1(k, x, \mu)$ is

$$\mu \frac{\partial f^1(k, x, \mu)}{\partial x} + \Sigma(k) f^1(k, x, \mu) = \frac{1}{2} \Sigma(k) \left[\int_{-1}^{1} f^1(k, x, \mu')\, d\mu' - C^0 S(\mu) \right], \quad \text{(VI.1)}$$

with the boundary conditions

$$f^1(k, a, \mu) = 0 \quad \text{for} \quad -1 \leqslant \mu < 0 \quad \text{and} \quad f^1(k, -a, \mu) = 0 \quad \text{for} \quad 0 < \mu \leqslant 1. \quad \text{(VI.2)}$$

Here $\Sigma(k) \propto k^4$ is the wave number dependent total cross section of all scatterers in a unit volume for Rayleigh scattering of phonons, k is the modulus of the vector $\mathbf{k}$ phonon wave (which plays the role of the particle momentum) and μ is the cosine of the angle θ between $\mathbf{k}$ and the x axis. Note that in this example of the transport problem, $\Sigma(k)$ does not depend on x, and furthermore $\lambda c(x) = 1$. The function $S(\mu)$ is defined by

$$S(\mu) = \begin{cases} 1 & \text{for} \quad 0 < \mu \leqslant 1 \\ -1 & \text{for} \quad -1 \leqslant \mu < 0 \end{cases} \quad \text{(VI.3)}$$

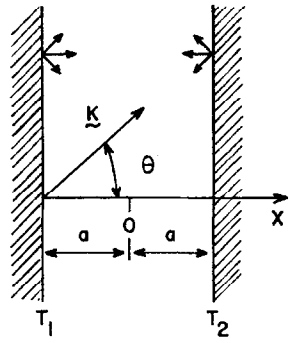

FIG. 2. Boundary conditions for the phonon transport problem. Two infinite planes acting as thermal reservoirs at temperatures T_1 and T_2 ($T_1 > T_2$) emit black-body radiation phonons into a slab of thickness $2a$. Phonons incident on the wall from within the slab are fully absorbed. Phonons are elastically scattered in the slab. $\mathbf{k}$ = wave vector of a phonon.

and

$$C^0 = f^0(T_1) - f^0(T_2), \tag{VI.4}$$

independent of x and μ. Here,

$$f^0(T) = [\exp(\hbar c_s k_B^{-1} k/T) - 1]^{-1} \tag{VI.5}$$

is the Bose distribution function, with $\hbar$ = Planck's constant = 1.05×10^{-27} erg sec, k_B = Boltzmann's constant = 1.38×10^{-16} erg/°K and c_s = velocity of sound in the material = 10^5 cm sec^{-1}. As in the previous sections, the wave number k occurs only as a parameter in the coefficient of the integrodifferential equation for f^1. Hence in the sequel this parameter is omitted, keeping in mind that the final results depend on k.

In accordance with Section II., Eq. (VI.1) is discretized in x; however, for convenience in storing subscripted variables in a computer array, we choose the smallest subscript to be 1 instead of 0. Setting $f(x_i, \mu) \equiv f_i(\mu)$ the result is

$$f_i^1(\mu) = \eta f_{i-1}^1(\mu) + \frac{1}{2}\frac{\alpha}{\mu + \alpha}[\Phi_i + \Phi_{i-1} - 2C^0 S(\mu)], \qquad \text{for} \quad i = 2,..., n. \tag{VI.6}$$

The discretization parameter is

$$\Delta x = x_i - x_{i-1} = 2a/(n-1) \qquad \text{for} \quad i = 2,..., n, \tag{VI.7}$$

and at the boundaries

$$x_1 = -a, \qquad x_n = a.$$

We use the notation

$$\alpha = \tfrac{1}{2}\Sigma\Delta x, \tag{VI.8}$$

$$\Phi_i = \int_{-1}^{1} f_i^1(\mu)\, d\mu, \tag{VI.9}$$

and η is defined in Eq. (IV.2).

With the definitions

$$\begin{aligned} f_i^+(\mu) &= f_i^1(\mu) \qquad \text{for} \quad \mu > 0, \\ \text{and} \qquad & \\ f_i^-(\mu) &= f_i^1(-\mu) \qquad \text{for} \quad \mu > 0, \end{aligned} \tag{VI.10}$$

and using Eq. (VI.3), Eq. (VI.6) can be written as the following set of coupled equations:

$$\begin{aligned} f_{i-1}^+(\mu) &= \eta f_i^-(\mu) + \frac{1}{2}\frac{\alpha}{\mu+\alpha}[\Phi_i + \Phi_{i-1} - 2C^0] \qquad \text{for} \quad \mu > 0,\ i = 2,..., n, \\ \text{and} \qquad & \\ f_{i-1}^-(\mu) &= \eta f_i^-(\mu) + \frac{1}{2}\frac{\alpha}{\mu+\alpha}[\Phi_i + \Phi_{i-1} + 2C^0] \qquad \text{for} \quad \mu > 0,\ i = 2,..., n. \end{aligned} \tag{VI.11}$$

Equations (VI.11) constitute a set of $2(n-1)$ equations in $2n$ unknowns $f_1^+,..., f_n^+$ and $f_1^-,..., f_n^-$. The remaining two unknowns are determined by the boundary conditions Eq. (VI.2), which by virtue of Eq. (VI.10) now read:

$$\begin{aligned} f_1^+(\mu) &= 0, \qquad \text{for} \quad 0 < \mu \leqslant 1 \\ \text{and} \qquad & \\ f_n^-(\mu) &= 0, \qquad \text{for} \quad 0 < \mu \leqslant 1. \end{aligned} \tag{VI.12}$$

Following the procedure outlined in Section III, one finds after making use of Eq. (VI.12)

$$\begin{aligned} f_i^+(\mu) &= \frac{1}{2}\frac{\alpha}{\mu+\alpha}\sum_{l=1}^{i-1}\eta^{i-l-1}[\Phi_l + \Phi_{l+1} - 2C^0] \qquad \text{for} \quad \mu > 0, i = 2,..., n, \\ \text{and} \qquad & \\ f_i^-(\mu) &= \frac{1}{2}\frac{\alpha}{\mu+\alpha}\sum_{l=1}^{n-i}\eta^{n-i-l}[\Phi_{n-l} + \Phi_{n+1-l} + 2C^0] \qquad \text{for } \mu > 0,\ i = 1,..., n-1. \end{aligned} \tag{VI.13}$$

In order to determine the fluxes Φ_i at each point x_i, we substitute the expressions Eq. (VI.13) into Eq. (VI.9), which by virtue of (VI.10) now reads

$$\Phi_i = \int_0^1 [(f_i^+(\mu) + f_i^-(\mu)]\, d\mu \qquad \text{for} \quad i = 1,..., n. \tag{VI.14}$$

The integrations over μ may be carried out analytically (as shown in Section III, this is always the case) yielding

$$\Phi_i = \frac{\alpha}{2}\left[(1-\delta_{i,1})\sum_{l=1}^{i-1} P_{i-l}(\Phi_l + \Phi_{l+1}) + (1-\delta_{i,n})\sum_{l=1}^{n-i} P_{n+1-i-l}(\Phi_{n-l} + \Phi_{n+1-l})\right]$$

$$- \alpha C^0\left[(1-\delta_{i,1})\sum_{l=1}^{i-1} P_{i-l} - (1-\delta_{i,n})\sum_{l=1}^{n-i} P_{n+1-i-l}\right], \qquad \text{for} \quad i = 1,\ldots,n. \tag{VI.15}$$

Equations (VI.15) form a linear algebraic system which can be written in a concise matrix form corresponding to Eq. (III.14) as follows:

$$\sum_{l=1}^{n} (\delta_{i,l} - M_{i,l})\,\Phi_l = Z_i \qquad \text{for} \quad i = 1,\ldots,n. \tag{VI.16}$$

The matrix elements in (VI.16) are

$$M_{i,l} = \frac{\alpha}{2}\,[(1-\delta_{l,n})(\theta_{i,l+1}P_{i-l} + \theta_{l,i}P_{l+1-i})$$

$$+ (1-\delta_{l,1})(\theta_{i,l}P_{i+1-l} + \theta_{l-1,i}P_{l-i})], \qquad \text{for} \quad i,l = 1,\ldots,n, \tag{VI.17}$$

and the inhomogeneous terms read:

$$Z_i = \alpha C^0 \sum_{l=1}^{n} (\theta_{l,i}P_{l+1-i} - \theta_{i,l+1}P_{i-l}) = \alpha C^0 \sum_{l=1}^{n-1} P_l\,, \qquad \text{for} \quad i = 1,\ldots,n. \tag{VI.18}$$

Here $\theta_{i,l}$ is defined in Eq. (III.11) and $P_l \equiv P_{1,l-1}$, as defined in Eq. (IV.8). The quantities P_l satisfy the recursion relations

$$P_l = \frac{1}{l-1}\left[(-1)^{l-1} - \left(\frac{1-\alpha}{1+\alpha}\right)^{l-1}\right] + P_{l-1}\,, \qquad \text{for} \quad l = 2,\ldots,n, \tag{VI.19}$$

with

$$P_1 = \ln(1 + 1/\alpha).$$

B. *Reduction of the Set of Equations and Their Formal Solution*

Note that the dimension of the matrix which determines the fluxes is equal to n, the number of discretization points. Because of round off errors and a matrix inversion time proportional to n^3 for Gaussian elimination (we used this method in tandem with an iterative improvement), it was found practical to limit the dimension of the matrix to $n = 23$.

However in the region of impurity concentration, where $10^{-1} < 2a < 10$, (and therefore $\alpha \simeq 1/(2n-2)$), the function $f^1(k, x, \mu)$ varied rapidly with x and it was necessary to use 46 discretization points to resolve $f_i^1(\mu)$ accurately for almost all values of x and μ. Only in a small angular interval around $\mu = 0$ near $x = \pm a$, does $\partial f^1/\partial x$ vary so rapidly that 46 points were not sufficient to obtain accurate values of the function f^1.

The influence of the number of discretization points n on the computational accuracy of the function $f_i^-(\mu)$ can be seen in Fig. 3.

In order to carry out the actual computer calculation for all values of the parameter k, it was found necessary to perform several more analytical manipulations.

Considerable computer time saving was achieved by the reduction of the order of the matrices involved by a factor of two. (In the Gaussian elimination technique the saving is a factor of eight.) This reduction is accomplished by choosing n *even* and noting the following properties of Eqs. (VI.17) and (VI.18):

$$M_{n+1-i,n+1-l} = M_{i,l}, \quad \text{for} \quad \begin{matrix} i = 1,\ldots, n, \\ l = 1,\ldots, n, \end{matrix} \tag{VI.20}$$

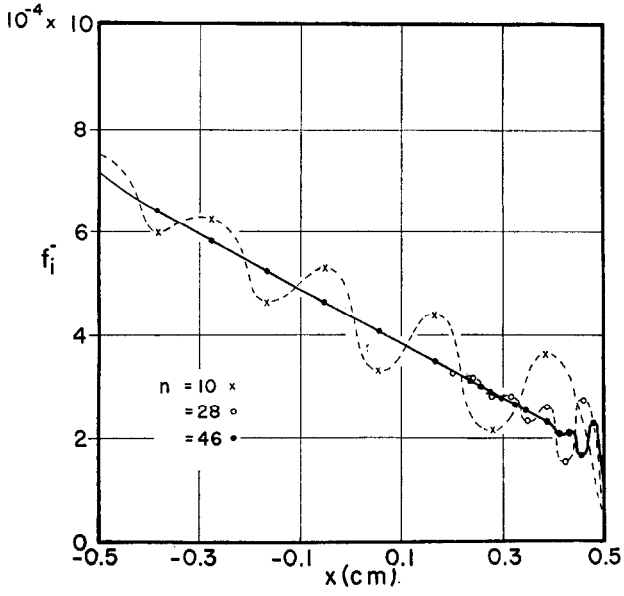

FIG. 3. Influence of the number n of discretization points on the computational accuracy. The function f_i^- ($\mu = 0.0087$) (phonon number) is plotted as a function of position (x_i) for $2a\Sigma = 1$. The phonons move at the angle 90.5° with respect to the x axis.

For larger numbers n the function smooths out, except very near to $x = 0.5$.

and

$$Z_{n+1-i} = -Z_i, \qquad \text{for} \quad i = 1,..., n. \tag{VI.21}$$

Introduction of the new subscripts $j = n + 1 - i$ and $k = n + 1 - l$ into the matrix equation (VI.16) and using (VI.20) and (VI.21) yields

$$\sum_{i=1}^{n} (\delta_{j,i} - M_{j,i}) \Phi_{n+1-i} = -Z_j, \qquad \text{for} \quad j = 1,..., n. \tag{VI.22}$$

Comparison of Eq. (VI.22) with Eq. (VI.16) shows that the following must be true:

$$\Phi_{n+1-i} = -\Phi_i, \qquad \text{for} \quad i = 1,..., n. \tag{VI.23}$$

Hence, half the number of the unknown fluxes Φ_i may be diposed of.

The original set of n equations (VI.16) can now be reduced to $n/2$ equations of the form

$$\sum_{l=1}^{n/2} R_{i,l} \Phi_l = Z_i, \qquad \text{for} \quad i = 1,..., n/2, \tag{VI.24}$$

where

$$R_{i,l} = \delta_{i,l} - M_{i,l} + M_{i,n+1-l}; \qquad \text{for} \quad \begin{matrix} i = 1,..., n/2 \\ l = 1,..., n/2 \end{matrix} \tag{VI.25}$$

We conclude this section by writing out explicitly the elements of the matrix $R_{i,j}$. These are needed in the subsequent section.

To simplify the notation we define

$$q_l = [(-1)^l - (1 - \alpha)^l (1 + \alpha)^{-l}]/l \tag{VI.26}$$

and iterate Eq. (VI.19) to give

$$P_l = \sum_{j=1}^{l-1} q_j + \ln(1 + 1/\alpha). \tag{VI.27}$$

With the further definition

$$(l, m) = \frac{\alpha}{2} \sum_{j=l}^{m} q_j \tag{VI.28}$$

the matrix elements $R_{i,l}$ can be written as

$$\begin{aligned}
R_{1,1} &= 1 + (1, n - 2), \\
R_{1,l} &= (l - 1, n - l) + (l, n - l - 1), \qquad \text{for} \quad l = 2,..., n/2, \\
R_{i,1} &= (i - 1, n - i - 1), \qquad \text{for} \quad i = 2,..., n/2, \\
R_{l,l} &= 1 + (1, n - 2l + 1) + (1, n - 2l), \qquad \text{for} \quad l = 2,..., n/2,
\end{aligned}$$

and

$$R_{l,i} = R_{i,l} = (l - 1, n - i - l + 1) + (l - i + 1, n - i - l),$$
$$\text{for} \quad i = 2,..., \frac{n}{2} - 1, \quad l = 2,..., n/2. \tag{VI.29}$$

Note that the logarithmic term $P_1 = \ln(1 + 1/\alpha)$ cancelled out in the process of reducing the matrix $M_{i,l}$ to $R_{i,l}$. Finally, the inhomogeneous terms (VI.18) can be written as

$$Z_i = 2C^0 \sum_{l=i}^{n-i} [(1, l - 1) + \tfrac{1}{2}\alpha \ln(1 + 1/\alpha)], \qquad \text{for} \quad i = 1,..., n/2. \tag{VI.30}$$

At this point the problem of finding the change $f_i^1(\mu)$ in the phonon distribution function at each point x_i has been formally solved. One needs only to invert the matrix $R_{i,l}$ in Eq. (VI.24), and apply it to the vector Z_i to solve for the vector Φ_i and substitute the components back into Eq. (VI.13) to determine $f_i^1(\mu)$.

C. *Convergence Improvement*

The expressions developed in the preceding section for the matrix elements $R_{i,l}$ cannot be used for numerical calculations for all values of the parameter α. The reason for this is that the matrix $R_{i,l}$ is singular to order α^{-1}, hence for large values of α the numerical results are inaccurate.

We recall that α is proportional to the product of the concentration and cross section of scattering centers [see Eq. (VI.8)].

Work with a computer utilizing 14 significant digits showed that the loss of accuracy through the singular nature of $R_{i,l}$ becomes intolerable for $\alpha > 3 \times 10^3$. Hence, expansions of the matrix elements $R_{i,l}$ and of the inhomogeneous terms Z_i were carried out analytically in inverse powers of α, up to order α^{-2}.

In this section these expansions are developed. For this purpose it is convenient to introduce the following abbreviation for an often occurring alternating sum of powers of integers

$$T_l^m(n) = \sum_{j=l}^{m} (-1)^j j^n. \tag{VI.31}$$

The following relation is immediately verified.

$$T_l^m(n) = T_1^m(n) - T_1^{l-1}(n). \tag{VI.32}$$

It is possible to write $T_1^m(n)$ in terms of $T_1^m(1),..., T_1^m(n - 1)$. Table III gives the values needed.

TABLE III

Values of $T_1^m(n) = \sum_{j=1}^{m} (-1)^j j^n$

	m even	m odd
$T_1^m(0)$	0	-1
$T_1^m(1)$	$m/2$	$-(m+1)/2$
$T_1^m(2)$	$m(m+1)/2$	$-m(m+1)/2$
$T_1^m(3)$	$m^2(2m+3)/4$	$-(m+1)^2(2m-1)/4$

As may be seen from (VI.28) and (VI.29), the matrix elements $R_{i,l}$ contain the quantities q_j, which are functions of α.

Expansion of $\frac{1}{2}\alpha q_j$ to order α^{-2} gives

$$\tfrac{1}{2}\alpha q_j = (-1)^j [1 - j/\alpha + (1 + 2j^2)/3\alpha^2]. \tag{VI.33}$$

Using (VI.33) we write (VI.28) as

$$(l, m) = T_l^m(0) - T_l^m(1)/\alpha + [T_l^m(0) + 2T_l^m(2)]/3\alpha^2. \tag{VI.34}$$

Referring to Table III, this expression becomes

$$(l, m) = \begin{cases} (-1)^l\{1 - (l+m)/2\alpha + [m(m+1) + l]/3\alpha^2\}, & \text{for } m - l \text{ even.} \\ (-1)^l\{(m - l + 1)/2\alpha + [m(m+1) - l + 1]/3\alpha^2\}, & \text{for } m - l \text{ odd.} \end{cases} \tag{VI.35}$$

The matrix $R_{i,l}$, expanded to order $1/\alpha$ is singular and of rank one. Since the inversion of such a matrix (needed to solve (VI.24)) leads to numerical inaccuracies, a new set of equations is formed. The new equations are linear combinations of the equations (VI.24). Their matrix elements are

$$\begin{aligned} R'_{1,l} &= R_{1,l}, && \text{for } l = 1,..., n/2, \\ R'_{i,l} &= R_{i,l} + (-1)^i R_{1,l}, && \text{for } \begin{matrix} i = 2,..., n/2, \\ l = 1, 2,..., n/2, \end{matrix} \end{aligned} \tag{VI.36}$$

and their inhomogeneous terms are

$$\begin{aligned} S_1' &= S_1, \\ S_i' &= S_i + (-1)^i S_1, \qquad \text{for } i = 2,..., n/2. \end{aligned} \tag{VI.37}$$

With the use of Eqs. (VI.29), (VI.35), and (VI.36) we obtain

$$\begin{aligned} R'_{1,1} &= 1 - (n-2)[1/2\alpha - (n-1)/3\alpha^2], \\ R'_{1,l} &= 2(-1)^{l-1}[1/2\alpha - (n-1)/3\alpha^2], \\ R'_{i,1} &= (-1)^i[2(n-i)(i-1) - 1]/3\alpha^2, \\ R'_{l,l} &= (4l-5)/3\alpha^2, \end{aligned} \tag{VI.38}$$

and finally

$$R'_{l,i} = R'_{i,l} = 4(-1)^{i+l}(i-1)/3\alpha^2, \qquad \text{for} \quad \begin{matrix} i = 2,\ldots, n/2 - 1, \\ l = 2,\ldots, n/2. \end{matrix}$$

To formulate the inhomogeneous terms we substitute $(1, l-1)$ from (VI.35) into (VI.30) and expand the logarithmic term to order α^{-2}. The results for l even and l odd are combined to give

$$\begin{aligned} S_i = C^0 \Big\{ &-T_i^{n-i}(0) + [T_i^{n-i}(1) - 1/2T_i^{n-1}(0)]/\alpha \\ &- \Big[T_i^{n-i}(0) - 4\sum_{j=i}^{n-1} T_1^{j-1}(2)\Big]\Big/3\alpha^2 \Big\}, \qquad \text{for} \quad i = 1,\ldots, n/2. \end{aligned}$$

From this, using Eq. (VI.31), Table III, and the fact that $n - 2i$ is even, follows

$$S_i = C^0(-1)^i\{-1 + (n-1)/2\alpha - [1 - n + 2(-1)^i T_i^{n-1}(2)]/3\alpha^2. \tag{VI.39}$$

According to the definition (VI.37), the inhomogeneous terms are now given by

$$\begin{aligned} &S_1' = C^0\{1 - (n-1)[1/2\alpha - (n-1)/3\alpha^2]\} \\ \text{and} \qquad &S_i' = 2C^0(-1)^i\,(n-i)(i-1)/3\alpha^2 \qquad \text{for} \quad i = 2,\ldots, n/2. \end{aligned} \tag{VI.40}$$

In terms of (VI.38) and (VI.40), the new set of equations, equivalent to (VI.24), is

$$\sum_{l=1}^{n/2} R'_{i,l}\Phi_l = S_i' \qquad \text{for} \quad i = 1,\ldots, n/2. \tag{VI.41}$$

At this point we have derived expressions which are suitable for all values of α to accurately solve for the fluxes Φ_i. As pointed out in Section VI.B, substituting Φ_i into Eq. (VI.13) gives the function f^1, hence a complete solution of the problem is obtained. A graphical representation of the solutions is shown in Fig. 4, a, b and c.

D. *Integral Quantities Obtained from the Distribution Function*

To illustrate the use of the solution and to examplify the necessity of the expansions in inverse powers of α we shall describe the calculation of the x component of the phonon momentum density. At each point x_i this quantity is defined as

$$\mathscr{P}_i = \mathscr{P}_0 + \Omega\hbar \int k\mu f_i^1 \, d^3k, \tag{VI.42}$$

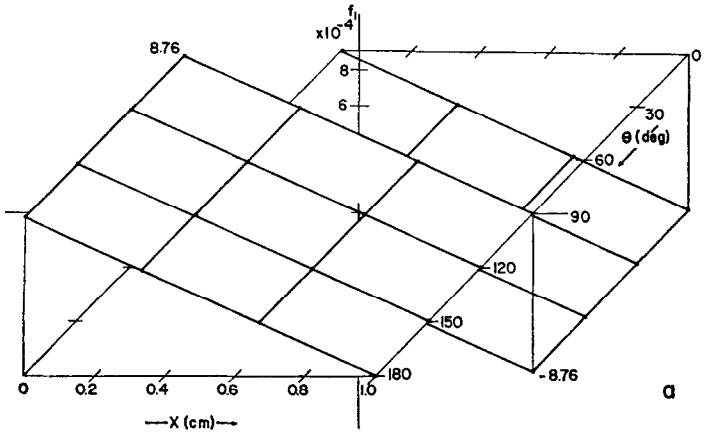

FIG. 4.

where $\mathscr{P}_0$ is the momentum density in the absence of scattering [6]. Thus $\mathscr{P}_0$ is given by

$$\mathscr{P}_0 = \Omega\hbar \int k\mu f^0 \, d^3k = \pi\Omega\hbar \int_0^\infty k^3 C^0 \, dk, \tag{VI.43}$$

where C^0 is given by (VI.4) in terms of the equilibrium distribution function f^0, and $\Omega\hbar$ is a numerical constant. Substitution of the discretized solutions f_i^+ and f_i^- given by (VI.13) into (VI.42) and integration over the angular variable μ yields

$$\mathscr{P}_i = \mathscr{P}_0 + \pi\Omega\hbar \int_0^\infty k^3 \Big\{ (1 - \delta_{i,1}) \sum_{l=1}^{i-1} \alpha^2 (Q_{i-l} + Q_{i-l+1})(\Phi_l + \Phi_{l+1} - 2C^0)$$

$$- (1 - \delta_{i,n}) \sum_{l=1}^{n-i} \alpha^2 (Q_{n-i-l+1} + Q_{n-i-l+2})(\Phi_{n-l} + \Phi_{n-l+1} + 2C^0) \Big\} \, dk. \tag{VI.44}$$

The quantities Q_m are defined as

$$Q_1 = 1/2\alpha,$$

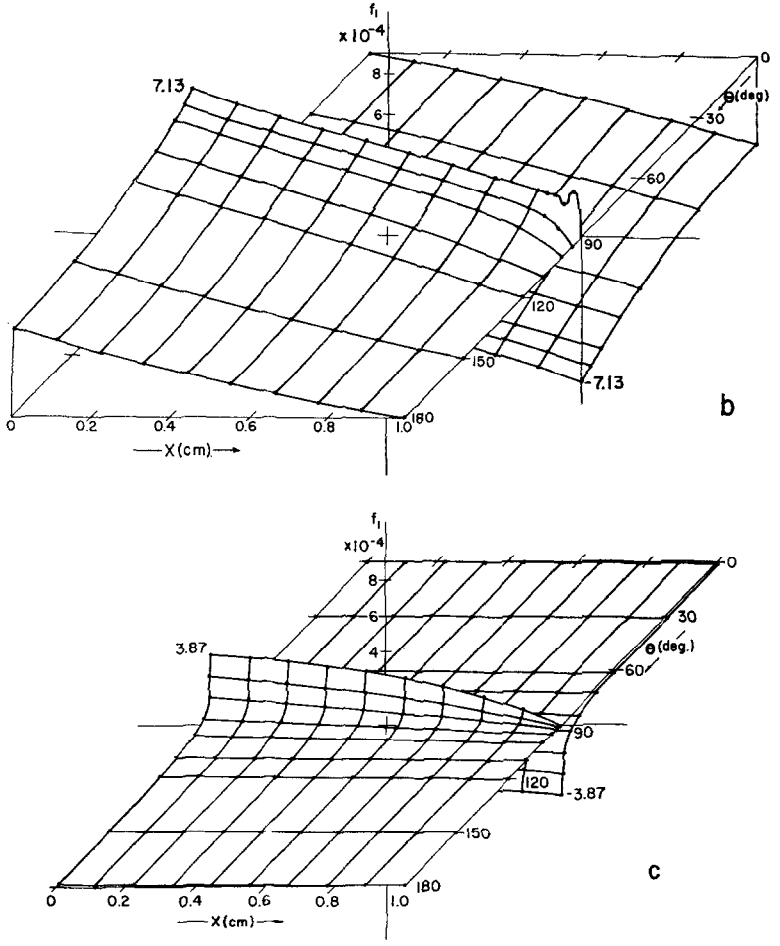

FIG. 4. Relief diagram of the contribution $f^1(x, \theta)$ to the phonon distribution function through scattering. The function has been obtained as a solution of (VI.1), using a maximum of 46 discretization points. Horizontal axes: coordinate x across slab, $\theta = \sphericalangle(\mathbf{k}, \hat{\mathbf{x}})$. Parameters: $\hbar c_s k_B^{-1} = 7.61 \times 10^{-7}$ cm °K (cf. Eq. VI.5), center temperature $T_m = 1$ °K, temperature difference across slab $T = 10^{-2}$ °K, phonon wave number $k = 5 \times 10^6$ cm^{-1} and slab thickness $2a = 1$ cm.
Figures a, b, and c show f^1 for $2a\,\Sigma(k) = 1000$, 1.0, 0.01, respectively.

and

$$Q_m = P_{2,m-1} = u^{m-1}/(1-u) - \tfrac{1}{2}(-1)^{m-1} - (m-1)\,P_{m-1}\,, \qquad \text{for } m = 2,\ldots,n, \tag{VI.45}$$

where u is defined by (IV.6)

Initially Eq. (VI.44) was used to find the total momentum density $\mathscr{P}$ for all α by numerically integrating the second term over k and then adding $\mathscr{P}_0$ (VI.43) to it. This method yielded inaccurate results for large values of α (large total scattering cross section Σ) because in this limit $\mathscr{P}$ approaches zero and the integration produces a term approaching $-\mathscr{P}_0$. Regarding $\mathscr{P}_0$ as of order unity, we needed to know the total momentum density for values of such that $\mathscr{P} < 10^{-10}$. Therefore, the term $-\mathscr{P}_0$ needed to be analytically extracted from the integral in Eq. (VI.44). This was accomplished by expanding $\alpha^2 Q_m$ to order α^{-2} for large α.

Specifically, using (VI.27) to rewrite (VI.45) we have

$$\alpha^2 Q_{m+1} = \frac{1}{2}\alpha u^m - m\alpha^2\left[\frac{1}{2}q_m + \sum_{l=1}^{m-1} q_l + \ln(1 + 1/\alpha)\right], \tag{VI.46}$$

where q_m is defined by (VI.26). After expanding all terms in (VI.46) to order α^{-2}, and making use of Table III, we find

$$\alpha^2(Q_m + Q_{m+1}) = \tfrac{1}{2}(-1)^{m+1}\{1 - 2(2m-1)/3\alpha + [m(m-1) + \tfrac{1}{2}]/\alpha^2\}. \tag{VI.47}$$

By setting $m = i - l$ and $j = l + i - 1$, and substituting (VI.47) into the momentum density integrand (VI.44), the zero-th order term (α^0) multiplying C^0 is found to be

$$\pi\Omega\hbar \int_0^\infty k^3 C^0 \left\{(1 - \delta_{i,1}) \sum_{m=i-1}^{1} (-1)^m + (1 - \delta_{i,n} \sum_{j=i}^{n-1} (-1)^{n-j}\right\} dk$$

$$= \pi\Omega\hbar \int_0^\infty k^3 C^0\, dk \sum_{m=1}^{n-1} (-1)^m = -\pi\Omega\hbar \int_0^\infty k^3 C^0\, dk = -\mathscr{P}_0. \tag{VI.48}$$

The total momentum density at the point x_i can now be written as

$$\mathscr{P}_i = \pi\Omega\hbar \int_0^\infty k^3\alpha^2 \Big\{(1 - \delta_{i,1}) \sum_{l=1}^{i-1} [(Q_{i-l} + Q_{i-l+1})(\Phi_l + \Phi_{l+1})$$

$$- 2C^0(Q_{i-l} + Q_{i-l+1} + (1/2)\,\alpha^{-2}(-1)^{i-l})] - (1 - \delta_{i,n}) \sum_{l=1}^{n-i} [(Q_{n-i-l+1}$$

$$+ Q_{n-i-l+2})(\Phi_{n-l} + \Phi_{n-l+1}) + 2C^0(Q_{n-i-l+1} + Q_{n-i-l+2}$$

$$+ (1/2)\,\alpha^{-2}(-1)^{n-i-l+1})]\Big\}\, dk. \tag{VI.49}$$

This expression was used to compute the momentum density at the point x_i with the aid of the computer programs outlined in the next section. We note, that the accuracy of the calculation was checked by comparing values of the momentum

density at different points. Since there are no sources or sinks in the slab, the momentum density was found to be the same at all points, i.e., $\mathscr{P}_i = \mathscr{P}$ for all i.

VII. Computational Procedure

In this section we outline the numerical calculations carried out on the example of the phonon transport problem. For brevity, we do not include a description of the neutron transport calculations of Section V. Computer programs may be obtained from the authors.

The numerical calculations were carried out on a digital computer.[4] A code designated as BOZMA, consisting of a main program and five subroutines, was written in the language FORTRAN IV [7] for the purpose of calculating f_i^1 and carrying out the necessary k-space integrations for the energy and momentum densities.

The integrations are performed by the Romberg algorithm [8]. The function to be integrated vanishes exponentially for large values of its argument. The total range of integration over the variable k $(0 - \infty)$ is divided into regions whose upper limits are calculated from predetermined fractions of the integrand's maximum value, which is found by a routine called *peak seeker*. The development of peak seeker was necessary because the integrand is sharply peaked. By placing the upper limit of one of the integration regions at the peak, the number of points needed in conjunction with the Romberg algorithm to satisfy certain convergence criteria is reduced considerably. Two types of convergence criteria are used in the integration. In each region of integration the column of the trapezoid sums and

[redacted]

less than 10^{-6}.

The set of linear equations (VI.41) is solved for the fluxes Φ_i by three subroutines taken from the literature [9]. The first of these subroutines, DECOMP, is essentially a Gaussian elimination routine with partial pivoting. The second, SOLVE, uses an upper triangular matrix generated by DECOMP to solve the equations. The third, IMPRUV, is a relaxation algorithm, which uses as a first approximation in an iterative procedure the solutions obtained by the Gaussian elimination.

The detailed results obtained by these calculations are published elsewhere. (See [6].)

[4] Model 6400 computer made by Control Data Corporation, of the Florida State University, operated with the assistance of the U.S. National Science Foundation Grant GJ367.

For fixed values of all parameters of the problem, the phonon distribution function, the momentum density, the energy, and the number of particles at each (out of n) discretization point x_i was computed.

For a comparison of the computational times needed for this and other methods the reader is referred back to Section V, third paragraph.

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REFERENCES

1. L. D. LANDAU AND E. M. LIFSHITZ, "Statistical Physics," pp. 152, Pergamon Press Ltd., London/Paris, 1958.
2. For a comprehensive discussion of these methods the reader is referred to R. D. RICHTMYER AND K. W. MORTON, "Difference Methods for Initial-Value Problems," 2nd. ed., Wiley (Interscience), New York, 1967.
3. B. CARLSON, *Proc. Symp. Appl. Math. II, Soc.* (1959), 219–232.
4. K. LATHROP, Los Alamos Scientific Laboratory Report LA-3373, Los Alamos, N. M., 1965.
5. J. H. BENNET, Integral equation methods for transport problems, some numerical results, *Numer. Math.* **6** (1964), 49–54.
6. P. ERDÖS AND S. B. HALEY, *Phys. Rev.* **184** (1969), 951.
7. American Standards Association Proposed Standards for FORTRAN, *Comm. Assoc. Comp. Mach.* **7** (1964), 591; ibid. **8** (1965), 287.
8. F. L. BAUER, Ed. STIEFEL, AND H. RUTISHAUSER, *in Proc. Symp. Appl. Math.* (N. Metropolis, Ed.) **15**, p. 199, *Amer. Math. Soc.*, publisher, Providence, R.I. (1963).
9. G. FORSYTHE AND C. B. MOLER, Computer Solution of Linear Algebraic Systems *in* "Series in Automatic Computation," Prentice-Hall, Englewood Cliffs, N.J., 1967.