Solution of the Transport Integral Equation with Anisotropic Scattering

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Received February 8, 1972

The paper deals with the solution of the integral equation for particle transport in homogeneous material systems having plane and spherical symmetry. Emphasis is put on the explicit inclusion of anisotropic scattering (higher Legendre components of the scattering kernel). The present approach is based on a generalization of the Integral Transform method. The solution is represented as an expansion with respect to analytical basis functions with coefficients satisfying a certain linear system. The determination of this linear system and its matrix elements in a form convenient for numerical purposes is the central point of the paper.

For the computation of the matrix elements a computer program has been developed. It calculates the elements in the case of isotropic and linear anisotropic scattering in systems of plane and spherical symmetry as a function of the optical thickness of the system. Higher anisotropy is easily included. Numerical examples indicate the great practical importance of the method, due to the fact that the computational effort involved is very low, especially for small systems.

INTRODUCTION

Transport integral equations are linearized versions of the Boltzmann equation and occur in many branches of physics to describe the interaction of particles or quasiparticles with matter. Important examples are neutron transport in a reactor, radiative transfer, rarefied gas dynamics or migration of point defects in crystals. The first approaches to solve the transport equation had been done in the domain of radiative transfer and summarized in the standard textbooks of Chandrasekhar [4] or Kourganoff and Busbridge [5]. In the present paper we focus on the solution of the integral equation for neutron transport [1] due to anisotropic scattering of monoenergetic neutrons in material systems having plane or spherical symmetry. The tool to solve this integral equation is the Integral Transform or IT method, an analytical approach developed in the last years [10]. As compared to purely numerical methods like S_N [12] or *Monte Carlo* [13] it has the advantage that the influence of the parameters of the problem can be studied explicitly; moreover it serves as a standard for testing numerical approximations.

Other analytical methods to solve the neutron transport equation are the widely used normal mode approach of Case [14] and the Fourier transform method of Kiesewetter [15]. In both cases the problem generally reduces to the solution of a Fredholm type integral equation to be performed numerically. If anisotropic scattering has to be taken into account, this integral equation is replaced by a system of integral equations of a rather complex structure [16]. The main difference between these and our IT method lies in the opposite convergence behavior of the solutions. Whereas the methods mentioned converge the faster the larger (compared to a characteristic mean free path) the system is, our method is the faster the smaller the system is.

As has been shown elsewhere [17], in the simplest case of isotropic scattering the transport equations for plane and spherical symmetry can simultaneously be reduced to the same integral equation of displacement type with the kernel $E_1(|x - x'|)$. ($E_1(z)$ denotes the exponential integral, x and x' the distance of the reference point and scattering point from the symmetry plane of the slab or from the center of the sphere). In the case of anisotropic scattering the transport integral equation is much more complicated since every anisotropic component of the physical scattering law gives rise to an additional kernel. In plane geometry they can again be expressed by higher exponential integrals $E_n(|x - x'|)$. No analogy exists for spherical geometry due to the lack of rotational symmetry in the anisotropic case, preventing expression of the kernels as a function of the radial distance |r - r'|. This difficulty can be overcome in the Fourier transform space where both geometries can again be treated simultaneously as in the isotropic case.

In the following section the transport integral equation is Fourier transformed resulting in a new integral equation with a simpler displacement kernel. The essential step of the method is to reduce the new integral equation to a linear system of algebraic equations by the aid of a certain bilinear expansion for the kernel. This bilinear expansion is a generalization of an addition theorem for spherical Bessel functions. Since it seems to be new, the derivation is given in the Appendix. Truncation of the bilinear expansion after N terms constitutes the IT_N approximation to our method.

In the third section the matrix elements of the linear system of equations are investigated in detail. They are analytical functions of the "optical depth" or thickness measured in mean free paths (2α) of the physical system. The evaluation and the appropriate representation of the matrix elements is of central importance for the IT method. For numerical convenience they are represented as asymptotic expansions for large α ($\alpha \gtrsim 10$) and as rapidly converging series expansions for small α .

A computer program has been written to calculate the elements to any spatial truncation order N, but it is limited for the time being to linear anisotropy. The elements for higher anisotropy can easily be included on the basis of recurrence relations.

The fourth section contains the representation of the solution of the transport equation obtained by inversion of the Fourier transform. The solution is given in terms of special analytic functions in the angular (μ) and space (x) variables with coefficients satisfying the linear system. In the fifth section the solution is represented as a very convenient double series of Legendre polynomials $P_{l}(\mu)$ and $P_{n}(x)$ which can easily be generated on the computer.

The last section gives some numerical results illustrating the working of the method.

2. The IT Approach

The macroscopic distribution of neutrons in the coordinate and momentum space is generally described by the directional or angular flux $\psi(\mathbf{r}, \Omega)$. For monoenergetic neutrons interacting with the atoms of a homeogeneous uniform medium, the directional flux is obtained as the solution of the linearized Boltzmann Eq. [1]

$$\psi(\mathbf{r},\,\boldsymbol{\Omega}) = \int_{0}^{\infty} ds \, e^{-s\Sigma_{t}} \left\{ \int_{(4\pi)} d^{3}\boldsymbol{\Omega}' \boldsymbol{\Sigma}_{s}(\mathbf{r}',\,\boldsymbol{\Omega}'\to\boldsymbol{\Omega}) \, \psi(\mathbf{r}',\,\boldsymbol{\Omega}') + S(\mathbf{r}',\,\boldsymbol{\Omega}) \right\}.$$
(2.1)

Here **r** is the vector of the reference point $P, \mathbf{r}' = \mathbf{r} - s\Omega$ the vector of the collision point P', Ω denotes the flight direction of a neutron, $S(\mathbf{r}', \Omega)$ the external source density at P' in direction Ω . The "scattering kernel" $\Sigma_s(\mathbf{r}', \Omega' \to \Omega)$ expresses the probability that a neutron at the collision point changes its flight direction from Ω' to $\Omega; \Sigma_t$ is the total macroscopic cross section (including scattering, fission and absorption). The restriction to monoenergetic neutrons is only for convenience and not essential for the present approach.

We make the usual assumption that the material is of isotropic structure so that the scattering kernel depends only on the cosine of the angle Θ between the directions Ω' and Ω . The anisotropy of the scattering may be of degree L; that means we have L anisotropic Legendre components in the expansion of the scattering kernel

$$\Sigma_{s}(\mathbf{r}, \mathbf{\Omega}' \to \mathbf{\Omega}) = (1/4\pi) \sum_{l=0}^{L} (2l+1) \Sigma_{s,l}(\mathbf{r}') P_{l}(\cos \theta).$$
(2.2)

In the following the transport integral equation for systems with spherical and with plane symmetry will be derived and solved by the IT technique. Since the transform technique in the case of the sphere is not straightforward some essential details are presented.

We look for solutions of Eq. (2.1) which are bounded and absolutely integrable functions. This set of functions contains just the solutions of physical meaning. It follows from the structure of the integral equation and the nature of its kernel that the solutions satisfy a Hölder condition with respect to the space variable. This is sufficient for the existence and unicity of the Fourier transform and its inversion [19].



FIG. 1. Radius vector r and r' of the reference point P and collision point P' in a system with spherical symmetry. Ω' and Ω are the particle flight directions before and after the collision.

Spherical Systems (Fig. 1)

Due to the radial symmetry the angular flux $\psi(\mathbf{r}, \Omega) = \psi(r, \mu)$ is assumed to depend only on $r = |\mathbf{r}|$ and the cosine $\mu = \cos(\Omega, \mathbf{r})$ between the flight direction and the radius vector of the reference point. We introduce further the projections (Fig. 1) $\mu_0 = \cos(\Omega, \mathbf{r}')$ and $\mu' = \cos(\Omega', \mathbf{r}')$. The directed source density at the point \mathbf{r}' is then of the form $S(r', \mu_0)$. The further treatment requires the separation of the coupled scattering angles Ω and Ω' in terms of the projections μ, μ_0 and μ' . This is achieved on the basis of the addition theorem for the spherical harmonics [2] which allows to express $P_i(\cos \Theta)$ in terms of associate Legendre functions of the variables μ_0 and μ' . Integration of $P_i(\cos \Theta)$ with respect to the azimuth φ' of Ω' referred to the \mathbf{r}' -axis cancels all terms except $P_i(\mu') P_i(\mu_0)$, the latter being multiplied by 2π . If we introduce the moments of the angular flux by

$$\int_{-1}^{+1} d\mu' P_{i}(\mu') \psi(r',\mu') = \psi_{i}(r'), \qquad (2.3)$$

Eq. (2.1) can be written

$$\psi(r,\mu) = \int_0^\infty ds \exp(-s\Sigma_t) \Big\{ \sum_{l=0}^L (l+1/2) \Sigma_{s,l}(r') P_l(\mu_0) \psi_l(r') + S(r',\mu_0) \Big\}.$$
(2.4)

In the case of isotropic scattering (L = 0), Eq. (2.4) may be converted into an integral equation of displacement type for the total flux $\psi_0(r)$. On the basis of a (one-dimensional) Fourier transform with respect to r this integral equation is reduced to a linear system [10]. In the anisotropic case $(L \ge 1)$, however, this direct approach fails. We are faced with the actual three-dimentional character of the problem and have to use the transform

$$F(B,\eta) \equiv (2\pi)^{-3/2} \int_0^\infty dr \, r^2 \int_{-1}^{+1} d\mu \int_0^{2\pi} d\varphi \, \exp(-i \, \mathbf{B} \cdot \mathbf{r}) \, \psi(r,\mu), \qquad (2.5)$$

where **B** is the coordinate vector of the transformed space, $B = |\mathbf{B}|$, and $\eta = \cos(\mathbf{\Omega}, \mathbf{B})$. On the basis of the following

Lemma 1.

$$\int_{0}^{2\pi} d\varphi \exp(-i \mathbf{B} \cdot \mathbf{r}) = 2\pi \sum_{n=0}^{\infty} (-i)^n (2n+1) j_n(Br) P_n(\eta) P_n(\mu), \quad (2.6)$$

which is proved in the Appendix, the integration with respect to φ on the r.h.s. of Eq. (2.5) is settled. The j_n are the spherical Bessel functions [3]. With definition (2.3) of the angular moments, Eq. (2.5) can be written

$$F(B,\eta) = (2\pi)^{-1/2} \sum_{n=0}^{\infty} (-i)^n (2n+1) P_n(\eta) \int_0^\infty dr \, r^2 j_n(Br) \, \psi_n(r). \quad (2.7)$$

Let the integral with respect to r in (2.7) be denoted by $f_n(B)$. It represents a Hankel transform [9] of order (n + 1/2) of the function $\psi_n(r)$. The inversion of this transform is given by

$$\psi_n(r) = \frac{2}{\pi} \int_0^\infty dB \ B^2 j_n(Br) f_n(B).$$
 (2.8)

The right hand side of Eq. (2.4) depends in a rather complicated way on the

variables r and μ . These are contained in r' and μ_0 according to elementary geometrical relations valid in the triangle (Fig. 1), spanned by r, r' and s. When applying the operator (2.5) to the r.h.s. of Eq. (2.4) it is essential to recognize that the volume element written down in Eq. (2.5) can be substituted by the volume element $r'^2 dr' d\mu_0 d\varphi_0$. $(0 \le r' \le \infty; -1 \le \mu_0 \le 1; \varphi_0 = \varphi + \text{const}; s \text{ un-}$ changed). Owing to this substitution the integration is considerably facilitated. We split the exponential $\mathbf{B} \cdot \mathbf{r}$ in the operator (2.5) into $\mathbf{B} \cdot \mathbf{r}' + Bs\eta$. The transform of the r.h.s. of Eq. (2.4) consists of a fourfold integral with respect to s, φ_0 , μ_0 and r'. The s-integration can be done immediately yielding $(\Sigma_t + iB\eta)^{-1}$ as a prefactor. The φ_0 -integration introduces a simplification according to the orthogonality property of the Legendre polynomials. It remains a finite sum from O to L of integrals with respect to r' containing the angular moments $\psi_i(r')$. The scattering cross sections $\Sigma_{s,l}(r')$ are constant inside the sphere and vanish identically outside ("black absorber assumption") so that the r'-integration actually runs from r' = 0to the sphere radius a. In order to get an integral equation in the Fourier space we express the remaining $\psi_1(r')$ by the $f_1(B)$ according to (2.8) and find

$$F(B,\eta) = (\Sigma_{t} + iB\eta)^{-1} \sum_{l=0}^{L} (-i)^{l} (l + \frac{1}{2}) \Sigma_{s,l} P_{l}(\eta)$$
$$\cdot \left(\frac{2}{\pi}\right)^{3/2} \int_{0}^{\infty} dB' \ B'^{2} f_{l}(B') \ K_{l}(B', B) + Q(B, \eta).$$
(2.9)

The new source term $Q(B, \eta)$ is the transform of the uncollided flux due to the source $S(r', \mu_0)$ in the sense of Eq. (2.5).

In Eq. (2.9) we introduced the "partial kernels"

$$K_{l}(B', B) \equiv \int_{0}^{a} dr r^{2} j_{l}(B'r) j_{l}(Br). \qquad (2.10)$$

The essential step of the IT method is to replace the partial kernels of the type (2.10) by bilinear expressions and to reduce (2.9) to a linear system of algebraic equations. This aim is attained by the aid of

Lemma 2.

$$K_{l}(B',B) = \frac{a}{B'B} \sum_{m=l+1(2)}^{\infty} (2m+1) j_{m}(aB') j_{m}(aB), \qquad (2.11)$$

the proof of which is given in the Appendix. (The summation subscript is always increased by two: m = l + 1, l + 3,...).

If the projections of the $f_l(B)$ onto the $j_m(aB)$ are denoted by X_m^l (up to a constant normalization factor) Eq. (2.9) can be rewritten in the form

$$F(B,\eta) = \frac{2}{B} \sqrt{\frac{2}{\pi}} \sum_{l=0}^{L} (-1)^{l} (2l+1) \frac{a\Sigma_{s,l}}{\Sigma_{t} + iB\eta} P_{l}(\eta)$$
$$\cdot \sum_{m=l+1(2)}^{\infty} i^{m-1}(2m+1) j_{m}(aB) X_{m}^{l} + Q(B,\eta).$$
(2.12)

The coefficients X_m^l are reproduced on the 1.h.s. of (2.12) first by performing the angular moments with respect to $P_{l'}(\eta)$ followed by a projection onto the $j_{m'}(aB)$. The results of the double integration is the desired linear system for the coefficients X_m^l

$$X_{m'}^{l'} = \sum_{l=0}^{L} (2l+1) \, a \Sigma_{s,l} \sum_{m=l+1(2)} (2m+1) \, T_{m'm}^{l'l}(\alpha) \, X_m^l \, + \, Q_{m'}^{l'} \qquad (2.13)$$

(m' = l' + 1, l' + 3,...). The matrix elements turn out to be

$$T_{m'm}^{l'l}(\alpha) = (-1)^{(m'-m)/2} \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\beta}{\beta} j_{m'}(\beta) j_m(\beta) \int_{-1}^{+1} d\eta \, \frac{P_{l'}(\eta) \, P_{l}(\eta)}{\alpha/\beta + i\eta} \,. \tag{2.14}$$

They are real and depend only on the "optical thickness" $2\alpha = 2a\Sigma_t$ of the sphere. Due to the obvious symmetry properties $T_{mm'}^{ll'}(\alpha) = T_{mm'}^{l'l}(\alpha) = (-1)^{m'+m} T_{m'm}^{l'l}(\alpha)$, only those matrix elements for which $l' \ge l$ and $m' \ge m$ need to be evaluated. The source vectors $Q_m^{l'}$ are obtained as the projection of $Q(B, \eta)$ onto $P_{l'}(\eta)$ and $j_{m'}(aB)$ in the same way as the $X_{m'}^{l'}$ are obtained from $F(B, \eta)$.

Plane systems (Fig. 2)

Whereas in the sphere the angular density depends on the angle between flight direction Ω and the instantaneous radius vector, all angles in the plane system refer to the same fixed x-direction. The angular density $\psi(x, \mu)$ in the reference point P is to depend only on the distance x from the mid-plane of the slab and on $\mu = \cos(\Omega, \mathbf{x})$, the cosine of the angle between flight direction and the x axis. The directed source density in P' depends on x' and μ . The decomposition rule (2.2) and the addition theorem for $P_l(\cos \Theta)$ are applied as in the preceding case with the only difference that μ_0 has to be replaced by μ , since all angles now refer to the same axis. Azimuthal integration of $P_l(\cos \Theta)$ cancels again all higher harmonics except $P_l(\mu') P_l(\mu)$. With the abbreviation (2.3) for the angular moments the integral equation (2.1) reduces to

$$\psi(x,\mu) = \int_0^\infty ds \exp(-s\Sigma_t) \Big\{ \sum_{l=0}^L (l+\frac{1}{2}) \sum_{s,l} (x') P_l(\mu) \psi_l(x') + S(x',\mu) \Big\}.$$
(2.15)



FIG. 2. Location of reference point P resp. collision point P' at the distance x resp. x' from the symmetry plane x = 0 in the slab case.

The appropriate integral transform is the one-dimensional Fourier transform

$$F(B,\mu) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} dx \exp(-iBx) \,\psi(x,\mu). \tag{2.16}$$

Operation (2.16) applied to the r.h.s. of Eq. (2.15) leads to a double-integral over an (x, s)-domain. It is much more convenient to perform the integration in the (x', s)-domain defined by the substitution $x' = x - s\mu$ which is geometrically evident from the triangle POP' in Fig. 2. The area element $(dx \, ds)$ changes into $(dx' \, ds)$, again $-\infty \leq x' \leq \infty$. The effective range of the variable x', however, is $-a \leq x' \leq +a$ since $\Sigma_{s,l}(x')$ and the source density vanish in the vacuum outside the slab of half-thickness a. Moreover we take $\Sigma_{s,l}$ to be constant inside the slab of uniform material. The s integration is now immediate, yielding a prefactor $(\Sigma_t + iB\mu)^{-1}$. Proceeding as before in the case of the sphere, we arrive at an integral equation for the Fourier transform $F(B, \mu)$ of the angular flux with the kernel $K(B', b) = (B' - B)^{-1} \sin(aB' - aB)$. On the basis of a well-known bilinear expansion for this kernel in terms of spherical Bessel functions [6, 17] the solution of the integral equation can be given in the form

$$F(B,\mu) = \sqrt{\frac{2}{\pi}} \left(\Sigma_t + iB\mu \right)^{-1} \sum_{l=0}^{L} (2l+1) a \Sigma_{s,l} P_l(\mu)$$

$$\cdot \sum_{m=0}^{\infty} (-i)^m (2m+1) j_m(aB) X_m^l + Q(B,\mu), \qquad (2.17)$$

with coefficients satisfying the linear system

$$X_{m'}^{l'} = \sum_{l=0}^{L} (2l+1) \, a \Sigma_{s,l} \sum_{m=0}^{\infty} (2m+1) \, T_{m'm}^{l'l}(\alpha) \, X_{m}^{l} + Q_{m'}^{l'}.$$
(2.18)

The source vector $Q_{m'}^{l'}$ is defined in the same way as for the sphere. Also the matrix elements $T_{m'm}^{l'l}$ are the same functions of α as before [Eq. (2.14)]. Whereas in the case of the sphere the sums (m + l) as well as (m' + l') have to be odd numbers due to the structure of the partial kernels (2.11), the selection rule for the matrix elements of the slab is based upon the parity property of the integrand in (2.14). Since $j_m(-\beta) = (-)^m j_m(\beta)$ and $P_n(-\mu) = (-)^n P_n(\mu)$ it follows that (m' + l' + m + l) has to be even. Otherwise, $T_{m'm}^{l'l}(\alpha) \equiv 0$ if (m' + l' + m + l) is odd.

As a consequence the solutions of system (2.18) split up in two different symmetry classes, a first class with both (m' + l') and (m + l) even and a second class with both odd. According to as the source vector $Q_{m'}^{l'}$ has even or odd parity (m' + l') even or odd!), the first or second class of solutions is selected out.

3. MATRIX ELEMENTS

The matrix elements of the linear system (2.13) and (2.18) and their determination in a form suitable for numerical purposes are of central importance in the present approach. Although the matrix elements are expressible in closed form, we shall, in view of numerical requirements, confine ourselves to present them as expansions with respect to the parameter α . Since the power series expansions converge slowly for $\alpha \gg 1$ we also give asymptotic expansions in $1/\alpha$, valid for large α .

By means of elementary transformations it is possible to bring the expression (2.14) for the matrix elements into the form

$$T_{m'm}^{l'l}(\alpha) = \int_0^1 dq \ Q_{m'm}(q) \int_0^1 \frac{d\mu}{\mu} P_{l'}(\mu) \ P_l(\mu) \exp(-2\alpha q/\mu), \tag{3.1}$$

where the $Q_{m'm}(q)$, defined as the Fourier transform of the product of spherical Bessel functions contained in expression (2.14), are special polynomials in q which had been investigated in detail in a previous paper [7].

Asymptotic expansions

If we perform in Eq. (3.1) first in the integration with respect to q, we obtain a finite expression in powers of (μ/α) and a further contribution of the order of $\exp(-2\alpha)$. A second integration with respect to μ yields the representation of the matrix elements for large α

$$T_{m'm}^{l'l}(\alpha) = \sum_{\nu=0}^{m'+m+1} (2\alpha)^{-\nu-1} \frac{\nu!}{\nu+1} A_{\nu}^{m'm} L_{\nu}^{l'l} + O(e^{-2\alpha}/\alpha), \qquad (3.2)$$

where $A_{\nu}^{m'm}$ is the coefficient of q^{ν} in the polynomial $Q_{m'm}(q)$. For $m \ge m'$ we found [7] $A_0^{m'm} = (m + 1/2)^{-1} \delta_{mm'}$; $A_1^{m'm} = -2$ and in the case $2 \le \nu \le m' + m + 1$,

$$A_{\nu}^{m'm} = \frac{2(-1)^{\nu}}{\nu! (\nu-1)!} \prod_{\rho=1}^{\nu-1} (m+m'+1+\nu-2\rho)(m-m'+\nu-2\rho). \quad (3.3)$$

For m < m' all coefficients are multiplied by $(-)^{m'+m}$, in agreement with the symmetry properties of Eq. (2.14). The effect of anisotropy is reflected by the cofactors

$$L_{\nu}^{l'l} = (\nu + 1) \int_{0}^{1} d\mu \, \mu^{\nu} P_{l'}(\mu) \, P_{l}(\mu). \qquad (3.4)$$

For l = l' = 0 they have the value unity, so that in this case the matrix elements (3.2) reduce to the $T_{m'm}(\alpha)$ derived for isotropic scattering in Refs. [7, 10]. For $\alpha \ge \alpha^* = 10$, the error caused by neglecting the exponential contribution in (3.2) is at most of the order 10^{-10} . For $\alpha < \alpha^*$ the following series expansion is recommended.

Series Expansions

If the product of the Legendre polynomials is expanded into powers of μ the μ -integral in (3.1) can be expressed in terms of the standard exponential integral $E_{r+1}(2\alpha q)$, the expansion of which near $\alpha = 0$ consists of a power series in α and a logarithmic term. It is given in Ref. [8].

Using this expansion in (3.1) and performing the integration with respect to q we obtain the result

$$T_{m'm}^{l'l}(\alpha) = -2 \sum_{j=j^*}^{\infty} \frac{(-2\alpha)^j}{j(j+2)!} \chi_j^{m'm} L_{-j-1}^{l'l} + D_{m'm}^{l'l}(\alpha), \qquad (3.5)$$

where $j^* = l' + l + 1$ if $m' + m \le l' + l$ and $j^* = 0$ if m' + m > l' + l. The anisotropy coefficients in Eq. (3.5) are defined by

$$L_{-j-1}^{i'l} = \sum_{\substack{r=0\\(r\neq j)}}^{r-i'} \frac{J}{(j-r)r!} \left[\frac{d^r}{d\mu^r} P_{l'}(\mu) P_{l}(\mu) \right]_{\mu=0}.$$
 (3.6)

They are the counterparts to (3.4) for negative powers of μ . Again they reduce to unity for the isotropic case l' = l = 0.

The constants $\chi_j^{m'm}$ are [7]

$$\chi_{j}^{m'm} = \begin{cases} (-)^{m} \prod_{k=1}^{\left|\frac{m'-m}{2}\right|} \frac{(j+3-2k)}{(j+1+2k)} \prod_{l=1}^{\frac{m'+m}{2}} \frac{(j+2-2l)}{(j+2+2l)} & (m'+m = \text{even}), \\ \\ (-)^{m} \prod_{k=1}^{\left|\frac{m'-ml-1}{2}\right|} \frac{(j+2-2k)}{(j+2+2k)} \prod_{l=1}^{\frac{m'+m+1}{2}} \frac{(j+3-2l)}{(j+1+2l)} & (m'+m = \text{odd}). \end{cases}$$

$$(3.7)$$

It turns out that in the case (m' + m) > (l' + l) all contributions $D_{m'm}^{l'l}(\alpha)$ due to the logarithmic singularity in the expansion of the exponential integral vanish identically. This is always true in the case of spherical symmetry described by Eq. (2.13). Hence the matrix elements for the sphere are all regular analytic functions of the optical thickness 2α .

In the case of the slab, Eq. (2.18), also matrix elements with $(m' + m) \leq (l' + l)$ are needed. These elements have a logarithmic singularity near $\alpha = 0$. The logarithmic terms and the first terms of the expansion in α up to $\alpha^{l'+l}$ are evaluated separately and denoted by $D_{m'm}^{l'l}(\alpha)$. These terms satisfy the same symmetry properties as the matrix elements themselves.

For linear anisotropy $(0 \leq l', l \leq 1)$ five different functions $D_{m'm}^{l'l}(\alpha)$ have to be calculated. They are

$$D_{00}^{00}(\alpha) = (3/2) - \gamma - \log(2\alpha), \qquad (3.8a)$$

$$D_{10}^{10}(\alpha) = (1/3) - (\alpha/3)((19/12) - \gamma - \log(2\alpha)), \qquad (3.8b)$$

$$D_{00}^{11}(\alpha) = (1/2) - (2\alpha/3) + (\alpha^2/3)((25/12) - \gamma - \log(2\alpha)), \qquad (3.8c)$$

$$D_{11}^{11}(\alpha) = (2\alpha/15) - (\alpha^2/9)((7/4) - \gamma - \log(2\alpha)), \qquad (3.8d)$$

$$D_{20}^{11}(\alpha) = -(\alpha/15) + (\alpha^2/15)((97/60) - \gamma - \log(2\alpha)).$$
 (3.8e)

where $\gamma = 0.577215 \cdots$ is the Euler-Mascheroni constant.

The Computer Program for the Matrix Elements

For the numerical calculations a computer program for the evaluation of the matrix elements has been developed. This program admits any desired spatial trunction order N (defined as the upper limit for summation with respect to m in the system (2.18)) but is restricted for the time being to linear anisotropy (L = 1).

Extension to a higher degree of anisotropy is straightforward on the basis of the following recurrence relations:

$$(2l+1)[(k+2) T_{mn}^{k+2,l}(\alpha) + (k+1) T_{mn}^{kl}(\alpha)] = (2k+3)[(l+1) T_{mn}^{k+1,l+1}(\alpha) + lT_{mn}^{k+1,l-1}(\alpha)],$$
(3.9)

$$(2m+3)(2n+1)[(k+1) T_{m+1,n}^{k+1,l}(\alpha) + k T_{m+1,n}^{k-1,l}(\alpha)]$$

= $(2n+1)(2k+1) \alpha [T_{m+2,n}^{kl}(\alpha) - T_{mn}^{kl}(\alpha)] + i^{m-n} \delta_{kl}(\delta_{mn} + \delta_{m+2,n})$ (3.10)

 $(\delta_{m,n} = 1 \text{ or } 0 \text{ according to as } m = n \text{ or not})$. All these relations are valid as long as all indices are nonnegative. Equations (3.9) and (3.10) hold also for l = 0 and l' = 0, respectively. In that case they degenerate into a three-term formula for elements at the border of the matrix. Furthermore, due to symmetry properties of (2.14), we find that only the following matrix elements have to be calculated directly: $T_{2m,0}^{00}(\alpha)$; $T_{mm}^{00}(\alpha)$. All other elements can be derived recursively.

The evaluation of the matrix elements for values of $|\alpha| < 10$ is based on the series expansion (3.5) together with Eqs. (3.8a)–(3.8e). For larger α -values the asymptotic approximation, Eq. (3.2) has been used. Numerical experiments on an IBM 360/65 computer using double precision arithmetic have shown that in the range $10 < \alpha < 15$ the results of both Eqs. (3.2) and (3.5) coincide within six significant digits.

The form of the coefficients $\chi_j^{m'm}$, Eqs. (3.7), is very convenient for numerical computations since each coefficient can be calculated from one with a lower index by multiplication with a certain number.

4. Solutions in the Physical Space

1. Slab

Once that $F(B, \mu)$, Eq. (2.17), is known in terms of the solutions of the linear system the angular flux distribution $\psi(x, \mu)$ is obtained by Fourier inversion. Introducing the uncollided angular flux $\psi_s(x, \mu)$ due to the particles originating directly from the source, which is equal to the Fourier inverse of $Q(B, \mu)$, and the distributions functions

$$G_n\left(\frac{x}{a},\frac{\mu}{\alpha}\right) = (-i)^n \frac{\alpha}{\pi} \int_{-\infty}^{+\infty} dB(\Sigma_t + iB\mu)^{-1} \exp(iBx) j_n(aB), \qquad (4.1)$$

we can write

$$\psi(x,\mu) = \psi_s(x,\mu) + \sum_{l=0}^{L} (2l+1) \frac{\sum_{s,l}}{\sum_t} \sum_{m=0}^{\infty} (2m+1) X_m^l P_l(\mu) G_m\left(\frac{x}{a},\frac{\mu}{\alpha}\right). \quad (4.2)$$

For appropriate source distributions the uncollided flux can be calculated analytically.

The G_n are real and obey the following reciprocity relation

$$G_n\left(\frac{x}{a}, -\frac{\mu}{\alpha}\right) = (-)^n G_n\left(-\frac{x}{a}, \frac{\mu}{\alpha}\right)$$
(4.3)

They individually satisfy the exact slab boundary conditions (i.e., no incoming angular flux at the boundaries):

$$G_n\left(1,\frac{\mu}{\alpha}\right)=0$$
 for $x=a, \mu<0,$ (4.4a)

$$G_n\left(-1,\frac{\mu}{\alpha}\right)=0$$
 for $x=-a, \ \mu>0.$ (4.4b)

Statements (4.4) are based on the fact that for x = a the integrand in (4.1) is regular in the upper half plane. For $\mu < 0$ the only singularity originating of the denominator lies in the lower half plane. The path of integration can be closed in the upper half plane, hence the integral is zero. The validity of (4.4b) is a consequence of (4.4a) and the reciprocity relation (4.3).

The functions (4.1) can be evaluated analytically. We find under the condition $\mu > 0$:

$$G_n\left(\frac{x}{a},\frac{\mu}{\alpha}\right) = (-)^n \sum_{j=0}^n \frac{(n+j)!}{j! (n-j)!} \left(\frac{\mu}{2\alpha}\right)^j \left[Z_j\left(\frac{x}{a},\frac{\mu}{\alpha}\right) - \exp\left(-\frac{\alpha}{\mu}\left(1+\frac{x}{a}\right)\right)\right]$$
(4.5)

where

$$Z_{j}\left(\frac{x}{a},\frac{\mu}{\alpha}\right) = \sum_{k=0}^{j} \frac{1}{k!} \left[-\frac{\alpha}{\mu}\left(1+\frac{x}{a}\right)\right]^{k}$$
(4.5a)

2. Sphere

The Fourier inversion of Eq. (2.5) leads to the following representation for the angular flux

$$\psi(r,\mu) = \sum_{k=0}^{\infty} (k+\frac{1}{2}) P_k(\mu) \psi_k(r), \qquad (4.6)$$

where

$$\psi_k(r) = \sqrt{\frac{2}{\pi}} i^k \int_0^\infty dB \ B^2 j_k(Br) \int_{-1}^{+1} d\eta \ P_k(\eta) \ F(B, \eta)$$
(4.7)

and $F(B, \eta)$ is given by Eq. (2.12).

In contrast to the situation for the slab the expression (4.7) for the sphere is hardly amenable to analytical evaluation. Owing to the theorems of the following section we are not forced to evaluate the distributions (4.7) if we only want to know the distribution of the angle-integrated flux, which is of primary interest in reactor physics.

5. The $P_K - SP_N$ Approximation

Whereas the analytical representations (4.2) or (4.6) are more of principal interest, the approximations stated by the following theorems are of practical importance and of surprising computational simplicity.

THEOREM I. The angular flux distribution $\psi(x, \mu)$ inside the slab can be approximated (in the mean!) by the double Legendre polynomial expansion with respect to the angle and the space variable $(P_K - SP_N \text{ approximation})$

$$\psi(x,\mu) = \lim_{\substack{k \to \infty \\ N \to \infty}} \sum_{k=0}^{k} (2k+1) \sum_{n=0}^{N} (2n+1) X_{n}^{k} P_{k}(\mu) P_{n} \left(\frac{x}{a}\right).$$
(5.1)

The X_n^k is just the solution vector of the linear system (2.18).

Proof. Using the orthogonality properties of the Legendre polynomials, the expansion coefficients in (5.1) satisfy $(\xi \equiv x/a)$

$$X_{m'}^{l'} = \frac{1}{4} \int_{-1}^{+1} d\xi \ P_{m'}(\xi) \int_{-1}^{+1} d\mu \ P_{l'}(\mu) \ \psi(x,\mu).$$
 (5.2)

If we substitute for $\psi(x, \mu)$ the expression (4.2), we obtain on the r.h.s. two contributions. Due to the interconnection between Legendre polynomials and spherical Bessel functions [3] which plays here a fundamental role, the second contribution reproduces the term $T_{m'm}^{l'l}(\alpha)$. In a similar way the contribution of the uncollided flux $\psi_s(x, \mu)$ results in the source vector $Q_m^{l'}$ introduced earlier. Hence the coefficients $X_{m'}^{l'}$ of the expansion (5.1) indeed satisfy the linear system (2.18)

Of great importance for practical problems is the knowledge of the "angleintegrated flux," defined by $\psi_0(r)$ in the sense of Eq. (2.3). For the slab, it is given by

$$\psi_0(x) = \lim_{N \to \infty} \sum_{n=0}^{N} (4n + 2) X_n^0 P_n\left(\frac{x}{a}\right).$$
 (5.3)

In the case of the sphere a P_{K} -SP_N expansion for the angular flux similar

to (5.1) could not be found. For the angle-integrated flux $\psi_0(r)$, however, an analog to the result (5.3) can be established by the following

THEOREM II. The flux distribution $\psi_0(r)$ in the sphere can be approximated (in the mean) in the P_0 -SP_N approximation by

$$\psi_0(r) = \frac{4}{r} \lim_{N \to \infty} \sum_{n=1,3,5,\dots}^N (2n+1) X_n^0 P_n\left(\frac{r}{a}\right), \qquad (5.4)$$

where X_n^0 satisfies the linear system (2.13) with l' = 0.

The proof of Theorem II is step by step completely the same as for Theorem I. Since the Legendre polynomials $P_k(\mu)$ and $P_n(x/a)$ are easily generated on a computer up to arbitrary high degrees K and N the complete solution of the transport integral equation is given by Eqs. (5.1) and (5.3) in the plane case and by Eq. (5.4) in the case of the sphere, provided the coefficients X_n^k have been obtained solving the linear systems (2.18) and (2.13).

6. NUMERICAL RESULTS

For illustration we give here some numerical examples. We consider neutron transport in a bare homogeneous sphere. Since the main purpose of the paper is to show the essentials and the usefulness of our method rather than the solution of a physical problem, we restrict our considerations to monoenergetic neutrons and linear anisotropic scattering.

The scattering kernel in this case reads

$$\Sigma_{s}(\mathbf{\Omega}' \to \mathbf{\Omega}) = \frac{\Sigma_{s,0}}{4\pi} (1 + 3\bar{\mu}\cos\Theta), \tag{6.1}$$

where $\bar{\mu} = \Sigma_{s,1}/\Sigma_{s,0}$ is the average cosine of the scattering angle. Since by physical reasons the scattering probability (6.1) must not be negative, we have the restriction $|\bar{\mu}| \leq 1/3$.

As an example we have determined for a sphere the eigenvalue $c = \sum_{s,0} / \sum_t$ (the mean number of secondaries per collision necessary to maintain criticality) as a function of $\overline{\mu}$ and α . The value c was obtained iteratively from Rayleigh quotients, except for $\alpha = 100$, where the characteristic polynomial has been constructed and solved numerically. For large α , all eigenvalues tend to unity and may thus not be well separated by the iterative method.

In Table I we present the result of our computations. These six digit values were all obtained for N = 3 only. They are final and do not change if N = 6 is taken. The computing time on the IBM 360/65 is about a second in any case.

TABLE I

Number of secondary particles (c) per collision required to maintain criticality as a function of the sphere radius. a (measured in mean free paths) for different average cosines ($\bar{\mu}$) of the scattering angle (case of linear anisotropic scattering).

	/3	33	387 8 7	ر م ا	999 65 71	977 88 89	0483 0486
μ	+	15.873 18.86 18.96	3.723 4.398 4.410	2.22	1.12 1.20 1.20	1.03 1.06 1.06	1.00 1.00
	+0,3	14.7096 16.17 16.25	3.49282 3.831 3.846	2.11385 2.301 2.308	1.11354 1.1497 1.1501	1.03411 1.0471 1.0471	1.000404 1.000405
	+0,1	14.0153 14.61 14.68	3.35442 3.497 3.510	2.04596 2.126 2.132	1.10385 1.1190 1.1193	1.03084 1.0361 1.0361	1.000360 1.000360
	0 Ref. [15]	13,42	3,237	1,988	1,095	1,028	
	0+	13.4286 13.32 13.39	2.23718 2.219 2.230	1.98839 1.981 1.986	1.09576 1.0955 1.0957	1.02815 1.0281 1.0282	1.000324 1.000324
	-0,1	12.9237 12.24 12.30	3.13605 2.983 2.993	1.93871 1.859 1.862	1.08890 1.0775 1.0776	1.02590 1.0223 1.0223	1.000295 1.000295
	-0,2	12.4825 11.32 11.37	3.04755 2.781 2.790	1.89524 1.754 1.758	1.08299 1.0634 1.0635	1.02398 1.0178 1.0179	1.000271 1.000270
	-1/3	11.9718 10.28 10.33	2.94495 2.553 2.560	1.84486 1.638 1.641	1.07628 1.0493 1.0493	1.02184 1.0136 1.0136	1.000244 1.000244
	ષ્ઠ	0,1	0,5	1,0	5,0	10,0	100,0
	Method	$^{\rm IT}_{\rm N_s}$	IT _N S _i	$_{S_8}^{IIT_N}$	IT _N S ₈ S ₁₆	IT_N S_8 S_{16}	IT _N Asympt. Ref. [11]

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The value of c depends weakly, and almost linearly, on the anisotropy parameter $\bar{\mu}$. Clearly, for backward scattering ($\bar{\mu} < 0$), c is smaller than for forward scattering ($\bar{\mu} > 0$).

The agreement with S_8 or S_{16} reference calculations performed with the code DTF-IV [12] using 50 space points is satisfactory for small anisotropy values $\bar{\mu}$. For $|\bar{\mu}| = 1/3$ the difference between the two methods is remarkable. As compared to IT_N the DTF-IV version of the S_N approximation overestimates the dependence of c on $\bar{\mu}$. From asymptotic theory [11] it is easily deduced that the quantity (1 - 1/c) is proportional to $(1 - \bar{\mu})^{-1}$. More precisely,

$$(1 - 1/c)_{\bar{\mu} = 1/3}/(1 - 1/c)_{\bar{\mu} = -1/3} = 2 + O(\alpha^{-2}).$$
(6.2)

For $\alpha = 10$ this ratio amounts to 1.8 for IT_N but to 4.8 for S_{16} . Hence there is a strong indication that the IT_N results are the more accurate ones. We note the full agreement with the results of Kiesewetter *et al.* [15] which, however, are confined to isotropy only.

It should be emphasized that due to the regular analytical behavior of the matrix elements for the sphere near $\alpha = 0$ the system (2.13) has still solutions in the case of negative values of α . They are meaningful in time dependent problems.

If we look for the asymptotic behavior of a source-free pulsed neutron distribution decaying exponentially in time with a rate λ , it has been shown [10] that the amplitude satisfies an integral equation identical to Eq. (2.1) without source term, except that the total cross section Σ_t has to be replaced by $(\Sigma_t - \lambda/v)$, v being the speed of the monoenergetic neutrons. We are faced with an implicit eigenvalue problem for the decay rate λ . We note that α is then no longer the "optical half thickness" $a\Sigma_t$ of the sphere but has the form

$$\alpha = a\Sigma_t [1 - (\lambda/v\Sigma_t)]. \tag{6.3}$$

For sufficiently small spheres the decay constant may be so large that α defined by Eq. (6.3) becomes negative. In Table II the fundamental decay constant $(\lambda/v\Sigma_t)$ is calculated as a function of α for different parameters $\bar{\mu}$. In order to obtain the radius $(a\Sigma_t)$ of the sphere (measured in mean free paths) we have to divide the α values in the first column of Table II by the corresponding factor $(1 - \lambda/v\Sigma_t)$. Thus, for instance, the decay constant is 1.0936 for a sphere of radius (-0.1): (1 - 1.0936) = 1.068 mean free paths.

The decay rate is strongly influenced by the preferential direction $(\bar{\mu})$ of the scattering. As can be deduced from Table II preferential backward scattering $(\bar{\mu} < 0)$ tends to diminish the decay rate whereas forward biased scattering tends to increase it. In the limit of thick spheres $(\alpha \gg 1)$ we find $\lambda(\bar{\mu} = 1/3)/\lambda(\bar{\mu} = -1/3) = 2$.

TABLE II

Fundamental decay constant $(\lambda/v\Sigma_t)$ for a uniform sphere as a function of the parameter α , Eq. (6.3), for different average cosines $\bar{\mu}$ of the scattering angle in the case of linear anisotropic scattering

α	μ											
	-1/3	-0, 2	-0, 1	\pm 0	+0, 1	+0, 2	+1/3					
-1.0	2.7288	2.6082	2.5151	2.4192	2.3202	2.2172	2.0727					
-0.1	1.0936	1.0894	1.0860	1.0825	1.0787	1.0746	1.0686					
+0.1	0.9165	0.9199	0.9262	0.9255	0.9286	0.9320	0.9370					
+1.0	0.4580	0.4724	0.4842	0.4971	0.5112	0.5269	0.5510					
+10.0	0.02137	0.02342	0.02524	0.02738	0.02992	0.03298	0.03824					
+100.0	0.000244	0.000271	0.000295	0.000324	0.000360	0.000404	0.000483					
Asymptot. Ref. [11]	0.000244	0.000270	0.000295	0.000324	0.000360	0.000405	0.000468					

This result is in full agreement with asymptotic transport theory where the decay rate for large systems is given by [11]

$$\lambda \sim (vB^2/3\Sigma_t)(1-\bar{\mu})^{-1}.$$
 (6.4)

Here the "buckling" B^2 is connected with the radius by $B = \pi(a + \delta)^{-1}$. The "extrapolation distance" δ used to calculate the asymptotic values of Tables I and II is that of the half-infinite space, namely, $\delta = 0.710$ m.f.p. Although the IT_N approximation has its merits (high accuracy for low order N) mainly for the solution of transport problems in small systems, it shows also the correct asymptotic behavior for large systems.

CONCLUDING REMARKS

The main restriction to the present IT-approach is imposed by the geometry. Apart from plane and spherical systems that can be treated simultaneously, it is also possible to solve analytically transport problems in cylinders or layered slabs. For more general geometrical configurations, the explicit determination of the matrix elements may become a very difficult task or even be impossible to do analytically. In this case an essential advantage of the IT approach will be lost.

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Energy exchange due to the interaction of the particles with matter can be taken into account in a straightforward way. Then the matrix elements of the linear systems have two more indices, characterizing the transition between any two energy groups.

APPENDIX

A. Proof of Lemma 1

Denoting the cosine between **B** and **r** by τ , we use the following addition theorem:

$$\exp(-i\mathbf{B}\cdot\mathbf{r}) = \sum_{n=0}^{\infty} (-i)^n (2n+1) j_n(Br) P_n(\tau)$$
(A1)

("decomposition of a plane wave into spherical waves" [3, p. 440]). The $j_n(x)$ are the spherical Bessel functions [3]. We relate the vectors **B** and **r** to the fixed axis Ω with $\cos(\mathbf{B}, \Omega) = \eta$, $\cos(\mathbf{r}, \Omega) = \mu$ and denote the azimuthal angle between the planes (**B**, Ω) and (**r**, Ω) by φ . Applying the addition theorem for spherical harmonics [2] to $P_n(\tau)$ and performing the azimuthal integration over φ from 0 to 2π all terms except $P_n(\eta) P_n(\mu)$ cancel out, the latter being multiplied by 2π . Hence Lemma 1, Eq. (2.6), is immediate.

B. Proof of Lemma 2

According to a result [3, p. 484] for the integration of a product of Bessel functions, the integral (2.10) defining the partial kernel $K_l(B', B)$ can be written as

$$K_{l} = \frac{a^{3}}{\beta^{\prime 2} - \beta^{2}} \left[\beta^{\prime} j_{l+1}(\beta^{\prime}) j_{l}(\beta) - \beta j_{l+1}(\beta) j_{l}(\beta^{\prime})\right],$$
(B1)

where $\beta = aB$ and $\beta' = aB'$. We suppose $\beta \neq \beta'$.

Using twice the recurrence relation [3, p. 439] for spherical Bessel functions in the bracket of (B1) we obtain a new recurrance relation for the K_i themselves:

$$K_{l} = a^{3}(\beta'\beta)^{-1} (2l+3) j_{l+1}(\beta') j_{l+1}(\beta) + K_{l+2}.$$
(B2)

We may write down Eq. (B2) for l replaced by (l + 2), (l + 4),..., (l + 2N + 2) and add. We obtain

$$K_{l} - a^{3}(\beta'\beta)^{-1} \sum_{n=0}^{N} (2l + 4n + 3) j_{2n+l+1}(\beta') j_{2n+l+1}(\beta) = K_{2N+l+2}.$$
 (B3)

The remainder term on the r.h.s. can be estimated in the following way: From the integral representation of Bessel functions [3, p. 438] and an estimation for the Legendre polynomials [3, p. 786], we have for all real x and n

$$|j_n(x)| \leq \frac{1}{2} \left| \int_0^{\pi} P_n(\cos \Theta) \sin \Theta \, d\Theta \right| \leq \sqrt{2/\pi n}. \tag{B4}$$

Hence K_{l+2N+2} vanishes like N^{-1} for $N \to \infty$. Performing the limit $N \to \infty$, we obtain directly the relation which constitutes Lemma 2. The case $\beta = \beta'$ is already known [3, p. 484] and again confirms Lemma 2.

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