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A NEW CONCEPT FOR DEEP-PENETRATION TRANSPORT CALCULATIONS AND TWO NEW FORMS OF THE NEUTRON TRANSPORT EQUATION

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ABSTRACT

A new concept to solve radiation transport problems is developed bypassing the solution of the Boltzmann equation. A distribution function ψ is defined as the product of the conventional neutron flux and adjoint distributions. Two equations, one complex and linear, the other real and nonlinear are derived for ψ. A conservation law for ψ is established and a physical interpretation given for ψ as a flux distribution for a limited number of source particles which will necessarily contribute to the integral response of interest. The linear but complex form of the transport equation is solved analytically for a sample case of a pure absorber in slab geometry.

I. INTRODUCTION

It is well known[1] that neutron transport problems, as described by the linear Boltzmann equation, can be formulated in a "forward" or an "adjoint" mode; both formulations being equivalent. Using the nomenclature of Ref. 1 we have

$$L\phi = Q, \tag{1}$$

with

$$I = <R,\phi>, \tag{2}$$

as the forward formulation. L denotes the linear time-independent Boltzmann transport operator, $\phi \equiv \phi(\underline{r}, \underline{\Omega}, E)$ is the angular flux distribution, $Q \equiv Q(\underline{r}, \underline{\Omega}, E)$

is a given neutron source distribution, $R \equiv R(\underline{r}, \underline{\Omega}, E)$ is a given response function, and I is an integral effect of interest (response), where the symbol $<,>$ indicates integrations over the common domains of all independent variables $\underline{r}$ (position), $\underline{\Omega}$ (direction), and E (energy). The sole objective in most practical radiation transport applications is the calculation of I when Q and R are given. Fully equivalent is the adjoint formulation

$$L^{+}\phi^{+} = R, \tag{3}$$

with

$$I = <Q,\phi^{+}>, \tag{4}$$

where the adjoint source-term is chosen to be the response function R, and $\phi^{+} \equiv \phi^{+}(\underline{r}, \underline{\Omega}, E)$ is the adjoint angular flux. The adjoint transport operator L^{+} is defined by[1]

$$<\phi^{+}, L\phi> = <L^{+}\phi^{+},\phi>, \tag{4a}$$

and it is assumed that the boundary conditions on ϕ and ϕ^{+} are such that Eq. (4a) is satisfied.

It is clear from the above formulations, that in order to calculate I one must know either ϕ or ϕ^{+}, hence, solve either Eq. (1) or Eq. (3). In particular, in deep penetration or shielding type calculations, the spatial distance between the neutron source (Q) and the detector (R) may be very large in terms of mean-free paths of the source neutrons. Since the neutron flux at the detector position is needed to evaluate I from Eq. (2), the usual procedure in solving Eq. (1) is to calculate the entire flux distributions $\phi(\underline{r}, \underline{\Omega}, E)$ at <u>all</u> locations $\underline{r}$ in the system although it is needed only at the detector location. The calculation of ϕ at locations $\underline{r}$ between the source and detector locations seems to be an intrinsic requirement to obtain the needed ϕ at positions where $R \neq 0$. However, the calculation of ϕ at all locations except the detector location could be considered a waste of effort if it were not intrinsically required. It is intriguing that so much wasted information must be generated in order to calculate the one number of interest, I. The same, of course, is true for the adjoint formulation where the actual computation of ϕ^+ at the source location must proceed step by step starting at the detector location.

In sensitivity calculations using variational methods, e.g., Ref. 2, the product of $\phi \cdot \phi^+$ is used which seems to be an even larger waste of information and effort since ϕ and ϕ^+ must both be calculated although each one of them separately contains all the information ever needed for most radiation transport analyses. It is admitted, however, that such variational methods produce more useful information than just the value of I. Nevertheless, the question arises: why not calculate the product $\psi = \phi\phi^+$ directly? Additional incentive to calculate ψ directly is obtained by a very interesting analytic property of ψ which will also provide the connection with our original problem of calculating I.

II. A CONSERVATION LAW FOR $\psi = \phi\phi^+$

Let us rewrite Eqs. (1) and (3) for a purely absorbing medium (Σ is the macroscopic absorption cross section):

$$\underline{\Omega}\cdot\underline{\nabla}\phi + \Sigma\phi = Q, \tag{5}$$

$$-\underline{\Omega}\cdot\underline{\nabla}\phi^+ + \Sigma\phi^+ = R. \tag{6}$$

Multiplying Eq. (5) with ϕ^+ (from left) and Eq. (6) with ϕ(from left), and subtracting the second from the first equation gives

$$\phi^+(\underline{\Omega}\cdot\underline{\nabla}\phi) + \phi(\underline{\Omega}\cdot\underline{\nabla}\phi^+) = Q\phi^+ - R\phi. \tag{7}$$

Since $\underline{\Omega}\cdot\underline{\nabla}\phi = \underline{\nabla}\cdot\underline{\Omega}\phi$, the two terms on the left side of Eq. (7) can be combined to $\underline{\nabla}\cdot\underline{\Omega}\phi\phi^+ \equiv \underline{\nabla}\cdot\underline{\Omega}\psi$ which is the "divergence operator" ($\underline{\nabla}\equiv$div) acting on the vector field $\underline{\Omega}\psi$:

$$\mathrm{div}(\underline{\Omega}\psi) = Q\phi^+ - R\phi. \tag{8}$$

Now we consider three different volume integrals of Eq. (8), keeping in mind that each volume integral can be translated into an equivalent surface integral by Gauss's theorem[3]

$$\int \mathrm{div}(\underline{\Omega}\cdot\psi)\,dV \equiv \oint_F (\underline{n}\cdot\underline{\Omega})\psi dF, \tag{9}$$

where dF is a surface element on the volume V and $\underline{n}$ is a normal vector on F pointing outward from the volume V.

1. Integrating Eq. (8) over a volume V_R which includes the detector location but not the source location (see Fig. 1) yields for the left side of Eq. (8)

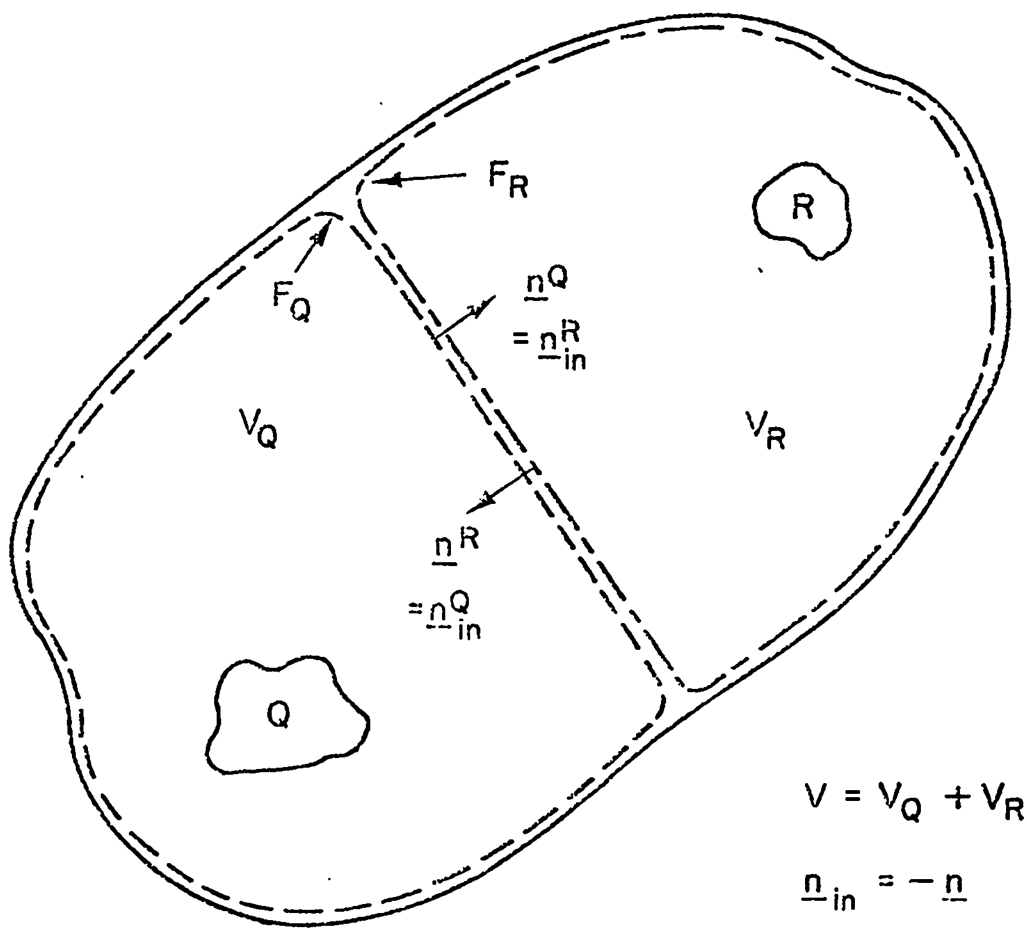

Fig. 1. Subdivision of the systems volume V.

$$\int_{V_R} \operatorname{div}(\underline{\Omega}\psi)\,dV = \oint_{F_R} (\underline{n}^R \cdot \underline{\Omega})\,\psi\; dF$$

$$= -\oint_{F_R} (\underline{n}^R_{in} \cdot \underline{\Omega})\,\psi\; dF, \tag{9a}$$

where $\underline{n}^R_{in} = -\,\underline{n}^R$ is the inward normal vector on F_R. The integral over the first term on the right side of Eq. (8) vanishes since the volume V_R was chosen so that $Q \equiv 0$ in V_R. The integral over the second term on the right side of Eq. (8) resembles Eq. (2) if we also integrate over all angles $\underline{\Omega}$ and all energies E. Therefore, integrating Eq. (8) over the volume V_R, all angles and energies, yields

$$I = \int_{-\infty}^{+\infty} \int_{(4\pi)} \oint_{F_R} (\underline{n}^R_{in} \cdot \underline{\Omega})\;\; \psi(\underline{r},\, \underline{\Omega},\, E)\;\, dF\; d^2\underline{\Omega}\; dE. \tag{10}$$

Hence, the effect of interest (response) I can be calculated from $\psi = \phi\phi^+$ directly by integrating the net inward current of the vector flux $\underline{\Omega}\cdot\psi$ over any surface F_R enclosing the detector, and also integrating over all angles and energies.

2. Similarly, integrating Eq. (8) over any volume V_Q which includes the neutron source but not the detector, we obtain

$$I = \int_{-\infty}^{+\infty} \int_{(4\pi)} \oint_{F_Q} (\underline{n}^Q \cdot \underline{\Omega})\;\; \psi(\underline{r},\, \underline{\Omega},\, E)\;\, dF\; d^2\underline{\Omega}\; dE, \tag{11}$$

where n^Q is the outward normal vector on the surface F_Q enclosing the volume V_Q.

3. Integration over the entire system V, including both source and detector, gives

$$\int_V \mathrm{div}(\underline{\Omega}\psi)\, dV = 0. \tag{12}$$

If ψ is interpreted as a particle flux, namely an importance weighted neutron flux $\phi^+\phi$, then Eqs. (10) through (12) allow very meaningful conclusions:

a. From Eq. (12) follows that the system never loses any ψ-particles; a conservation law for ψ.

b. From Eqs. (10) and (11) follows that the integral response I is given by summing up the net current of all ψ-particles which either enter any closed surface F_R around the detector or leave any closed surface F_Q around the source.

The above technique was derived from Ref. 4; the results are, therefore, probably not new. But the above interpretations are intriguing enough to formulate a new concept for the solution of deep-penetration transport problems with fixed sources. The idea is to establish an equation for ψ and then calculate I either from Eq. (10) or Eq. (11). From these equations follows that the distribution function $\psi(\underline{r}, \underline{\Omega}, E)$ contains the necessary and sufficient information to calculate I. The neutron distribution $\phi(\underline{r}, \underline{\Omega}, E)$ at any given point $\underline{r}$ outside the detector region gives information on all neutrons which traveled from the source to $\underline{r}$, disregarding whether these neutrons will ever reach the detector position or not; this is too much information if one only wants to calculate I. The distribution $\psi(\underline{r}, \underline{\Omega}, E)$, however, gives at any point $\underline{r}$ information only on those "ψ-particles" which will certainly contribute to the response I. Intuitively this interpretation for ψ may be obvious from its definition as an importance weighted neutron flux distribution $\phi^+\phi$. To calculate I from Eq. (10) or Eq. (11) it is sufficient to know $\psi(\underline{r}, \underline{\Omega}, E)$ only at any closed surface encompassing either R or Q. A graphical display of the multidimensional function $\psi(\underline{r}, \underline{\Omega}, E)$ can immediately identify radiation streaming effects of significance for the special problem under consideration: peaks in the spatial distribution of ψ will point to spatial streaming paths (heterogeneity effects), peaks in the energy distribution of ψ identify spectral streaming (e.g., due to cross-section minima), and peaks in the angular distribution will occur in directions which are of greatest importance to the problem.

III. DERIVATION OF THE ψ-EQUATIONS

In the following we restrict ourselves to the monoenergetic transport equation and for algebraic simplicity we consider only slab geometry with isotropic scattering. Equations (1) and (3) take then the form[1]

$$\mu \frac{\partial \phi(x,\mu)}{\partial x} + \Sigma \phi(x,\mu) = \frac{c}{2}\int_{-1}^{+1} \phi(x,\mu')\, d\mu' + Q, \tag{13}$$

$$-\mu \frac{\partial \phi^+(x,\mu)}{\partial x} + \Sigma \phi^+(x,\mu) = \frac{c}{2}\int_{-1}^{+1} \phi^+(x,\mu')\, d\mu' + R. \tag{14}$$

Since we want to derive an equation for $\phi\phi^+$ we define a complex flux distribution

$$\Psi(x,\mu) = \phi(x,\mu) + i\phi^+(x,\mu), \tag{15}$$

with $i = \sqrt{-1}$, then our unknown product $\psi = \phi\phi^+$ can be derived from Ψ as one-half of the imaginary part of Ψ^2:

$$\psi(x,\mu) \equiv \phi\phi^+ = \frac{1}{2}\, Im\, \Psi^2. \tag{16}$$

By summing and subtracting Eq. (13) and i-times Eq. (14) we obtain a coupled set of two equations for Ψ and its conjugate complex, Ψ^*:

$$\mu \frac{\partial \Psi^*}{\partial x} + \Sigma \Psi = \frac{c}{2}\int_{-1}^{+1} \Psi\, d\mu' + (Q + iR), \tag{17}$$

$$\mu \frac{\partial \Psi}{\partial x} + \Sigma \Psi^* = \frac{c}{2}\int_{-1}^{+1} \Psi^*\, d\mu' + (Q - iR). \tag{18}$$

To simplify further analysis we define a complex source term

$$S = Q + iR, \tag{19}$$

and assume for the following that the given functions Q and R are constants with respect to x and μ; also, Σ and c are assumed constants. Now we differentiate Eq. (18) with respect to x and obtain

$$\mu \frac{\partial^2 \Psi}{\partial x^2} + \Sigma \frac{\partial \Psi^*}{\partial x} = \frac{c}{2} \int_{-1}^{+1} \frac{\partial \Psi^*}{\partial x} d\mu' . \tag{20}$$

Eliminating $\partial\Psi^*/\partial x$ from Eq. (20) by using Eq. (17), gives the desired equation for Ψ:

$$- \mu^2 \frac{\partial^2 \Psi(x,\mu)}{\partial x^2} + \Sigma^2 \Psi(x,\mu) = (\Sigma - c\mu)S + \frac{c}{2} \mu \int_{-1}^{+1} \cdot \left[\frac{\Sigma}{\mu'} \Psi(x,\mu') - \frac{c}{2\mu'} \int_{-1}^{+1} \Psi(x,\mu'') \, d\mu''\right] d\mu' . \tag{21}$$

The left side of this equation, for the real part of Ψ, $\mathcal{Re}\,\Psi \equiv \phi$, has been derived earlier by other authors, e.g., Ref. 5, and is identified as the self-adjoint second-order derivative part of the nonself-adjoint first-order derivative portion of the original transport operator. It is interesting to note that Eq. (21) is valid for the complex function Ψ containing information on ϕ as well as ϕ^+.

Now, since $\Psi = \phi + i\phi^+$ does not give the desired product $\psi = \phi\phi^+$ directly, Eq. (16) must be applied to calculate it. Then the response I can be calculated via Eq. (10) or Eq. (11) which in slab geometry reduce to

$$I = \int_{-\infty}^{\infty} \int_{0}^{1} \mu\psi(x,\mu) \, \delta(x - x_S) \, d\mu dx, \tag{22}$$

where x_s is any space point separating source and detector. Location x_s can be thought of as an infinite plane between source and detector which closes to a full surface at infinity.

Since the new transport equation, Eq. (21), is an equation for the complex variable $\Psi = \phi + i\phi^+$, it actually represents two equations, one for the real part of Ψ, $Re\ \Psi = \phi$, and one for the imaginary part of Ψ, $Im\ \Psi = \phi^+$. In principle it must be possible, therefore, to derive from these two equations (through elimination processes) one equation for the product $\psi = \phi\phi^+$, which was our original goal. Rather than starting from Eq. (21), we may also start with the original Boltzmann Eqs. (13) and (14) to derive an equation for $\psi = \phi\phi^*$. For simplicity we chose c = 0, the case of a purely absorbing medium and follow the latter approach. The equation we obtain for ψ [a real function, not to be confused with the complex function Ψ of Eq. (21)] is nonlinear and takes the form

$$\mu^4 \left(\frac{\partial^2\psi}{\partial x^2}\right)^2 + 4\mu^2 QR \frac{\partial^2\psi}{\partial x^2} - \mu^2\Sigma^2 \left(\frac{\partial\psi}{\partial x}\right)^2 - 4\Sigma^2 QR\psi + 4Q^2R^2 = 0. \tag{23}$$

The fact that this equation is nonlinear follows from the process of elimination and substitution when Eq. (23) is derived from Eqs. (13) and (14). In this process, it was necessary to once differentiate and square the entire equation.

Intuitively, the process in deriving Eq. (21) and Eq. (23) from the Boltzmann Eqs. (13) and (14) can be viewed as a process of continuously reducing the information content of the equations. To obtain Eq. (21) a differentiation with respect to x was required which is always a loss of information. As Pomraning and Clark[5] point out, the second-order form of the transport equation is not consistent anymore with the continuity equation of classical diffusion theory since this information is lost by differentiation. Hence, Eq. (21) contains less information than Eqs. (13) and (14). Similarly, the additional "squaring-process" required to derive Eq. (23) indicates that this equation contains even less information than Eq. (21). However, such an information reduction process was exactly what we had originally intended. Since Eq. (23) describes the behavior of "ψ-particles" rather than neutrons, it is not surprising that neutron continuity conditions and neutron conservation conditions may be lost. We gained, however, the very simple and basic conservation law for ψ described in the previous section.

IV. A SAMPLE CALCULATION

To demonstrate the new concept and the applicability of the ψ-equations to deep-penetration fixed-source transport problems we chose a simple example for which the Boltzmann equation can be solved analytically exact: a point source at $x = 0$ with a point detector at $x = a$ in an infinite, purely absorbing medium, in slab geometry. To further simplify the example, we allow neutrons to travel only in one direction, $\mu = 1$. Then the forward and adjoint formulations of the Boltzmann equation describe the problem as follows (source and detector are normalized to 1.0; compare Fig. 2).

<u>Forward formulation:</u>

$$\left.\begin{aligned}
&\frac{d\phi(x)}{dx} + \Sigma\phi(x) = \delta(x), \\
&\text{with the boundary condition } \phi(0) = 1. \text{ The solution is: } \phi(x) = e^{-\Sigma x}, \\
&I = \langle R,\phi\rangle, \text{ with } R = \delta(x - a), \\
&\quad = \int_{-\infty}^{+\infty} e^{-\Sigma x}\,\delta(x - a)\,dx, = e^{-\Sigma a}\,.
\end{aligned}\right\} \quad (24)$$

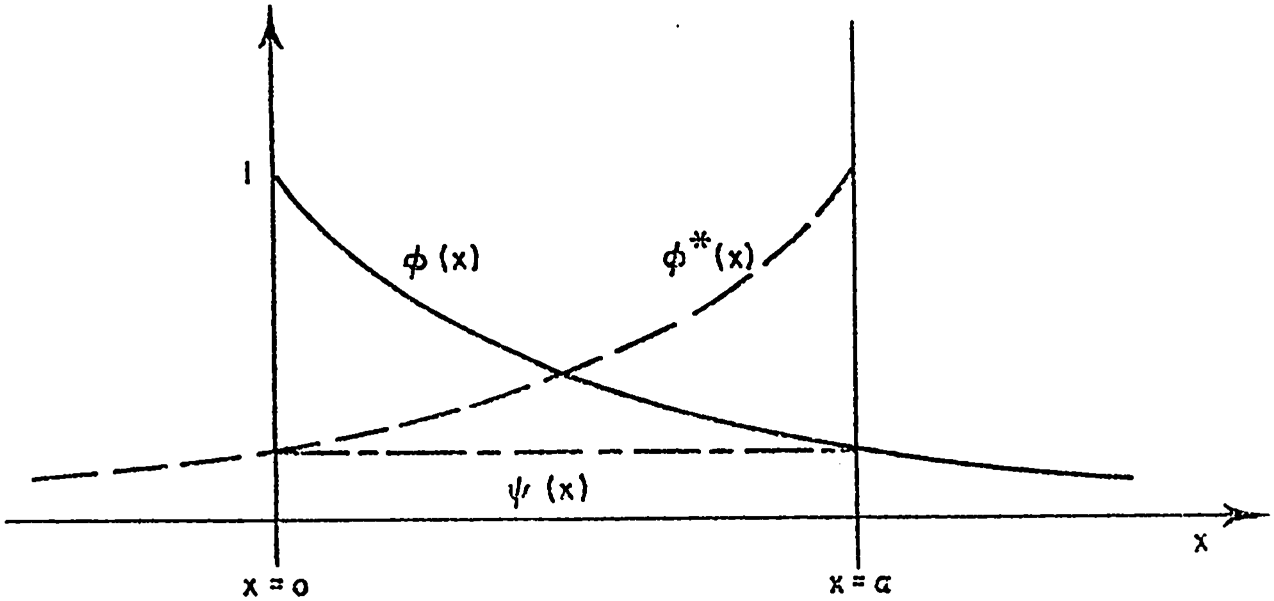

Fig. 2. Flux, adjoint, and ψ-distribution for sample problem with $Q = \delta(x)$ and $R = \delta(x-a)$.

Adjoint formulation:

$$\left.\begin{aligned}
&-\frac{d\phi^+(x)}{dx} + \Sigma\phi^+(x) = \delta(x-a), \\
&\text{with the boundary condition } \phi^+(a) = 1. \text{ The solution is: } \phi^+(x) = e^{\Sigma(x-a)}, \\
&I = \langle Q, \phi^+\rangle, \text{ with } Q = \delta(x), \\
&\quad = e^{-\Sigma a}.
\end{aligned}\right\} \quad (25)$$

Now, to exercise the new concept in calculating I we must either solve Eq. (23) for $\mu = 1$ and then perform integral (22):

$$\left.\begin{aligned}
&(\psi'')^2 + 4\delta(x)\delta(x-a)\psi'' - \Sigma^2(\psi')^2 - 4\Sigma^2\delta(x)\delta(x-a)\psi + 4\delta^2(x)\,\delta^2(x-a) = 0, \\
&I = \int_{-\infty}^{+\infty} \psi(x)\,\delta(x-x_s)\,dx = \psi(x_s);\ 0 < x_s < a,
\end{aligned}\right\} \quad (26)$$

or solve Eq. (21) for $c = 0$, $\mu = 1$, and exercise Eq. (16) and Eq. (22):

$$\left.\begin{aligned}
-\Psi'' + \Sigma^2\Psi &= \Sigma S \\
&= \Sigma\delta(x) + i\Sigma\delta(x-a), \\
\psi(x) &= \frac{1}{2}\,Im\,\Psi^2, \\
I &= \int_{-\infty}^{+\infty} \psi(x)\,\delta(x-x_s)dx = \psi(x_s);\ 0 < x_s < a \\
&= \frac{1}{2}\,Im\,\Psi^2(x_s).
\end{aligned}\right\} \quad (27)$$

For this sample case it appears that the equations in formulation (27) are solved easier than those in the nonlinear formulation (26). The general solution for $\Psi(x)$ is easily obtained as the sum of the general solution of the homogeneous equation (complementary solution) and a known or guessed particular integral for the inhomogeneous equation, since the equation for Ψ is an ordinary linear differential equation. It is easily verified that the general solution is

$$\Psi(x) = C_1 e^{\Sigma x} + C_2 e^{-\Sigma x} + \frac{S}{\Sigma}, \tag{28}$$

where C_1 and C_2 are two complex integration constants to be determined from boundary conditions. The necessary boundary conditions for Ψ are derived from those for ϕ and ϕ^+ given in Eqs. (24) and (25):

$$\left.\begin{array}{ll} 1. & \mathit{Re}\,\Psi(0) = \phi(0) = 1, \\ 2. & \mathit{Re}\,\Psi(+\infty) = 0, \\ 3. & \mathit{Im}\,\Psi(a) = \phi^+(a) = 1, \\ 4. & \mathit{Im}\,\Psi(-\infty) = 0. \end{array}\right\} \tag{29}$$

Since C_1 and C_2 are complex, it is required to have four conditions, and therefore the original by two boundary conditions for $\phi(0)$ and $\phi^+(a)$ must be augmented by flux and adjoint boundary conditions at $x \to \pm\infty$ as shown in Eqs. (29). Introducing $C_1 = a + ib$ and $C_2 = c + id$, the values for a through d are determined from Eqs. (29) as $a = d = 0$, $c = 1$, and $b = e^{-\Sigma a}$, which transform the general solution (28) into the full particular solution of our sample case:

$$\Psi(x) = e^{-\Sigma x} + ie^{-\Sigma a}e^{\Sigma x}. \tag{30}$$

Calculating the square of Eq. (30) yields

$$\Psi^2(x) = e^{-2\Sigma x} - e^{2\Sigma(x - a)} + 2ie^{-\Sigma a} \tag{31}$$

from which only the imaginary part is needed to calculate I according to Eqs. (27):

$$\begin{aligned} I &= \frac{1}{2}\,\mathit{Im}\,\Psi^2(x_s), \\ &= e^{-\Sigma a}, \text{ for any } x_s. \end{aligned} \tag{32}$$

Of course, this result [Eq. (32)] is verified immediately by comparison with Eqs. (24) or (25). The fact that $\psi(x) = \frac{1}{2}\, Im\, \Psi^2(x)$ is a constant in this case, is an immediate consequence of the conservation law discussed previously. Equation (12) reduces in our special case to

$$\frac{d\psi(x)}{dx} = 0, \text{ for } 0 < x < a, \tag{33}$$

and, that ψ therefore must be constant is obvious. However, to identify from first principles a boundary condition for $\psi(x)$ in Eq. (33) -- which would determine the value of the integration constant to be $e^{-\Sigma a}$ -- is not trivial.

V. OPEN QUESTIONS

Since the foregoing analysis is just a first attempt to find solutions to shielding-type problems without the need to solve the "almighty" Boltzmann equation, it appears as if more mathematical problems might be generated in the new approach than solved. Obviously, many questions need to be addressed before any conclusions about the usefulness of such a new approach may be drawn. The reader is invited to ask and answer any relevant questions, in particular those pertaining to the practicability of the new concept. Here is a list of such questions:

1. How can boundary conditions for ψ or Ψ be formulated in general?
2. Can Eq. (23) be generalized to include scattering media?
3. Can Eqs. (21) and (23) be generalized to other than slab geometries?
4. Can energy-dependence be treated?
5. What are the computational ramifications in solving complex or nonlinear equations of the form of Eqs. (21) and (23)?
6. Is it possible to derive from Eq. (23) or Eq. (21) an equation directly for I, by partial integration, e.g.?
7. What are the analytic properties of the new "transport operators" acting on ψ and Ψ?

VI. CONCLUSION

In an attempt to solve shielding-type problems through equations which have only the minimum necessary information content, two new forms of the neutron transport equation have been established. The equations are for a function $\psi = \phi^+\phi$ which obeys a conservation law and allows the direct calculation of the integral response $I = \langle R,\phi \rangle = \langle Q,\phi^+ \rangle$. The physical interpretation of ψ as the restricted number of source particles which will necessarily contribute to the integral response gives insight and understanding of the radiation transport process from a new perspective. The fact that these two new forms of the transport equation manifest themselves as either linear and complex, or nonlinear but real, is very interesting but can intuitively be understood because of the reduced information content of these equations. Boundary conditions for the new Ψ-equations have been treated only superficially but are felt to be extremely important in any general formulation. The fact that even the linear Boltzmann equation must be solved numerically for almost any problem of practical interest gives hope that there may be some practical problem existing for which the numerical solution of the new equations may prove advantageous.

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