Letters to the Editor

The Influence of Boundary Conditions on the Precision of the Eigenvalues of the Boltzmann Equation

Dahl and Sjöstrand[1] recently published a paper on a method for calculating the eigenvalues of the linear Boltzmann equation in plane and spherical geometries. They use the integral form of the transport equation and expand the space-dependent neutron flux in Legendre polynomials for the case of linear anisotropy in the elastic scattering kernel.

We do not intend to comment on the computational analysis of the Dahl and Sjöstrand results, but rather on the theoretical features of their method, which affect not only the values of the operator spectrum but also the corresponding angular distributions of the neutron fluxes.[2] The equation used in Ref. 1 has the form

$$\phi(x) = \frac{ac}{2}\left(\int_{-1}^{+1}\phi(y)\cdot E_1(a|x-y|)dy - 3\bar{\mu}(c-1)\right.$$
$$\times\left\{\int_{-1}^{+1}\phi(y)\cdot E_3(a|x-y|)dy - \frac{1}{2}\left[E_3(a|1-x|)\right.\right.$$
$$\left.\left.+(-1)^q E_3(a|1+x|)\right]\int_{-1}^{+1}\phi(y)y^q dy\right\}\Bigg) ,$$
$$\text{with } x,y \in [-1,1],\ q = 1 \text{ or } 2 . \qquad (1)$$

This equation is an exact one in the framework of the linear anisotropy approximation. However, Eq. (1) ceases to be exact as soon as one expands the neutron flux $\Psi(x,z)$ in a series of the type

$$\Psi(x,z) = \sum_{n=0}^{N}(2n+1)F_n(z)P_n(x) ,$$

which leads to

$$\phi(x) = \sum_{n=0}^{N}(2n+1)F_n\cdot P_n(x) \ ; \quad (N<\infty) , \qquad (2)$$

and in which only a few terms are considered. This is not a drawback if the convergence is fast enough. What is more interesting for the precision of the results presented in Ref. 1 is that Eq. (2) is the consequence of integration with respect to the angle variable, z ($z = \cos\theta$), of the equation

$$\Psi(x,z) = \sum_{n=0}^{N}(4n+1)F_{2n}(z)P_{2n}(x) \ ; \quad (z,x \in [-1,1]) , \qquad (3)$$

where $\Psi(x,z)$ is the angular neutron flux.

This expansion *does not exactly satisfy the boundary conditions*

$$\Psi(x,z) = 0 \ ; \qquad x = +1 \ , \quad z \in [-1,0]$$

and

$$\Psi(x,z) = 0 \ ; \qquad x = -1 \ , \quad z \in [0,1] , \qquad (4)$$

for a small number of terms (e.g., $N = 8$), a fact that is fundamental for the critical problem. In this sense, no analytical method except the methods of Refs. 3 and 4 rigorously satisfies the boundary conditions, Eqs. (4). The solutions given in Ref. 4 are of the form

$$\Psi_+(x,z) = \sum_{n=0}^{\infty}\left[S_n(x-a,z) - (-z)^n\exp\left(-\frac{x-a}{z}\right)\right]\cdot q_n \ ; \quad z>0 \qquad (5)$$

and

$$\Psi_-(x,z) = \sum_{n=0}^{\infty}\left[S_n(x-b,z) - (-z)^n\exp\left(-\frac{x-b}{z}\right)\right]\cdot p_n \ ; \quad z<0 . \qquad (6)$$

These expressions fulfill termwise the boundary conditions. The constants $\{p_n,q_n\ n = 0, 1, \ldots\}$ are related by $p_n = (-)^n q_n$. The polynomials $\{S_n(x,z)\}$, discovered recently,[5] possess the properties

$$S_n(x,0) = \frac{x^n}{n!} ,$$
$$S_n(0,z) = (-z)^n ,$$
$$\left(z\cdot\frac{\partial}{\partial x}+1\right)S_n(x,z) = \frac{x^n}{n!} , \qquad (7)$$

and are given by

$$S_n(x,z) = (-1)^n\left(z^n - \frac{z^n x}{1!} + \frac{z^{n-z}\cdot x^2}{z!} - \ldots\frac{x^n}{n!}\right) . \qquad (8)$$

These properties are substantial for the fulfillment of the boundary conditions.

In this respect, Eqs. (5) and (6) are of a different quality, and, therefore, the way to compare the results of Ref. 1 with those of Ref. 2 is not quite obvious, as might be implied from Ref. 1. Nevertheless, even on the level of numerical argumentation, one can clearly see that the results of the S_N method tend toward our results with increasing order of approximation of S_N. Consequently, also from the numerical point of

[1] E. B. DAHL and N. G. SJÖSTRAND, *Nucl. Sci. Eng.*, **69**, 114 (1979).

[2] C. SYROS and P. THEOCHAROPOULOS, *Ann. Nucl. Energy*, **4**, 495 (1977).

[3] K. M. CASE, *Ann. Phys.*, **9**, 1 (1960).

[4] C. SYROS, *Phys. Repts.*, **45**, 211 (1978).

[5] C. SYROS, *Lett. Nuovo Cimento*, **13**, 541 (1973).

view, the analysis makes clear the accuracies of the respective methods in question.

In addition, this conclusion would be much easier to see if angular neutron flux distributions were given in Ref. 1 as in Ref. 2 and, in particular, the values at the boundaries, which are the main source of the discrepancies. Finally, we should perhaps keep in mind the fact that not all references (Refs. 1 through 11) of Ref. 1 indeed rigorously satisfy the boundary conditions. For example, Ref. 6, which is labeled "exact," uses the discrete-ordinates method for the boundary conditions, e.g., $\Psi(t/2,\mu_j) = 0$ for $\mu_j > 0$ and $j = 1, 2, \ldots, 16$. Our method, being exact and completely analytic, corresponds to $\{\mu_j = \text{continuous}\}$ over the interval $[0,1]$.

On the other hand, while the "exact" method uses an accuracy limit of 10^{-8} in a number of interdepending iteration processes with possibilities for propagating numerical errors, we use the same accuracy limit only in two cases of matrix inversion. No approximate integrations or iterations are needed in our method.

The authors of Ref. 1 have probably observed that our eigenvalues are systematically lower than almost all calculated eigenvalues by other authors. This cannot, in our present view, be accidental: According to a theorem of the analysis of the linear operators, the lower the fundamental expectation value of a positive definite operator, the better the eigenfunction used for calculating it.

In conclusion, since our method is an exact one mathematically, both for the angular and the integrated distribution functions, the better agreement between the results of Refs. 1 and 7 should not surprise anyone because the approximate representation of the spatial dependence of the neutron fluxes is the same in both methods of these references.

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[6]K. D. LATHROP and A. LEONARD, *Nucl. Sci. Eng.*, **22**, 115 (1965).

[7]K. H. KSCHWENDT, *Nucl. Sci. Eng.*, **44**, 423 (1971).

Reply to "The Influence of Boundary Conditions on the Precision of the Eigenvalues of the Boltzmann Equation"

The calculations of eigenvalues of the transport equation[1] that Syros and Theocharopoulos[2] refer to are based on a development of the angular neutron flux in a sphere or infinite slab in the following way:

$$\psi(x,\mu) = \frac{1}{2}\sum_{n=0}^{\infty}(2n+1)P_n(\mu)\psi_n(x) \quad . \qquad (1)$$

In our work, we solved an integral equation for $\psi_0(x)$. This equation for the flux is exact and contains the boundary condition of no incoming neutrons, facts that Syros and Theocharopoulos[2] also point out. Similarly, it is possible to derive an integral equation for the neutron current $\psi_1(x)$ and then to obtain $\psi_2(x)$ and higher order functions. In this way, one should be able to calculate the angular neutron flux in Eq. (1).

Since our work was restricted to the exact integral equation for the neutron flux $\psi_0(x)$, the angular distribution of the neutrons was not involved. Therefore, solving the integral equation by expanding $\psi_0(x)$ in Legendre polynomials in the spatial variable x should give the correct eigenvalues of the equation.

However, as pointed out by Syros and Theocharopoulos,[2,3] their eigenvalues are systematically smaller than almost all other published data. The relative deviation between their values and ours is between 1.0×10^{-4} and 1.3×10^{-3}, which is outside the estimated limits of uncertainty in our calculations. Examples for isotropic neutron scattering in an infinite slab are given in Table I. The systematic difference raises the question of whether we have had an inadequate convergence in our computations of the eigenvalues. To investigate this further, we have repeated some of our calculations with 20 terms in the series of spatial Legendre polynomials instead of 9. The results are given in Table I. It can be seen that the values obtained with 9 polynomials are in agreement with the 20 polynomial values within one unit in the 8th figure, which is the stated uncertainty.[1]

As a further check, the integral equation for the neutron current $\psi_1(x)$ has been solved with 20 polynomials in the development and for the same parameter values. As can be seen in Table I, it is not possible to get as high an accuracy as for the flux equation, but the disagreement does not start until the 8th figure.

Syros and Theocharopoulos[2] state that the fact that our results agree with those of Kschwendt[4] can be explained by a similar development of the spatial dependence. However, our results also agree with those of Kaper et al.,[5] who applied the method of Case. Some of their values are shown in Table I. They claim that the errors are less than one unit in the last decimal place, which is probably the highest accuracy obtained in a calculation of this type. The deviation between their values and ours is at most two units in the last figure given. This deviation is probably not caused by an insufficient number of terms in the development but by the limitations of our numerical procedure.

That calculations of our type do converge properly is corroborated by the work by Sanchez,[6] who used up to 150 polynomials in a similar method of solving the transport equation with linear anisotropic scattering for infinite cylinders. For the same range of anisotropy as in our work, the maximum relative deviation between his eigenvalues for 10 and 100 polynomials is 1.8×10^{-6} (see p. 90 of Ref. 6), but it is usually much less.

The evidence presented leads us to believe that our results[1] are accurate to within the error limits given. We cannot explain

[1]E. B. DAHL and N. G. SJÖSTRAND, *Nucl. Sci. Eng.*, **69**, 114 (1979).

[2]C. SYROS and P. THEOCHAROPOULOS, *Nucl. Sci. Eng.*, **73**, 108 (1980).

[3]C. SYROS and P. THEOCHAROPOULOS, *Ann. Nucl. Energy*, **4**, 495 (1977).

[4]H. KSCHWENDT, *Nucl. Sci. Eng.*, **44**, 423 (1971).

[5]H. G. KAPER, A. J. LINDEMAN, and G. K. LEAF, *Nucl. Sci. Eng.*, **54**, 94 (1974).

[6]R. SANCHEZ, "Généralisation de la méthode d'Asaoka pour le traitement d'une loi de choc linéairement anisotrope; données de référence en géométrie cylindrique," CEA-N-1831, Centre d'Etudes Nucléaires de Saclay (1975).