Quadrature With Arbitrary Weight for the Numerical Solution of the Critical Slab Neutron Transport Equation

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Abstract

A standard procedure for the solution of singular integral equations is applied to the one-dimensional transport equation for monoenergetic neutrons. The results obtained with two versions of the procedure, differing only in the extent of the basic region to which they are applied, are compared with analytically derived results available for benchmarking. The procedures considered yield consistent results for the calculated neutron densities and eigenvalues. Several approximate expressions of the neutron density are used to render closed-form formulas for the densities which can then be analytically operated on to obtain expressions for extrapolation distances or angular densities or serve other purposes that require an analytical expression of the neutron density.

1. INTRODUCTION

The neutron density ρ(x) of monoenergetic neutrons in an infinite, homogeneous, isotropic, critical slab, obeys the singular integral equation [1,2]:

$$\rho(x) = \frac{c}{2} \int_0^a E_1(|x-x'|) \rho(x') dx', \ x \in [0,a]$$  \hspace{1cm} (1)

where c is the number of secondary neutrons per collision and a is the slab width, measured in mean free paths. The exponential integral function of order one $E_1(z)$, has a singularity in $z=0$.

For the solution of Eq.(1) we employ in this note a standard numerical scheme suitable for the treatment of singular integral equations with a displacement kernel, as described by Delves and Walsh [3] and by Press et al [4]. This approach consists in obtaining an eigensystem that can be regarded as a projection in a finite-dimensional space of the original eigenvalue problem posed by Eq.(1) and whose solution yields approximate values of the neutron density at a finite number of specified points, together with the corresponding eigenvalue which is directly related to c, the number of secondaries per collision required for criticality. In a fashion similar to the subtraction of the singularity method [5,6] and the collision probability method, [7,8] the present procedure
owes its practicality to the fact that the kernel in Eq.(1) i.e. the function \( E_1 \), not only is integrable but its integrals are known functions also.

It should be noted that an exact solution of Eq.(1) can be obtained by either the Wiener-Hopf technique [9] or the singular eigenfunction expansion method of Case [1]. This latter method ultimately provides a solution in terms of a system of integral Fredholm equations of the first kind for the coefficients of the eigenfunction expansion; this system can in principle be solved by an iterative procedure and in this manner one obtains successive closed-form approximations to the solution; tabulations of the main functions required exist and in this sense the problem is considered solved. Extraction of accurate numerical values from this analytical solution is however, not trivial [9]. Successful approaches include those of Kaper et al. [10] who provided benchmark results for planar and cylindrical systems and of Sanchez and Ganapol [11] who completed the set of one-dimensional problems by providing results for systems with cylindrical symmetry. Our intention here is to show that the conceptually simpler present approach produces accurate enough results and gives rise to “natural” closed-form approximations of the neutron density in terms of the \( E_n \) functions.

### 2. QUADRATURE WITH ARBITRARY WEIGHT [3,4,5]

In order to describe this numerical technique we introduce an operator \( A \) whose domain is a normed function space \( X \) and such that,

\[
A \phi = \int_0^a E_1( |x-x'| ) \phi(x') \, dx', \quad \text{for all } \phi \in X. \tag{2}
\]

Notice that the singular kernel \( E_1 \) is integrable. With this notation, Eq.(1) is

\[
A \rho = \frac{2}{c} \rho(x) \tag{3}
\]

an operator \( A_M \) is now chosen in such a manner that

\[
A_M f = \sum_{j=1}^{M+1} w_j(x) f(x_j) \tag{4}
\]

for all functions \( f \in X \) and where \( x_1, x_2, \ldots, x_{M+1} \) define a partition of \([0,a]\).

The functions \( w_j(x) \) are determined by the requirement that

\[
A q_M = A_M q_M \tag{5}
\]

for all polynomials \( q_M \) of degree \( \leq M \). We will denote by \( \| \cdot \| \) the norm of the space \( X \) and assume that \( \| A \phi - A_M \phi \| \to 0 \) as \( M \to \infty \), under relatively mild conditions to be satisfied by \( \phi \).
By substituting the operator $A$ in Eq. (3) by the operator $A_M$ with a given $M$, and making $x$ to assume the values $x_i$, with $i = 1, 2, 3, ..., M + 1$, one obtains an eigensystem whose solution provides approximate values of $\rho$ at the points of the partition. The resulting approximation to the solution of Eq. (1) is then said to be of accuracy $\mathcal{O}[M]$. In practice, a relatively low value of $M$ is used and in order to achieve a given precision, the scheme is successively applied in as many subintervals of $[0,a]$ as needed, as explained below.

2.A. Derivation of an $\mathcal{O}[3]$ Formula for a Single Subinterval

We will consider the partition of $[0,a]$ given by $\{x_1, x_2, x_3, ..., x_{N+1}\}$ with $x_1=0$ and $x_{N+1}=a$, and will apply the prescription given by Eq. (4) to each one of the subintervals defined by the partition. In each subinterval $(x_k, x_{k+1})$ the abscissae intervening in the formula are chosen to be $x_{k-1}, x_k, x_{k+1}, x_{k+2}$ so that the $\mathcal{O}[3]$ approximation takes the form,

$$\int_{x_k}^{x_{k+1}} E_i\big(|x-x'|\big) \rho(x') \, dx' = \sum_{j=1}^{M} w_j^{(k)}(x) \rho(x_{k-2+j}), \quad x \in [0,a], \quad (5a)$$

for $2 \leq k \leq N - 1$. The functions $w_j^{(i)}$ are the weights corresponding to the subinterval starting at $x_i$.

For the first and last intervals, in accordance with Eq. (4) we will set, respectively,

$$\int_{x_1}^{x_2} E_i\big(|x-x'|\big) \rho(x') \, dx' = \sum_{j=1}^{M} w_j^{(1)}(x) \rho(x_j), \quad x \in [0,a], \quad (5b)$$

$$\int_{x_N}^{x_{N+1}} E_i\big(|x-x'|\big) \rho(x') \, dx' = \sum_{j=1}^{M} w_j^{(N)}(x) \rho(x_{N-3+j}), \quad x \in [0,a],$$

It should be noted that we allow $x$ to be located anywhere in the interval $[0,a]$. The particular choice of the set of abscissae is such that the interior subintervals are symmetrically located with respect to the intervening abscissae.

For an $\mathcal{O}[3]$ formula the determination of the weights is accomplished by requiring the fulfillment of the conditions

$$\sum_{j=1}^{M} \left(x_{k-2+j}\right)^q w_j^{(k)} = \int_{x_k}^{x_{k+1}} \left(x'\right)^q E_i\big(|x-x'|\big) \, dx';$$

$$q = 0, 1, 2, 3; \quad k = 2, 3, 4, ..., N - 1; \quad (6)$$

for $k=1$ and $k=N$, the conditions should be modified in the obvious way implied by Eq. (11b). It should also be noted that for each subinterval, Eq. (6) gives rise to a set of four linear equations from which the weight functions for that subinterval are to be determined, but a general solution...
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can be found in which \( x_k \) appears as a parameter that specifies the solution as pertaining to a given subinterval.

Assuming that the functions \( w_j^{(k)}(x) \) are known, Eq. (1) becomes,

\[
\rho(x) = \frac{c}{2} \left( \sum_{j=1}^{i=4} w_j^{(1)}(x) \rho(x_j) + \sum_{k=2}^{N-1} \sum_{j=1}^{i=4} w_j^{(k)}(x) \rho(x_{k-2+j}) + \sum_{j=1}^{i=4} w_j^{(N)}(x) \rho(x_{N-3+j}) \right)
\]

(7)

and making \( x \) take the values \( x_1, x_2, \ldots, x_{N+1} \), one obtains the eigensystem

\[
\lambda f = W f, \quad \text{with } \lambda = \frac{2}{c}
\]

(7a)

where \( f = (\rho(x_1), \rho(x_2), \rho(x_3), \ldots, \rho(x_{N+1}))^T \), and where the elements of \( W \) are determined after factoring out each one of the \( \rho(x_i) \).

2.B. An \( Q(3) \) Formula for Three Subintervals

A somewhat simpler scheme results when the integrals to be approximated cover at once three subintervals: First we write Eq. (1) in the form

\[
\rho(x) = \frac{c}{2} \sum_{k=0}^{N-1} \left[ \int_{x_{3k+1}}^{x_{3k+4}} \rho(x') E_1(|x - x'|) \, dx' \right], \quad \forall x \in [0, a]
\]

(8)

and then make

\[
\int_{x_{3k+1}}^{x_{3k+4}} \rho(x') E_1(|x - x'|) \, dx' = \sum_{j=1}^{i=4} w_j^{(3k+1)}(x) \rho(x_{j+3k})
\]

(9)

so that

\[
\frac{2}{c} \rho(x) = \sum_{k=0}^{N-1} \sum_{j=1}^{i=4} w_j^{(3k+1)} \rho(x_{j+3k}).
\]

(10)

The weights are now determined by the conditions

\[
\sum_{j=1}^{i=4} \left( x_{3k+j} \right)^q w_j^{(3k+1)} = \int_{x_{3k+1}}^{x_{3k+4}} (x')^q E_1(|x - x'|) \, dx';
\]

(11)
and in this manner one sets the eigensystem

\[
\frac{2}{c} \rho(x_i) \approx \sum_{k=0}^{N-1} \sum_{j=1}^{\frac{N}{3}} w_j^{(3k+1)}(x_i) \rho(x_{j+3k}); \quad i = 1, 2, 3, \ldots N + 1
\]

Once the eigensystem is solved, i.e. once the \( \rho(x_i) \) and \( c \) are determined, Eqs. (7) and (10) provide the closed-form, interpolation formulas for the neutron density for the case of integration over one and three subintervals, respectively.

### 3. CLOSED-FORM EXPRESSIONS OF THE DENSITY

One can use as an interpolating formula the expression for the density that is obtained after applying a quadrature formula. This is described in general in Ref.(4) where the assessment of this device, performed by Delves and Mohamed in Ref.(3), is cited; a formal evaluation of the accuracy so achieved is given by Gavurin [13].

As an example, we now list the formulas that can be extracted from two well-known approaches: the **Subtraction of the Singularity** and the **Collision Probabilities** methods. In the formulas given below, the number of secondaries per collision \( c \), and the values of the neutron density \( \rho(x_j) \) at the discrete set of abscissae chosen, are assumed to have been determined by the corresponding methods or by any other schemes. \( N \) indicates the number of subintervals considered in the approximations.

#### 3.a Subtraction of the singularity

This is a well-known method for the solution of singular integral equations which is described in a general setting in Ref.(4) and Ref.(5); specific applications to neutron transport are described by Sanchez and McCormick [6]. When applied to Eq.(1) this method can be made to yield the following expression for the neutron density:

\[
\rho(x) \approx \frac{2h}{3} \sum_{j=1}^{N+1} w_j \rho(x_j) E_i \left( \left| x - x_j \right| \right)
- \frac{2}{c} \sum_{j=1}^{N+1} w_j \left( x_j \right) + \frac{2h}{3} \sum_{j=1}^{N+1} w_j E_i \left( \left| x - x_j \right| \right) \]

\( x \neq x_j, \quad j = 1, 2, 3, \ldots, N + 1. \)

\( = \rho(x_j) \) otherwise.

The weights \( w_j \) correspond to Simpson's Rule as applied for the evaluation of the required integrals:
The function \( d_g(x; a) \) is given by
\[
d_g(x; a) = 2 - E_2(x) - E_2(a - x),
\]
where \( E_2 \) is the exponential integral function of order 2.

3.b Collision Probabilities

This method has been used by many authors to solve many different problems in this field. Recent references include Stacey [7] and M.M.R. Williams [8]. The method can be used to obtain the following formula, analogous to Eq. (12):
\[
\rho(x) = \hat{\rho} \sum_{i=1}^{N} \hat{\rho}_i I_i(x)
\]
where
\[
I_i(x) = \begin{cases} 
E_2(x_{i+1} - x) - E_2(x_i - x), & \text{if } x \leq x_i, \\
E_2(x-x_i) - E_2(x-x_{i-1}), & \text{if } x \geq x_i, \\
2 - E_2(x-x_{i-1}) - E_2(x_i - x), & \text{if } x \in [x_{i-1}, x_i], 
\end{cases}
\]
and \( \hat{\rho}_i \) is a “flat flux” approximation to \( \rho(x) \) in \([x_{i-1}, x_i]\). (One should recall that the Collision Probability method assumes a sectionally constant density). Eq.(14) is relatively simpler than the interpolation formula obtained from the quadrature with arbitrary weight method, Eq.(7) or Eq.(8). It is also worth mentioning that the interpolation formulas suggest that the density can independently be expressed approximately in terms of the \( E_n \) functions.

4. RESULTS AND CONCLUSIONS

The described schemes were coded employing a system capable of symbols manipulation [12] and were ran in a personal computer. The benchmark numerical values given in Ref.(10) (denoted as K L L) were used for comparison. Our own results are generally consistent with those of Ref.(10) and the absolute values of the discrepancies, are no larger than \( 2 \times 10^{-7} \) for the values of \( c \). In the following table we present the values of the number of secondaries per collision needed for criticality; the number of subintervals employed, was arbitrarily set to 100 for the Quadrature with Arbitrary Weight for Centered subintervals (QAWC), and to 102 for the Quadrature with Arbitrary Weight for three subintervals (QAW3) approaches.
As regards to the neutron density, the results obtained with the QAWC approach, for the same slab thicknesses included in the table above, are given below. Reducing the step-size one can increase the number of significant digits in the values of the density yet the size of the computer word-length employed seems to slow this process.

We assumed that ill-conditioning would manifest itself in that small changes in the slab thickness would produce relatively large changes in both \( c \) and the neutron density. Neither this or any other indications of ill-conditioning were observed. This could be due to the fact that although the method employed can be considered to be a Gaussian quadrature-like method, the particular choice of the collocation points and the use of functions of position as weights, in contrast to the usual quadrature methods, results in a very tractable matrix (it is a central-symmetric matrix). As a rudimentary test of the robustness of the method, very thin slabs were considered (with thicknesses of 0.00999, 0.01 and 0.01001 mean free paths) where some quadrature methods could be expected to fail; this resulted in small variations in \( c \) and in \( \rho(x) \) about the
corresponding values for \(a=0.01\) and the variations observed were in the correct direction, that is, to the wider thickness corresponded a smaller value of \(c\) and vice versa.

The time required by each calculation is short, the longest times for a personal computer with a clock frequency of 850kHz, and with about 400 subintervals, do no exceed 5 minutes for the QAWC approach and is shorter for the other approach. We did not exploit the central symmetry of the resulting matrices that permits to reduce the numerical work in half. Obviously, the problem considered here is of only academic interest and computer time is not an issue.

The interpolation formulas that result with the total number of subintervals employed in this note are too unwieldy for human manipulation, but do not present any problems for the Mathematica system that we used.

The fact that the \(E_n\) functions appear naturally in these formulas suggests that approximations to the density with a reduced number of terms containing these functions could be independently derived.

An extension of this device to more than one dimension could in principle be made, provided that the integrals of the general kernel \(e^{-r}/r^2\) exist and can be expressed in terms of tractable functions.

**REFERENCES**

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