JOURNAL OF COMPUTATIONAL PHYSICS 33, 417–424 (1979)

Note

On the Properties of Collision Probability Integrals in Annular Geometry. II. Evaluation

1. Introduction

To calculate neutron flux distributions in infinitely long annular regions, the inner–outer and outer–outer transmission probabilities P^{io} and P^{oo} are required. Efficient algorithms for the computation of these probabilities as functions of two variables (the ratio of inner/outer radii κ, and cross section Σ) are given for $0 \leqslant \kappa \leqslant 1$ and all $0 < \Sigma$, with fractional errors less than 2×10^{-5}.

In a previous paper [1], referred to as I, the analytic evaluation of two integrals fundamental to neutron transport calculations in annular geometry was derived. The integrals were expressed as an infinite sum of Meijer's G-function. The purpose of this note is to report an efficient method for the numerical evaluation of two of the most commonly calculated probabilities, p^{00} and p^{i0}, where

$$P^{oo} = \frac{4}{\pi} \int_{\sin^{-1}\kappa}^{\pi/2} Ki_3(2x \cos\theta) \cos\theta \, d\theta,$$

$$P^{io} = \frac{4}{\pi} \int_{0}^{\sin^{-1}\kappa} Ki_3(xR) \cos\theta \, d\theta,$$

$$R = (1 - \kappa^2 \sin^2\theta)^{1/2} - \kappa \cos\theta,$$

and Ki_3 are the Bickley–Naylor functions, together with $0 \leqslant \kappa \leqslant 1$ and $x \geqslant 0$.

These probabilities form the basis of the $J^{\pm}$ method [2, 3] of solving the transport equation and certain of them are used extensively in transport codes [4–8] Methods for numerical evaluation are given in [4, 9, 10], all of which are accurate to two or three significant figures over a range of both variables, but break down [4] in certain limits. Numerical integration can be used [6, 7, 11] but in typical problems where the routines are called several thousand times, this can be slow and expensive [7, 11].

The analytic expansions from I have been used to isolate the singularities of the integrals in both variables, and the remaining functions—represented by infinite series—were fitted with rational REMES minimax approximations [12, 13] in one variable, demanding a relative accuracy in the final answer to better than 2×10^{-5} over all physical ranges of both variables. All integrations to check the claimed accuracy of the fits were performed using the CADRE algorithm [14], and a Bickley–Naylor minimax fit [15] accurate to 13 significant digits.

0021-9991/79/120417-08$02.00/0

To summarize, computational accuracy in P^{oo} and P^{io} to better than 2 parts in 10^5 is claimed for any combination of radius and cross section in the range $0 \leqslant \kappa \leqslant 1$ and $0 \leqslant \Sigma$. The following sections deal with the evaluation of P^{oo} and P^{io}, respectively.

2. Evaluation of P^{oo}

It is convenient to employ different representations for P^{oo} according to the value of z and κ. Explicitly, for $0 \leqslant \kappa \leqslant 1$ and $0 \leqslant z \leqslant 1.4$, using Eq. (4.3) of Ref. [1], $\lambda^2 = 1 - \kappa^2$, $z = x\lambda$ and $w = 2z^2/(1 + \kappa)$,

$$P^{oo} = (1 - \kappa)\Big[1 + 2w(1 - \tfrac{1}{3}(1 - \kappa)) + w^{1/2}F_{-1}(\kappa) + w^{3/2}\sum_{i=0}^{I} w^i(H_i(\kappa) + F_i(\kappa)\log w)\Big]. \tag{2.1}$$

Analytic expressions and minimax approximations to the function $F_i(\kappa)$ and $H_j(\kappa)$ are given elsewhere [16], and we find that

$$I = [3.65852z + 0.878]$$

gives sufficient terms in the series to achieve a fractional error of less than 1×10^{-5} where [ ] means the greatest integer less than the bracketed quantity.

As the value of I increases in Eq. (2.1), the functions get more difficult to fit to a constant accuracy, without unduly increasing the order of the rational polynomials. However, the contribution of the higher-order terms to the accuracy of the final answer decreases, so *we accept lower accuracy fits for higher-order terms.* This stratagem is used throughout, and results in a slight loss of precision from the goal of five significant digits, but repays itself by the resulting efficient algorithms. It is worth noting, that if the geometrical functions $F_i(\kappa)$ and $H_i(\kappa)$ are precomputed, considerable arithmetic will be saved if z remains in the range $0 \leqslant z \leqslant 1.4$ throughout an ensuing burnup and/or slowing-down calculation.

Finally, note that for $w \approx 0$, the variable w will underflow faster than $\log w$ will overflow in Eq. (2.1), and so the product $w^{3/2}\log w$ has no numerical singularities if a test is made for $w = 0$. This remark is true for all logarithmic singularities that superficially appear in this note.

For $1.4 < z \leqslant 7.5$, the minimum number of terms in the series is found by using expansions about $\lambda^2 = 1$ or $\lambda^2 = 0$. For $0 \leqslant \lambda^2 < 0.696$, Eq. (4.3) of Ref. [1] suggests

$$P^{oo} = (1 - \kappa)\sum_{l=0}^{I_1} (1 - \kappa)^l A_l(w), \tag{2.2}$$

where

$$A_l(w) = \frac{2}{\pi l!}(-1/2)^l\, G_{3.5}^{3,2}\left(w \,\middle|\, \begin{matrix} 0, -l; 2 \\ 0, 1/2, 3/2; l, -1-l \end{matrix}\right).$$

Rational minimax approximations to $A_l(w)$ are given in [16]. The integer I_1 in Eq. (2.2) may be chosen according to the value of w and κ by means of empirical approximations [16].

For $1.4 < z \leqslant 7.5$ and $0.696 \leqslant \lambda^2 \leqslant 1$, we find from Eq. (4.1) of Ref. [1]

$$P^{oo} = P_{CYL}(x) - \lambda^2\kappa \exp(-2z)\, z^{-1/2} \sum_{l=0}^{I_2} (\kappa^2 z)^l\, B_l(z)(z - z_0(l)), \tag{2.3}$$

where

$$B_l(z) = \frac{\exp(2z)\, z^{1/2-l}}{\Gamma(\frac{3}{2}+l)} \frac{G_{2.4}^{3,1}\left(z^2 \,\middle|\, \begin{matrix} -1/2-l; 2 \\ 0, 1/2, 3/3; -1/2 \end{matrix}\right)}{(z - z_0(l))}$$

and

$$P_{CYL}(x) = \pi^{-1/2} G_{2.4}^{3,1}\left(x^2 \,\middle|\, \begin{matrix} 0; 2 \\ 0, 1/2, 3/2; -1/2 \end{matrix}\right) \tag{2.4}$$

is the transmission probability for a cylinder. Again, approximations to $B_l(z)$, $P_{CYL}(x)$ and I_2 may be found elsewhere [16].

For $x > 7.7$, it is possible to derive an asymptotic form using G-function properties [17]. We find

$$P_{CYL}(x) = \pi^{-3/2} x^{-2} \sum_{l=0}^{I_3} \frac{\Gamma(\frac{3}{2}+l)\,\Gamma(\frac{3}{2}+l)\,\Gamma(\frac{5}{2}+l)}{\Gamma(3+l)\, x^{2l}} \tag{2.5}$$

and tables of I_3 are given in Ref. [16].

Finally, for $z > 7.5$, an asymptotic form for P^{oo} is found from Eq. (5.1) or (4.3) of I. Since the asymptotic series for P^{oo} and $P_{CYL}(x)$ coincide, it is convenient to use Eq. (4.3) of I and write

$$P^{oo} = P_{CYL}(x) - \frac{\lambda^2 \pi^{-1/2} w^{-3/4} \exp(-2w)}{2(1+\kappa)} \tag{2.6}$$

giving the required accuracy for all values of λ^2 when $z > 7.5$. We have tested these algorithms using 40 000 pseudo-random values of $0 \leqslant x$ and $0 \leqslant \kappa \leqslant 1$. The average time required for one evaluation of P^{oo} was 0.233 ms on a CDC 6600 computer, about 76 times faster than numerical integration to the same accuracy. Of these cases, 0.3 % had a fractional error greater than 10^{-5}, the largest fractional error observed was 1.66×10^{-5}.

3. Evaluation of P^{io}

The properties of p^{io} are very different from P^{oo} and the function is more difficult to calculate. Two formulas obtained from I are employed. The first—Eq. (3.9) of Ref. [1]—is

$$P^{io} = \frac{z}{2}\left[\sum_{l=0}^{I} (-\eta)^{l+1/2}\, g_l(z) - \sum_{l=0}^{I} (-\eta)^l\, h_l(z)\right] \tag{3.1}$$

with

$$g_l(z) = G^{3,1}_{2,4}\left(\frac{z^2}{4}\,\middle|\, \begin{matrix} -l;\, 3/2 \\ 0,\, 1/2,\, 1;\, l \end{matrix}\right)\Big/(\Gamma(l+1)\,\Gamma(l+2)),$$
$$\eta = -\kappa^2/\lambda^2, \tag{3.2}$$

and

$$h_l(z) = g_{l-1/2}(z) - 2\delta_{l,0}/z \tag{3.3}$$

The second is Eq. (5.6) of I which gives

$$P^{io} = \left(\frac{1+\kappa}{\kappa}\right)(\mathscr{I}_1 - \mathscr{I}_2), \tag{3.4}$$

where

$$\mathscr{I}_1 = \sum_n \gamma^{2n} \sum_r e_n(r)\, \mathscr{I}_1^{n+r}(z\gamma^{1/2}) \tag{3.5}$$

and

$$\mathscr{I}_2 = \sum_n \gamma^{2n} \sum_r e_n(r)\, \mathscr{I}_2^{n+r}(z, \gamma) \tag{3.6}$$

with

$$\mathscr{I}_1^{n+r}(z\gamma^{1/2}) = \frac{4}{\pi}\int_1^\infty t^{2(n+r-1)} Ki_3(z\gamma^{1/2}t)(t^2-1)^{-1/2}\, dt \tag{3.7a}$$

$$= \frac{1}{\pi^{1/2}}\, G^{4,0}_{2,4}\left(\frac{z^2\gamma}{4}\,\middle|\, \begin{matrix} ;\, 2,\, 3/2 - n - r \\ 1 - n - r,\, 0,\, 1/2,\, 3/2; \end{matrix}\right), \tag{3.7b}$$

$$\mathscr{I}_2^{n+r}(z, \gamma) = \frac{4}{\pi}\int_{\gamma^{-1/2}}^\infty t^{2(n+r-1)} Ki_3(z\gamma^{1/2}t)(t^2-1)^{-1/2}\, dt, \tag{3.8}$$

$$e_n(r) = (-)^r \frac{\Gamma(\frac{1}{2}+n-r)}{\Gamma(2-r)\,\Gamma(\frac{1}{2})\,\Gamma(n-r+1)},$$

and

$$\gamma = (1-\kappa)/(1+\kappa)$$

It is convenient to subdivide the segment of the (κ^2, z) plane of interest into six regions defined in Ref. [16], and described below. In each region, a different numerical evaluation method is appropriate, as detailed in the following sections labeled A–F corresponding to the respective areas.

Case A $\kappa^2 \approx 0, z \gtrsim 5.0$

The basic formula here is Eq. (3.1), which converges slowly for increasing values of η. In addition, the functions $g_l(z)$ are oscillatory, which makes it difficult to determine the integer I simply, and the power series expansion of $g_l(z)$ suffers from severe numerical instability. Accordingly, invoke the recursion formula [17]

$$g_{l+1}(z) = [\tfrac{3}{4}zg_l'(z) - l(l+1)\,g_l(z) + \tfrac{1}{4}z^2 g_l''(z)]/((l+1)(l+2)). \tag{3.9}$$

A similar result holds for $h_{l+1}(z)$ according to Eq. (3.3). From Ref. [1] identify

$$g_0(z) = 2Ki_2(z), \tag{3.10}$$

$$h_0(z) = -(4/z)\,Ki_3(z), \tag{3.11}$$

where $Ki_n(z)$ are the Bickley–Nayler functions, which obey

$$\frac{d^n}{dz^n} Ki_m(z) = (-)^n\, Ki_{m-n}(z) \tag{3.12}$$

and negative order functions can be calculated by the (numerically stable) recursion formula

$$Ki_{n-3}(z) = \frac{n-1}{z} Ki_n(z) - \frac{n-2}{z} Ki_{n-2}(z) + Ki_{n-1}(z). \tag{3.13}$$

So taking $I = 10$ in Eq. (3.1), applying Eqs. (3.9)–(3.13) to each of $g_l(z)$ and $h_l(z)$ and evaluating the sum algebraically [18], it is possible to express P^{io} in the form

$$P^{io} = \tfrac{1}{2}z[Ki_0(z)\,P_0(z,\eta) + Ki_1(z)\,P_1(z,\eta) + Ki_2(z)\,P_2(z,\eta)], \tag{3.14}$$

where $P_i(z, \eta)$ are polynomials in z, η and $(-\eta)^{1/2}$.

The analytic (unnested) form of these functions is given in Ref. [16].

Case B. $0 \leqslant \kappa^2 \leqslant 0.5, z \lesssim 5.0$

In this range, employ the series expansions for $g_l(z)$ and $h_l(z)$ in Eq. (3.1) and transpose the sums. The result for $y = \frac{1}{4}z^2$ is

$$P^{io} = 1 + y^{1/2}\left[Q_{-1}(\eta) + y^{1/2}R_{-1}(\eta) + y\sum_{i=0}^{I} y^i(R_i(\eta) - \log y Q_i(\eta))\right], \tag{3.15}$$

where Q and R, functions of the geometry only, may be precomputed in some applications. Analytic expressions and rational minimax approximations for $Q(\eta)$ and $R(\eta)$, and estimates of I in Eq. (3.15) are given in Ref. [16].

Case C. $0.5 < \kappa^2 \leqslant 1.$, $z \lesssim 5.0$

In this range, perform the analytic continuation $\eta \to 1/\eta$ as outlined in Eq. (4.5) of I. The result (using $y = \frac{1}{4}z^2$) is

$$P^{io} = 1 + y^{1/2}\left[(-\eta)^{-1/2}\, T_{-1}\left(\frac{1}{\eta}\right) + y^{1/2} S_{-1}\left(\frac{1}{\eta}\right) - \lambda^2 y \sum_{i=0}^{I} y^i \left[S_i\left(\frac{1}{\eta}\right) - \log y T_i\left(\frac{1}{\eta}\right)\right]\right]. \tag{3.16}$$

Rational minimax approximations to and analytic expressions for the functions S and T and estimates of the values of I in Eq. (3.16) are recorded in Ref. [16].

Case D. $\kappa^2 > 0$, *z intermediate*

Here we discuss the evaluation of P^{io} for intermediate values of z; the governing equation is (3.4). As indicated in I, the function $\mathscr{I}_2$ vanishes like $\exp(-2)$, whereas $\mathscr{I}_1$ has the asymptotic exponential behavior $\exp(-z\gamma^{1/2})$.

Thus for some area of the plane, $\mathscr{I}_2$ does not contribute, and so use Eq. (3.5) to write (setting $v = z\gamma^{1/2}$)

$$P^{io} = P_1^{io} = \left(\frac{1+\kappa}{\kappa}\right)\left\{\mathscr{I}_1^{\,0}(v) + \frac{\gamma^2}{2}\,\mathscr{I}_1^{\,1}(v) + \frac{1}{\pi^{1/2}} \sum_{n=2}^{I_1} \gamma^{2n} \mathscr{I}_1^{\,n}(v)\left[\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n+1)} - \gamma^2 \frac{\Gamma(n-\frac{3}{2})}{\Gamma(n-1)}\right]\right\}, \tag{3.17}$$

where values of I_1 and the identification of the functions $\mathscr{I}_1^{\,n}(v)$ is recorded in Ref. [16].

Case E. $\kappa^2 > 0$, *z intermediate*

In that region of the plane in which $\mathscr{I}_2$ contributes, it is possible to identify

$$\mathscr{I}_2^{\,n} = \gamma^{1-n} \exp(-z)\, z^{-3/2} \sum_l \frac{(\frac{1}{2})_l\, \gamma^l}{l!}\, H_{n-l}(z) \tag{3.18}$$

using Eq. (3.8). The triple sums in Eq. (3.6) are then reordered and the result is

$$\mathscr{I}_2 = \gamma \exp(-z)\, z^{-3/2} \sum_{n=0}^{I_2} \gamma^n \mathscr{H}_n(z) \tag{3.19}$$

together with

$$P^{io} = P_1^{io} - \left(\frac{1+\kappa}{2\kappa}\right)\mathscr{I}_2 \tag{3.20}$$

because of Eqs. (3.17) and (3.4).

The functions $H_{n-1}(z)$ and $\mathscr{H}_n(z)$ are identified, rational minimax approximations to $\mathscr{H}_n(z)$ are given, and estimates of values of I_2 in Eq. (3.19) are recorded in Ref. [16].

Case F. $\kappa^2 > 0$, $z\gamma^{1/2}$ large

In this range of values the only contributions come from $\mathscr{I}_1$ in Eq. (3.4). Extract the first few terms of the asymptotic series for the G-function defined in Eq. (3.7b) and analytically [18] sum the series (3.5) over n and r. The result is an asymptotic series given by

$$P^{io} = \left(\frac{1+\kappa}{\kappa}\right)\frac{\exp(-v)}{v}(1-\gamma^2)^{1/2}\sum_{n=0}^{I}\frac{P_{2n}(\gamma)}{[v(1-\gamma^2)]^n} \tag{3.21}$$

where $P_{2n}(\gamma)$ is a polynomial in γ of degree $2n$ identified in Ref. [16] where required values of I that depend on the value of $v = z\gamma^{1/2}$ are also given.

The algorithms described in this section were used in a computer routine to calculate P^{io} using pseudo-random values of $0 \leqslant x$ and $0 \leqslant \kappa \leqslant 1$. The average time for one calculation of P^{io} (with no precalculation of geometrically invariant functions) was 0.67 ms on a CDC 6600 computer, about 40 times faster than simple numerical integration with the same accuracy. Of 80 000 cases, 0.15 % had a fractional error greater than 1×10^{-5}; the largest fractional error observed was 0.19×10^{-4}.

4. Summary

Algorithms are given which permit the swift and accurate evaluation of the collision probabilities P^{io} and P^{oo} as a function of two variables lying in the range $0 \leqslant \kappa \leqslant 1$ and $0 \leqslant z$. The method gives results which are correct to a fractional error of less than 2×10^{-5}; six other probabilities may be evaluated simultaneously with no loss of significant figures.

The method is designed to take advantage of characteristics of a large set of problems for which the probabilities are required. In these cases–nuclear transmutation or neutron slowing-down—the geometry remains invariant and only the cross section varies. Precalculation of geometrical quantities thus leads to extremely efficient evaluations because in a majority of practical cases the variable z is small and only a few terms in the series are needed.

For practical applications however, the method is superior in both speed and accuracy in comparison to contemporary techniques of evaluation, and may have potential application to other functions of two variables (e.g. Sievert's integral).

REFERENCES

1. M. S. MILGRAM, *J. Mathematical Phys.* **18** (1977), 2456.
2. H. MÄRKL, Int. Conf. on the Peaceful Uses of Nuclear Energy, paper P/640, Session 3.1, Geneva, 1964, A/CONF. 28/.
3. D. EMENDÖRFER, Proceedings of the 1973 Conference on Mathematical Models and Computational Techniques for Analysis of Nuclear Systems, 1973, Paper VII (5), VII–136.
4. M. S. MILGRAM, Atomic Energy of Canada Limited Report AECL–5036, 1975; G. J. PHILLIPS AND J. GRIFFITHS, Atomic Energy of Canada Limited Report AECL–3857, 1970.
5. S. JABBAWY *et al.*, "Symposium on Applications of Nuclear Data in Science and Technology," p. 147, Conf. IAEA–SM–170/8, STI/PUB/343, Intern. At. Energy Agency, Vienna, 1973.
6. P. H. KIER AND A. A. ROBBA, Argonne National Laboratory Report ANL–7326, 1967; R. N. HWANG AND B. J. TOPPEL, *in* "Proceedings, 1979 ANS Topical Meeting on Computational Methods in Nuclear Engineering," Papers 7-7, 7-8.5.
7. H. C. HONECK, Module CREEP, DPSTM–500, 1970.
8. A. JONSSON, AEEW–R253, 1963.
9. R. BONALUMI, *Energia Nucleare* **8** (1961), 326.
10. A. MÜLLER AND E. LINNARTZ, *Nukleonik* **5** (1963), 23.
11. G. DOHERTY, AAEC/TM489, 1969.
12. F. S. ACTON, "Numerical Methods That Work," Harper & Row, New York, 1970.
13. J. H. JOHNSON AND J. M. BLAIR, Atomic Energy of Canada Limited Report AECL–4210, 1973.
14. M. B. CARVER AND V. J. JONES, Atomic Energy of Canada Limited Report AECL–5605, 1977.
15. J. M. BLAIR, C. A. EDWARDS, AND J. H. JOHNSON, *Math. Comp.* **32** (1978), 876.
16. M. S. MILGRAM AND K. N. SLY, Atomic Energy of Canada Limited Report AECL–6479, 1979.
17. Y. LUKE, "The Special Functions and Their Approximations," Vol. I, Academic Press, New York, 1969.
18. *Comput. Phys. Comm.* **8** (1974), 1.

RECEIVED: November 8, 1978; REVISED: February 12, 1979

MICHAEL S. MILGRAM AND KENNETH N. SLY

Applied Mathematics Branch
Atomic Energy of Canada Limited
Chalk River, Ontario, K0J 1J0, Canada