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COMPUTATION OF THE GOUDSMIT-SAUNDERSON DISTRIBUTION IN ELECTRON TRANSPORT

DAVE WALTER VANDE PUTTE

Isotopes and Radiation Division, Atomic Energy Board, Private Bag X256, Pretoria, South Africa

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Equations leading to the Goudsmit–Saunderson electron multiple scattering distribution are examined from a numerical point of view. Shorter methods are proposed for their solution.

1. Introduction

This paper deals with the computation of the electron multiple scattering distribution $f(\theta, t)$, according to Goudsmit and Saunderson's theory[1]).

One defines $f(\theta, t) \sin\theta \, d\theta$ as the probability that an electron will be deflected to an angle between θ and $\theta + d\theta$, relative to its initial direction, for a fractional residual path length equal to t.

The need to calculate $f(\theta, t)$ arises when solving electron transport problems by random sampling techniques on a digital computer. Since such techniques are generally time and memory consuming, in view of the many particle histories to be sampled, one has to devise the quickest methods of evaluating the distributions involved. In this respect, the present article considers the effect of double-precision arithmetic in calculating $f(\theta, t)$, as well as the cumulative distribution $F(\omega, t)$, in mono-elemental materials. $F(\omega, t)$ is the probability that $\cos\theta \geqslant \cos\omega$, for a given t.

The equations used in evaluating $f(\theta, t)$ and $F(\omega, t)$ appear in section 2, whereas the numerical aspects are treated in section 3.

2. Equations

Here, mathematical relations appear in a sequence that respects the order in which they are used in computations. A more conventional presentation is given by Berger[2]).

2.1. Ratio of Mott to Rutherford cross sections for single scattering: σ_m/σ_r

If $\theta = 0°$: $\sigma_m/\sigma_r = 1$.

If $0° < \theta \leq 10°$:

$$\sigma_m/\sigma_r = 1 + (\pi\beta^2 q/\sqrt{2}) \cos\gamma (1 - \cos\theta)^{\frac{1}{2}},$$

where

$$\beta^2 = \tau(\tau+2)/(\tau+1)^2,$$

and

$$\tau = E/0.510976,$$

with 0.510976 = electron rest mass energy (MeV),

E = electron energy (MeV),

$$q = \frac{Z}{137} \frac{\tau+1}{[\tau(\tau+2)]^{\frac{1}{2}}},$$

Z = atomic number of element through which the electron travels,

$$\cos\gamma = \mathrm{Re}\left[\frac{\Gamma(\frac{1}{2} - iq)}{\Gamma(\frac{1}{2} + iq)} \frac{\Gamma(1+iq)}{\Gamma(1-iq)}\right],$$

Γ = gamma function.

If $10° < \theta < 180°$:

$$\sigma_r = \frac{7.961759 \times 10^{-26} \times Z^2 \times (\tau+1)^2}{\tau^2(\tau+2)^2(1 - \cos\theta)^2},$$

$$\sigma_m = \frac{7.944723 \times 10^{-26} \times Z^2}{\tau^2(\tau+2)^2} |F_0 + F_1|^2 \operatorname{cosec}^2(\tfrac{1}{2}\theta) + \frac{1.491145 \times 10^{-21}}{\tau(\tau+2)} |G_0 + G_1|^2 \sec^2(\tfrac{1}{2}\theta), \quad (1)$$

where

$$F_0 = (i/2) \exp[iq \ln(\sin^2 \tfrac{1}{2}\theta)] \frac{\Gamma(1-iq)}{\Gamma(1+iq)},$$

$$G_0 = -iqF_0 \cot^2(\tfrac{1}{2}\theta),$$

$$F_1 = (i/2) \sum_{l=0}^{\infty} [lD_l + (l+1) D_{l+1}] P_l(\cos\theta), \quad (2)$$

$$G_1 = (i/2) \sum_{l=0}^{\infty} (-1)^l [l^2 D_l - (l+1)^2 D_{l+1}] P_l(\cos\theta),$$

$$D_l = \frac{\exp(-i\pi l)}{l+iq}\frac{\Gamma(l-iq)}{\Gamma(l+iq)} - \frac{\exp(-i\pi\rho_l)}{\rho_l+iq}\frac{\Gamma(\rho_l-iq)}{\Gamma(\rho_l+iq)},$$

$$\rho_l = [l^2-(Z/137)^2]^{\frac{1}{2}}, \qquad (2)$$

$P_l(\cos\theta)$: lth order Legendre polynominal.

If $\theta = 180°$: relation (1) no longer holds; in that case one assumes:

$$(\sigma_m/\sigma_r)_{180°} = (\sigma_m/\sigma_r)_{179°}.$$

2.2. Auxiliary function $h(E, \theta)$

$$h(E,\theta) = (\sigma_m/\sigma_r) - 1 - \left(\frac{\pi q}{\sqrt{2}}\right)\cos\gamma(1-\cos\theta+2\eta)^{\frac{1}{2}},$$

where

$$\eta = 1.7\times10^{-5}Z^{\frac{2}{3}}[\tau(\tau+2)]^{-1}(1.13+3.76q^2).$$

$h(E, \theta)$ must be approximated by a fifth-degree polynomial:

$$h(E,\theta) = \sum_{j=1}^{5} h_j(E)(1-\cos\theta+2\eta)^{j/2}. \qquad (3)$$

2.3. Expansion coefficients $G_l(E)$

$$G_l(E) = \frac{0.301314\,\rho Z(Z+1)}{W}\left[\frac{\tau+1}{\tau(\tau+2)}\right]^2 \times$$

$$\times\{p(-2,l)+[h_1(E)+(\pi q/\sqrt{2})\cos\gamma]\,p(-\tfrac{3}{2},l) +$$

$$+\sum_{j=2}^{5} h_j(E)\,p[\tfrac{1}{2}(j-4),l]\},$$

with W: atomic weight and ρ: density.

The $p(m, l)$ coefficients are obtained through a set of recursion relations:

$$p(m,0) = 0,$$

$$p(-2,1) = \ln(1+\eta^{-2}) - (1+\eta^{-1}),$$

$$lp(-2,l+1) = (2l+1)(1+2\eta)\,p(-2,l) - (l+1)\,p(-2,l-1) - (2l+1)(1+\eta)^{-1}, \quad (l \geq 1),$$

$$p(-\tfrac{3}{2},1) = 2(2\bar{\eta})^{\frac{3}{2}}(1+\bar{\eta})^{-1},$$

$$p(-\tfrac{3}{2},l+1) = \bar{\eta}\,p(-\tfrac{3}{2},l) + p(-\tfrac{3}{2},1), \quad (l \geq 1),$$

$$p(m+1,l) = (1+2\eta)\,p(m,l)+p(m,1) - \frac{l+1}{2l+1}\,p(m,l+1) - \frac{l}{2l+1}\,p(m,l-1),$$

where

$$\bar{\eta} = 1-2\eta[-1+(1+\eta^{-1})^{\frac{1}{2}}].$$

2.4. $f(\theta, t)$ and $F(\omega, t)$

By introducing the continuous slowing-down approximation, a one-to-one correspondence is established between the particle's energy, path length and fractional residual path length. It then follows that:

$$f(\theta,t) = \sum_{k=0}^{\infty}(k+\tfrac{1}{2})\exp\left(-\int_0^s G_k^*(s')\,ds'\right)P_k(\cos\theta), \qquad (4)$$

where

$$\int_0^s G_k^*(s')\,ds' = \frac{S_t C_1}{C_2}\frac{\bar{G}_k(1)}{\bar{G}_1(1)}\ln\left[\frac{t+C_2}{t(1+C_2)}\right],$$

S_t is the total path length corresponding to the initial energy,

s is the path length corresponding to the fractional residual path length t,

C_1 and C_2 are obtained by writing[2])

$$\overline{G_1}(t) = \frac{C_1}{t(t+C_2)},$$

for two values of t and then solving the system,

$G_k(s)$ is obtained from $G_k(E)$ when passing from E to s,

$\bar{G}_k(t)$ is obtained from $G_k(E)$ when passing from E to t.

In random sampling one uses $F(\omega, t)$ rather than $f(\theta, t)$.

$$F(\omega,t) = \tfrac{1}{2}(1-\cos\omega) + \sum_{k=1}^{\infty}\tfrac{1}{2}C_k[P_{k-1}(\cos\omega) - P_{k+1}(\cos\omega)], \qquad (5)$$

where

$$C_k = \exp\left(-\int_0^s G_k^*(s')\,ds'\right).$$

3. Numerical aspects

3.1. Ratio of Mott to Rutherford single scattering cross section

Because of their slow convergence, the series (2) have to be transformed[4,5]):

If

$$g(\theta) = \sum_{k=0}^{\infty} a_k P_k(\cos\theta),$$

then

$$(1-\cos\theta)^m g(\theta) = \sum_{k=0}^{\infty} a_k^{(m)} P_k(\cos\theta), \qquad (6)$$

where

$$a_k^{(m)} = a_k^{(m-1)} - \frac{k+1}{2k+3} a_{k+1}^{(m-2)} - \frac{k}{2k-1} a_{k-1}^{(m+1)},$$

$$a_k^{(0)} \equiv a_k, \qquad a_{-1}^{(i)} \equiv 0,$$

m: order of the transformation,
an accepted procedure being $m = 3$, summation over 150 terms in single-precision.

In the present study, eleven elements were considered ($Z = 6$, 12, 13, 26, 29, 47, 50, 74, 79, 82, 92) together with seven energies (100, 10, 4, 0.7, 0.4, 0.1 and 0.05 MeV) and angles ranging from 10° to 179°. (For angles less than 10°, no series have to be summed.)

Direct summation (i.e. no transformation) and transformations up to the fifth order were investigated in both single and double-precision arithmetic. In no instance were more than 200 terms used. Results of double-precision arithmetic are summarised in table 1.

As can be seen from table 1, double-precision offers two procedures, namely $m=2$ or $m=3$. The maximum discrepancy between them is approximately 0.03% and appears in the case of angles between 10° and 20°. Only 16 terms suffice to attain convergence; in the case of 200 terms results are within 0.001% of those obtained with 16 terms.

In single-precision, no summation procedure showed convergence for all Z, E and θ envisaged. Consequently, double-precision with a second-order transformation and 16 terms is the optimum method of summing series (2). Furthermore, throughout the investigation, identical calculations carried out in single and double-precision required only 15% more machine time in the latter case (IBM. SYST/370-MODEL 155-IH). And since far fewer terms are required, an overall time-economisation is achieved.

3.2. Polynomial expansion of $h(E, \theta)$

One requires a set of coefficients $\{h_j(E)\}$ such that

$$h(E,\theta) = \sum_{j=1}^{5} h_j(E)(1-\cos\theta+2\eta)^{j/2},$$

$$0 \le \theta \le \pi, \text{ for a given } E.$$

Although one can determine $h(E, \theta)$ exactly for any combination of (E, θ), it is not known a priori that this function is in fact a linear combination of powers of $(1-\cos\theta+2\eta)^{\frac{1}{2}}$. Two attitudes are therefore possible. Either the approximating function can be required to be equal to $h(E, \theta)$ for five values of θ ($\{h_j(E)\}$ is then solution of a set of five linear equations) or one can use a least squares approximation. Both methods are sensitive to the way in which the input data are chosen, but the latter requires more than five values of $h(E, \theta)$ to be of interest. Seeing that each of these values requires an evaluation of series (2), the first attitude is adopted.

Although discrepancies of up to 1.2% occurred

Table 1

Results obtained when calculating σ_m/σ_r in double-precision arithmetic Z: atomic number, E: electron energy, θ angle

Order of transformation	Effect specifically due to Z	Effect specifically due to E	Effect specifically due to θ
Direct summation	20% overestimation at $\theta<90°$ for heavy elements	—	No convergence for $\theta>90°$
$m=1$	—	300% overestimation in light elements if $E>1$ MeV	5% error if $\theta<90°$
$m=2$	Convergence for all Z	Convergence for all E	Convergence for all θ
$m=3$	Convergence for all Z	Convergence for all E	Convergence for all θ
$m=4$	3% underestimation if $\theta<90°$ for light elements and 200% overestimation for heavy elements if $10°<\theta<20°$	—	3% underestimation if $\theta<90°$ for light elements and 200% overestimation for heavy elements if $10°<\theta<20°$
$m=5$	No convergence	No convergence	No convergence

TABLE 2

Results obtained when calculating $f(\theta,t)$ in double-precision arithmetic.

Direct summation	Fails for $Z = 5$, 12, 13, for $E_s = 5$ to 10 MeV and for penetration of the order of 0.99 (small penetrations)
$m = 1$	Converges for all E_s, Z, t, θ
$m = 2$	Fails for small penetrations ($t \approx 0.90$), at small angles (1°–5°) when $E_s = 5$ to 10 MeV

between the true and approximating functions, choosing this particular method did not influence the final values of $f(\theta, t)$ and $F(\omega, t)$.

3.3. GOUDSMIT–SAUNDERSON DISTRIBUTION

Next, series (4) is to be summed. Eleven materials were selected ($Z = 6$, 12, 13, 26, 29, 47, 50, 74, 79, 82, 92). Angles ranged from 0 to π and fractional residual path lengths from approximately 0.99 to 0.1. Starting energies E_s (MeV) were chosen so that radiation energy losses equalled at the most 10% of collisional losses, in order that the continuous slowing-down approximation introduced in eq. (4) be valid[3]). This implies $E_s \leq 66Z$.

First of all, the $p(m, l)$'s of section 2.3 are to be evaluated. The use of single or double-precision was found to have no effect on the subsequent behaviour of series (4). Up to 200 terms were introduced and transformation eq. (6) was used to improve convergence, except for $\theta = 0$ where it is not valid.

The results of double-precision computations are summarised in table 2.

Contrary to series (2), no general "recipe" can be given for summing eq. (4). The number of terms in eq. (4) for $m = 1$ varies greatly with t, Z, E_s and θ, a general tendency being that the smaller the penetrations, Z, θ and the greater E_s, the more terms are needed, e.g. 150 terms for $Z = 6$, $E_s = 10$ MeV, $\theta = 2°$, $t = 0.99068$, while only eight terms for $Z = 82$, $E_s = 1$ MeV, $t = 0.45$, at all angles. The most dramatic effect is due to decreasing Z.

Single-precision proved inadequate, except in cases of deep penetrations ($t \approx 0.5$–0.1), low initial energies, or high Z materials.

3.4. CUMULATIVE DISTRIBUTION

One has to sum series (5) to obtain $F(\omega, t)$. Direct summation in double-precision was found to be adequate in all cases. Here again, the number of terms in eq. (5) varies greatly with Z, E_s and t. Usually 10 to 20 terms suffice; however, for light elements ($Z = 6$, 12, 13) and low penetrations ($t \approx 0.99$), up to 120 terms are required (see table 3).

TABLE 3

$f(\theta,t)$ and $F(\omega,t)$ for $Z = 6$, $E_s = 10$ MeV, $t = 0.99068$.

θ(°)	$f(\theta,t)$	ω(°)	$F(\omega,t)$: 50 terms	$F(\omega,t)$: 90 terms	$F(\omega,t)$: 120 terms
1.00	972.8693	1.00	0.1018	0.1401	0.1441
2.00	467.0296	2.00	0.3622	0.3622	0.4491
5.00	27.4013	5.00	1.0195	0 9234	0.9298
10.00	0.7978	10 00	0.9895	0 9930	0.9900
15.00	0.9387	15 00	0.9387	0 9994	0.9961
30.00	0.0117	30.00	0.9676	1.0023	0.9992
60.00	0.0009	60.00	1.0189	0.9977	0.9999
90.00	0.0002	90.00	1.0155	1.0012	1.0000
120.00	0.0001	120.00	0.9887	0.9996	1.0000
150.00	0.0000	150.00	0.9920	0.9998	1 0000
165.00	0.0000	165.00	0.9998	1.0006	1.0000
180.00	0.0000	180.00	1.0000	1.0000	1.0000

In cases such as those of table 3, single-precision fails, otherwise, its results agree to within 0.01% with those of double-precision arithmetic.

4. Conclusion

Double-precision arithmetic emerges as being superior to single-precision arithmetic. It speeds up convergence and produces it even in cases where single-precision fails. However, it does not increase the accuracy of calculations when no convergence problems occur. Its use should be generalized in this type of calculation.

Transformation (6) proves useful, but one must not "overdo it" by applying it too repeatedly to a series (table 1).

Finally, there is considerable advantage in computing the cumulative distribution directly.

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