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A Monte-Carlo Method for Calculations of the Distribution of Angular Deflections due to Multiple Scattering

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A Monte Carlo method for calculation of the distribution of angular deflections of fast charged particles passing through thin layer of matter is described on the basis of Molière theory of multiple scattering. The distribution of the angular deflections obtained as the result of calculations is compared with Molière theory. The method proposed is useful to calculate the electron transport in matter by Monte Carlo method.

I. INTRODUCTION

When fast charged particles pass through the matter, they are deflected laterally from their original path by multiple Coulomb scattering. The theory of multiple scattering has been developed in considerable detail and elegance in many papers.[1~7] In all the theories the thickness of matter is assumed to be thick enough so that the number of collisions is large but thin enough so that energy loss is negligible. Of these theories, the Molière theory has often been used for Monte Carlo calculations of electron transport in matter because of its simplicity and reasonable accuracy.[8~10] Messel *et al.*[11] have proposed a random sampling technique of angular deflections on the basis of Molière theory. Their method uses combination of the composition and rejection techniques, and was recently modified by Sugiyama.[9] In the previous work,[10] we tested the validity of the method of Messel *et al.* and Sugiyama. However, this method is tedious and time consuming. In view of the many particle histories to be sampled, it is hoped to devise simpler method.

The main purpose of the present paper is to present a quick and simple method to calculate the angular deflection due to Molière scattering by using the direct sampling technique. The numerical values used for sampling are calculated numerically and given in the table. The validity of the present method has been tested by comparing the angular distribution obtained as the result of our Monte Carlo calculations with that of Molière theory.

II. METHOD OF CALCULATION

According to the Molière theory, the probability that an electron will have angle between Θ and $\Theta+d\Theta$ after traversing distance t can be written by

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$$f(\Theta)\mathrm{d}\Theta=\theta\mathrm{d}\theta[f^{(0)}(\theta)+f^{(1)}(\theta)/B+f^{(2)}(\theta)/B^2+\cdots\cdots\cdots], \tag{1}$$

where the reduced angle θ is

$$\theta=\Theta/(\chi_c B^{1/2}). \tag{2}$$

The parameter χ_c depends on the thickness as well as the energy and is defined as

$$\chi_c{}^2=4\pi Nt\, e^4\, Z(Z+1)/(pv)^2, \tag{3}$$

where N is the number of atoms per cm^3, e the charge of the electron, and p and v the momentum and the velocity of the electron, respectively. The parameter B is obtained by solving the transcendental equation:

$$B-\ln B=b, \tag{4}$$

where

$$b=\ln(\chi_c/\chi_a)^2+1-2C. \tag{5}$$

Here $C=0.5772156\ldots$ is the Euler constant. The screening angle χ_a is defined as

$$\chi_a{}^2=\chi_0{}^2[1.13+3.76(Ze^2/hv)^2], \tag{6}$$

and the angle χ_0 is

$$\chi_0=\lambda\!\!\!^{-}/(0.885a_0\, Z^{-1/2}), \tag{7}$$

where $\lambda\!\!\!^{-}$ is the de Broglie wave length of the electron and a_0 is the first Bohr radius.

It has been shown by Bethe[6] that the function $f^{(0)}$ to $f^{(2)}$ are sufficient to determine the distribution function to about 1% or better for any angle. The functions $f^{(0)}$, $f^{(1)}$, and $f^{(2)}$ are expressed in terms of $x=\theta^2$ as[3]

$$f^{(0)}=2e^{-x}, \tag{8}$$

$$f^{(1)}=2\mathrm{e}^{-x}(x-1)[\overline{\mathrm{Ei}}(x)-\ln x]-2(1-2\mathrm{e}^{-x}), \tag{9}$$

$$f^{(2)}=\mathrm{e}^{-x}\Big([\psi^2(2)+\psi(2)](x^2-4x+2)+4\int_0^1 y^{-3}\mathrm{d}y[\ln y/(1-y)-\psi(2)]$$
$$\times[(1-y^2)\mathrm{e}^{xy}-1-(x-2)y-(x^2/2-2x+1)y^2]\Big), \tag{10}$$

where $\psi(n)=\mathrm{d}\{\ln\Gamma(n+1)\}/\mathrm{d}n$, $\overline{\mathrm{Ei}}(x)$ is the exponential integral defined by Jahnke and Emde.[12]

According to Bethe,[6] the integral in Eq. (10) can be written in a power series as obtained by Goldstein;

$$\text{Integral}=\sum_{n=0}^{\infty}\frac{1}{n+1}[\psi(n)+C-\psi(2)]\left(\frac{x^{n+3}}{(n+3)!}+\frac{2x^{n+2}}{(n+2)!}+\frac{x^{n+1}}{(n+1)!}\right). \tag{11}$$

In order to sample the angular defelction from Eq. (1), the direct sampling technique was used. Let r be a random number uniformly distributed over the interval (0, 1). Then a set of random numbers $\{\theta\}$, which has the density function $f(x)$, can be obtained from[13]

$$r=\int_{-\infty}^{\theta(r)} f(u)\mathrm{d}u. \tag{12}$$

Since the lower limit of θ is 0, the integration should be made between 0 and ∞. From Eqs. (1) and (12), we obtain a random number by solving the equation for θ:

$$r=\sum_{i=0}^{2}F^{(i)}(\theta)/B^i, \tag{13}$$

where

$$F^{(i)}(\theta)=\int_0^\theta f^{(i)}(u)\mathrm{d}u. \tag{14}$$

For this purpose, it is useful to present a table of $F^{(i)}$ as a function of θ.

III. RESULTS AND DISCUSSION

From Eqs. (8), (9), and (10), we calculated the functions $f^{(0)}$, $f^{(1)}$, and $f^{(2)}$ on the FACOM M-190 computer of the Data Processing Center of Kyoto University. In general, agreement between the present results and the previous values of Molière[3] and of Bethe[4] is good.

The calculations of the integrals $F^{(i)}(\theta)$ have been made numerically by the use of the $f^{(i)}(\theta)$ values calculated above. The results are listed in table I. It should be noted that the integral of the function $f^{(0)}$ from 0 to ∞, $F^{(0)}(\infty)$, yields to be unity, whereas other two integrals, $F^{(1)}(\infty)$ and $F^{(2)}(\infty)$, become zero. By using these values and Eq. (13), random sampling from the Molière distribution can be made.

In order to test the validity of the present method, the Monte Carlo calculations of angular deflections have been performed and comparison has been made with the Molière theory. Figure 1 shows the result of 50,000 events for $B=5$. It can be seen from the figure that the distribution is in good agreement with the Molière distribution calculated analytically.

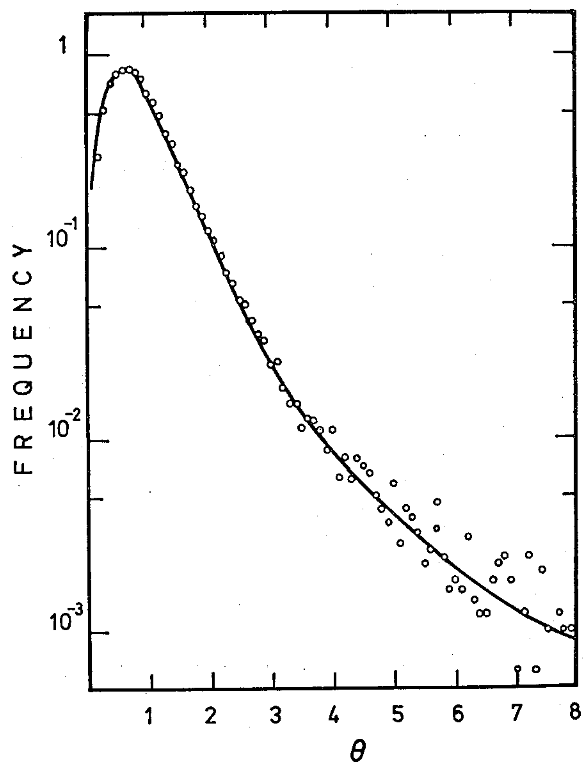

Fig. 1. Comparison of the distribution of random variates with the Molière theory.

Table I. Functions $F^{(0)}(\theta)$, $F^{(1)}(\theta)$, and $F^{(2)}(\theta)$ of the Moliere scattering.

θ	$F^{(0)}\theta$	$F^{(1)}\theta$	$F^{(2)}\theta$
0.0	0.0	0.0	0.0
0.2	0.0392106	0.0154745	0.0455467
0.4	0.1478562	0.0464374	0.1373463
0.6	0.3023236	0.0580940	0.1838614
0.8	0.4727075	0.0218099	0.1321979
1.0	0.6321205	−0.650543	0.0126277
1.2	0.7630722	−0.1782689	−0.0936320
1.4	0.8591415	−0.2824504	−0.1234883
1.6	0.9226952	−0.3500982	−0.0733350
1.8	0.9608361	−0.3718558	0.0128890
2.0	0.9816844	−0.3549602	−0.0844011
2.2	0.9920929	−0.3148239	0.1147103
2.4	0.9968489	−0.2665861	0.1062038
2.6	0.9988408	−0.2205301	0.0765804
2.8	0.9996063	−0.1814935	0.0435778
3.0	0.9998766	−0.1504422	0.0173933
3.2	0.9999643	−0.1264022	0.0006926
3.4	0.9999905	−0.1078331	−0.0080980
3.6	0.9999976	−0.0933110	−0.0117323
3.8	0.9999995	−0.0817399	−0.0125431
4.0	0.9999999	−0.0723401	−0.0120307
4.2	1.0000000	−0.0645705	−0.0110082
4.4	1.0000000	−0.0580535	−0.0098628
4.6	1.0000000	−0.0525197	−0.0087585
4.8	1.0000000	−0.0477718	−0.0077546
5.0	1.0000000	−0.0436619	−0.0068653
5.2	1.0000000	−0.0400768	−0.0060865
5.4	1.0000000	−0.0369281	−0.0054076
5.6	1.0000000	−0.0341457	−0.0048167
5.8	1.0000000	−0.0316736	−0.0043019
6.0	1.0000000	−0.0294663	−0.0038528
6.2	1.0000000	−0.0274864	−0.0034602
6.4	1.0000000	−0.0257032	−0.0031160
6.6	1.0000000	−0.0240910	−0.0028134
6.8	1.0000000	−0.0226283	−0.0025468
7.0	1.0000000	−0.0212968	−0.0023110
7.2	1.0000000	−0.0200811	−0.0021021
7.4	1.0000000	−0.0189680	−0.0019165
7.6	1.0000000	−0.0179460	−0.0017510
7.8	1.0000000	−0.0170054	−0.0016032
8.0	1.0000000	−0.0161377	−0.0014708
8.2	1.0000000	−0.0153355	−0.0013515
8.4	1.0000000	−0.0145922	−0.0012450
8.6	1.0000000	−0.0139021	−0.0011485
8.8	1.0000000	−0.0132604	−0.0010613
9.0	1.0000000	−0.0126624	−0.0009823
9.2	1.0000000	−0.0121043	−0.0009107
9.4	1.0000000	−0.0115826	−0.0008455
9.6	1.0000000	−0.0110942	−0.0007861
9.8	1.0000000	−0.0106362	−0.0007320
10.0	1.0000000	−0.0102063	−0.0006824

The computation time of the present method is about 1/5 of the conventional method of Messel *et al.*[11] for this example.

In conclusion, the present method is quicker than the conventional method and reasonably accurate. Therefore, the present method can be successfully used in electron Monte Carlo calculations to determine angular deflections due to multiple scattering.

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