Multiple Scattering of High-Energy Electrons from Beryllium

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The multiple-scattering distribution function for high-energy electrons scattered from a beryllium foil has been calculated, following a method discussed in an earlier paper. Calculations were done with Thomas-Fermi as well as Hartree-Fock potentials for the beryllium atom. The results obtained with the Hartree-Fock potential were found to be in better agreement with the experimental results.

I. INTRODUCTION

In an earlier paper[1] (henceforth referred to as I), we discussed a method for calculating the distribution function for multiple scattering of high-energy Dirac particles from thin foils. Molière's[2] representation for the Thomas-Fermi potential of the scattering atom was considered, and in the case of a heavy scatterer, the calculated results were found to be in agreement with the experimental results of Hanson, Lanzl, Lyman, and Scott.[3] However, for beryllium, the calculated $1/e$ width of the distribution function $\chi_{1/e}$ was higher than the experimental value. Reed,[4] who followed the method of Nigam, Sundaresan, and Wu,[5] found a still higher value, but not much different from the value obtained in I. In the method of Nigam *et al.*, the multiple-scattering distribution function was calculated starting from the second Born-approximation results of Dalitz[6] for single scattering. On the other hand, we utilized in I the single-scattering results obtained by following the method of Mukherjee and Majumdar.[7] It is not difficult to see why the two methods which gave different results for heavy scatterers should give almost similar results for beryllium. The first Born approximation is sufficiently good for small-angle scattering from beryllium at the energy considered, and any correction to it (either by the Dalitz formula or by the method we followed in I) is not very significant. In fact, any approximate scattering solution gives in this case multiple-scattering results close to those obtained by the first Born approximation. The large discrepancy between the theoretical and the experimental results for multiple scattering, therefore, cannot be due to the approximate nature of the solution for single scattering and can be removed only by considering a more accurate potential than is given by the Thomas-Fermi model. The model is known to be sufficiently accurate for heavy atoms, and the calculations in I also confirm this. The same, however, is not true in the case of light atoms.[8] It is, therefore, worth while to compare the results obtained with the more accurate Hartree-Fock potential. The purpose of this paper is to report the results of the calculations done with the Hartree-Fock potential for beryllium.

Hartree and Hartree[9] calculated the atomic potential $v(r)=-Z_p(r)e^2/r$ for beryllium, where $Z_p(r)$ is the effective atomic number at the distance r. Fleischmann[10] fits the numerical values of $Z_p(r)$, which includes the contributions of the exchange terms, by the expression

$$Z_p(r)=4[\exp(-2.45r/a_0)+1.43(r/a_0)^2 \times\exp(-2.00r/a_0)+0.001(r/a_0)^4\exp(-r/a_0)], \quad (1)$$

where a_0 is the Bohr radius. This agrees within 1% with the calculation of Hartree and Hartree for $0<r/a_0\leq 4$. The expression, however, is not very convenient for multiple-scattering calculations, the presence of the terms with r^2 and r^4 introducing very long and almost unmanageable calculations. We tried to find an alternative analytic expression of the form

$$Z_p(r)=4[a_1\exp(-b_1r/r_0)+a_2(r/r_0)\exp(-b_2r/r_0)] \quad (2)$$

and obtained the best fit[11] with the following values of the constants:

$$a_1=1.00, \qquad b_1=1.09r_0/a_0,$$
$$a_2=-1.54r_0/a_0, \qquad b_2=3.28r_0/a_0, \quad (3)$$

where r_0 is the Thomas-Fermi radius. The value of $\chi_{1/e}$ calculated with this potential shows better agreement with the experimental value, supporting the belief that for light atoms the Hartree-Fock potential is more reliable than that obtained by the Thomas-Fermi method. A further improvement is likely if the modifications in the atomic potential due to the crystalline structure of beryllium metal is taken into account. Unfortunately, this cannot be done by an analytical approach and will not be considered here.

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[11] This agrees with Fleischmann's expression for Z_p within 0.008 for $0\leq r/a_0<2.5$ and within 0.002 elsewhere.

II. SINGLE-SCATTERING AMPLITUDES

The single-scattering matrix $T(\mathbf{P}, \mathbf{P}')$[1,7] for the potential (2) involves integrals like

$$I_0=\int r^{-1}\exp[(i\mathbf{q}\cdot\mathbf{r}-\lambda r)]F(ia\epsilon/p,\ 1,\ ipr-i\mathbf{P}\cdot\mathbf{r})\,d\mathbf{r}, \tag{4}$$

as well as

$$I_1=\int \exp[(i\mathbf{q}\cdot\mathbf{r}-\lambda r)]F(ia\epsilon/p,\ 1,\ ipr-i\mathbf{P}\cdot\mathbf{r})\,d\mathbf{r}, \tag{5}$$

where all the symbols have the same significance as in I. The integrals can be evaluated following Mukherjee and Majumdar,[7] and we get

$$T(\mathbf{P}, \mathbf{P}')=\exp[(1/2)\pi a\epsilon/p]\frac{\Gamma(1-ia\epsilon/p)}{\Gamma(1+ia\epsilon/p)}[2\epsilon a+a\boldsymbol{\alpha}\cdot(\mathbf{P}'-\mathbf{P})]$$
$$\times\left\{\frac{a_1}{[4p^2\sin^2(\tfrac{1}{2}\theta)+b_1^2/r_0^2]}\left(\frac{4p^2\sin^2(\tfrac{1}{2}\theta)+b_1^2/r_0^2}{b_1^2/r_0^2-2ippb_1/r_0}\right)^{ia\epsilon/p}+\frac{a_2}{r_0}\left[\frac{2(1-ia\epsilon/p)(b_2/r_0)}{[4p^2\sin^2(\tfrac{1}{2}\theta)+b_2^2/r_0^2]^2}\right.\right.$$
$$\left.\left.+\frac{i(a\epsilon/p)(2b_2/r_0-2ip)}{(b_2^2/r_0^2-2ipb_2/r_0)[4p^2\sin^2(\tfrac{1}{2}\theta)+b_2^2/r_0^2]}\left(\frac{4p^2\sin^2(\tfrac{1}{2}\theta)+b_2^2/r_0^2}{b_2^2/r_0^2-2ipb_2/r_0}\right)^{ia\epsilon/p}\right]\right\}. \tag{6}$$

The scattering amplitudes $f(\theta)$ and $g(\theta)$ were calculated from (6) following the method discussed in I. With terms of order $a^2\epsilon^2/p^2$ neglected, the quantity $J(\theta)$ may be written in the small-angle approximation as

$$J(\theta)=f^*f+\theta^2g^*g$$
$$=\exp(\pi\bar{a})\frac{4\bar{a}^2}{p^2}\left[1+\theta^2\frac{(\epsilon-1)^2}{4\epsilon^2}\right]\times\left\{\frac{a_1^2}{(\theta^2+\theta_1^2)^2}s_1+\frac{4a_2^2\theta_0^2\theta_2^2}{(\theta^2+\theta_2^2)^4}s_2+2\ \mathrm{Re}\ \frac{(-i\bar{a})a_2^2\theta_0^2(4\theta_2^2-4i\theta_2)}{(\theta_2^2-2i\theta_2)(\theta^2+\theta_2^2)^3}s_2\right.$$
$$\left.+2\ \mathrm{Re}\left[\frac{2a_1a_2\theta_0\theta_2(1+i\bar{a})}{(\theta^2+\theta_1^2)(\theta^2+\theta_2^2)^2}+\frac{a_1a_2\theta_0(-i\bar{a})(2\theta_2+2i)}{(\theta_2^2+2i\theta_2)(\theta^2+\theta_1^2)(\theta^2+\theta_2^2)}\right]\left(\frac{\theta^2+\theta_1^2}{\theta^2+\theta_2^2}\right)^{i\bar{a}}s_{12}\right\}, \tag{7}$$

where

$$\bar{a}=a\epsilon/p,$$
$$s_1=\exp[-2\bar{a}\tan^{-1}(2/\theta_1)],$$
$$s_2=\exp[-2\bar{a}\tan^{-1}(2/\theta_2)],$$
$$s_{12}=[(\theta_2^2+2i\theta_2)/(\theta_1^2-2i\theta_1)]^{i\bar{a}}, \tag{8}$$

and $\theta_0=1/pr_0$ and $\theta_i=b_i\theta_0$. The contribution of the term θ^2g^*g is very small and will be neglected subsequently.

III. SCREENING ANGLE AND MULTIPLE-SCATTERING DISTRIBUTION FUNCTION

To calculate the multiple-scattering distribution function $f(x)$, we shall have to evaluate the integral

$$\tilde{j}(\xi)-\tilde{j}_0=2\pi nt\int\theta d\theta J(\theta)\,[J_0(\xi\theta)-1], \tag{9}$$

where n is the number of scattering centers per unit volume, and t is the path traversed by the particles. The integrals occurring in (9) may be evaluated following I. It will be convenient, however, to express $\tilde{j}(\xi)-\tilde{j}_0$ in terms of a screening angle θ_α defined by

$$\lambda\ln\theta_\alpha=-\tfrac{1}{2}\lambda-\lim_{\theta_s\to\infty}\left[\int_0^{\theta_s}\frac{q(\theta)}{\theta}\,d\theta-\lambda\ln\theta_s\right], \tag{10}$$

where $q(\theta)$ is defined by (2.13) of I, and λ is given by

$$\lambda = \exp(\pi\bar{a})\left[a_1^2 s_1 + 2\,\mathrm{Re}\,\frac{a_1 a_2(-i\bar{a})\theta_0(2\theta_2+2i)}{(\theta_2^2+2i\theta_2)}\,s_{12}\right]. \tag{11}$$

The screening angle is then given by

$$\lambda\ln\theta_a^2 = \lambda\ln\theta_0^2 + \exp(\pi\bar{a})\left\{a_1^2 s_1\ln b_1 - \frac{a_2^2}{3b_2^2}s_2 + \mathrm{Re}\,\frac{(i\bar{a})a_1a_2}{b_2}s_{12} + \mathrm{Re}\,a_1a_2s_{12}\left[\frac{i\bar{a}}{b_2} - \frac{(1+i\bar{a})2b_2}{b_2^2-b_1^2}\right]\right.$$
$$\times\left[\frac{b_1^2\ln b_1^2 - b_2^2\ln b_2^2}{b_2^2-b_1^2} - i\bar{a}\mathfrak{L}_2\left(\frac{b_2^2-b_1^2}{b_2^2}\right) + \tfrac{1}{2}(i\bar{a})\frac{b_1^2}{b_2^2-b_1^2}\ln^2\frac{b_1^2}{b_2^2}\right]$$
$$\left. - \mathrm{Re}\,a_1a_2s_{12}\frac{(1+i\bar{a})2b_2}{b_2^2-b_1^2}\left[1 + \ln b_2^2 + i\bar{a}\sum_{k=1}^{\infty}\frac{1}{k^2(k+1)}\left(\frac{b_2^2-b_1^2}{b_2^2}\right)^k\right]\right\}, \tag{12}$$

where $\mathfrak{L}_2(x)$ is Euler's dilogarithm[12] defined by

$$\mathfrak{L}_2(x) = \sum_{n=1}^{\infty}\frac{x^n}{n^2} = -\int_0^x \frac{\ln(1-y)}{y}\,dy. \tag{13}$$

$\tilde{j}(\xi)-\tilde{j}_0$ may be expressed in terms of this screening angle as

$$\tilde{j}(\xi)-\tilde{j}_0 = \tfrac{1}{4}\lambda\theta_c^2\xi^2\ln(\gamma^2\xi^2\theta_a^2/4e), \tag{14}$$

where $\ln\gamma$ is Euler's constant, and θ_c is the characteristic angle for the particular scattering experiment. The multiple-scattering distribution function can be written now in the familiar form of Molière, viz.,

$$f(\varphi) = (2\pi)^{-1}\int\eta d\eta\, J_0(\varphi\eta)\,\exp[-\tfrac{1}{4}\eta^2 + (\eta^2/4B)\ln(\tfrac{1}{4}\eta^2)], \tag{15}$$

where $\eta = \xi\theta_c(\lambda B)^{1/2}$, and $\varphi = \chi/\theta_c B^{1/2}\lambda^{1/2}$ is the reduced angular variable. The parameter B satisfies Eq. (2.16) of I, with λ given by (11) of the present article.

The integral (15) was evaluated numerically for different values of φ by an IBM 1620 digital computer and the $1/e$ width of the distribution function calculated. We have compared in Table I the different results for the scattering of 15.24-MeV electrons from a beryllium foil. It is seen that with the Hartree-Fock potential for beryllium, the value of $\chi_{1/e}$ calculated by the present method shows improved agreement with the experimental results of Hanson *et al.* The discrepancy that still remains is noticeable and may possibly be accounted for by considering the crystalline structure of metallic beryllium. An expression for $Z_p(r)$ which fits the Hartree-Fock calculations better than the expression (2) may also give a little improvement.

TABLE I. Multiple scattering of 15.24-MeV electrons from beryllium; $\rho_0 t = 491.3$ mg/cm^2; $\theta_c = 1.506°$.

	λ	B	$\chi_{1/e}$(degrees)
Experiment[a]			4.25
Hartree-Fock	0.9991	10.003	4.438
Thomas-Fermi	0.9993	10.263	4.507
Thomas-Fermi (Reed,[b] $\mu=1.00$)		10.267	4.523

[a] Hanson *et al.* (Ref. 3).
[b] R. D. Reed (Ref. 4).

[12] K. Mitchell, Phil. Mag. **40**, 351 (1949), gives tables for $\mathfrak{L}_2(x)$ for $-1\leq x\leq 1$.

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