THE SCATTERING OF ELECTRONS BY FREE NEUTRAL ATOMS IN THE THOMAS-FERMI MODEL

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In this paper using the approximate solution of the Thomas-Fermi equation for free neutral atom given by BUCHDAHL we derive an analytical formula for the scattered intensity by a group of free atoms. The scattered intensity concerns the elastic and inelastic scattering for singly scattered electrons by free atoms in the Thomas-Fermi model. A comparison with the numerical results shows that our formula for the sacttered intensity is very accurate.

I. Introduction

When a beam of electrons strikes a free atom, the intensity of scattered electrons varies with the scattering angle in a way dependent upon the nuclear charge and electronic structure of the atom, and the energy of the incident electrons. In this paper we obtain an analytical formula for the scattered intensity $I(s)$ by a group of free atoms. BORN[1] and MOTT[2], as known. were the first, who obtained the scattered intensity $I(s)$ for elastic scattering, MORSE[3] extended the Born approximation to include inelastic scattering, obtaining the expression for singly scattered electrons

$$I(s) = \frac{I_0 N}{R^2}\left(\frac{8\pi^2 me^2}{h^2}\right)^2 \frac{1}{s^4}\{[Z - F(s)]^2 + Z\,S(s)\}, \tag{1}$$

where I_0 is the intensity of the incident electron beam, N the number of independently scattering atoms intercepted by the beam, R the distance between the point of observation of the scattered electrons, s the variable $\left(4\pi \sin\frac{1}{2}\Theta\right)/\lambda$, λ is the de Broglie wavenlength of the incident beam, Θ the scattering angle, Z the atomic number of the atoms, $F(s)$ the x-ray atomic scattering factor of the atoms, and $S(s)$the x-ray incoherent scattering function of the atoms. The term $[Z - F(s)]^2$ represents the elastic scattering and the term $S(s)$ represents the inelastic scattering.

[1] M. BORN, Z. Phys., **38**, 803, 1926.
[2] N. P. MOTT, Proc. Roy. Soc. (London) (A), **124**, 425, 1928; **127**, 658, 1930.
[3] P. M. MORSE, Z. Phys., **33**, 443, 1932.

II. Theory

Since the exact values of the Thomas-Fermi function $\varphi_0(x)$ are given only for the discrete values of the argument x, the evaluation of the atom form factor $F(s)$ of the Thomas-Fermi atom[4] of the atomic number Z

$$F(s) = \int_0^\infty \frac{\sin sr}{sr} \varrho\, 4\pi r^2\, dr \tag{2}$$

$$= Z\left[1 - s\mu \int_0^\infty \sin s\mu x \cdot \varphi_0(x)\, dx\right], \tag{3}$$

where μ is the Thomas-Fermi unit, was carried out by BRAGG and WEST[5] in such a way that exact values were taken for φ_0 and the integral was approximated by a sum. The results can be given naturally only in tabular form, so that the dependence on Z as well as on s is at first sight not clear except the similarity rule that the F-curves for an atom Z_0 is transformed so as to be suitable for any other atom Z by multiplying F and s by Z/Z_0 and $(Z/Z_0)^{1/3}$, respectively. Moreover, owing to the oscillating nature of sine, it is necessary to take the summation in as small steps as possible. The term $S(s)$ responsible for the inelastic scattering, as known[6], is given by

$$S(s) = 1 - \int_0^{x_0} \left\{\left[\frac{\varphi_0(x)}{x}\right]^{1/2} - w\right\}^2 \left\{\left[\frac{\varphi_0(x)}{x}\right]^{1/2} + \frac{1}{2} w\right\} x^2\, dx, \tag{4}$$

where w is defined by

$$w = \frac{0{,}176 \cdot 10^{-8}\,\mathrm{cm}}{Z^{2/3}}\, s, \tag{5}$$

and x_0 is the root of the following equation

$$\left[\frac{\varphi_0(x)}{x}\right]^{1/2} = w. \tag{6}$$

[4] P. GOMBÁS, Die statistische Theorie des Atoms und ihre Anwendungen, Wienna 1949; p. 245.
[5] W. L. BRAGG and J. WEST, Z. Krist. u. Mineral., **69**, 118, 1929.
[6] W. HEISENBERG, Phys. Z., **51**, 213, 1932.

III. Procedure and result

Since the exact solution of the Thomas-Fermi equation

$$\varphi_0''(x) = \varphi_0^{3/2}(x)/x^{1/2} \tag{7}$$

is available only numerically, its approximate expression in a closed analytical form is desirable for practical purposes. Hitherto[7] several different forms have been given. A detailed consideration of the author has shown that the best approximate solutions of the Thomas-Fermi equation (7) for free neutral atoms which fulfil the boundary conditions

$$\varphi_0(0) = 1\,, \qquad \varphi_0(\infty) = 0\,, \qquad \varphi_0'(0) = \text{const.} \tag{8}$$

are the Tietz[8] approximate solution

$$\varphi_{Ti}(x) = (1 + ax + bx^2)^{-3/2}$$

with

$$a = 0.7105\,, \quad b = 0.03919\,. \tag{9}$$

and the Buchdahl[9] approximate solution

$$\varphi_{Bn}(x) = \frac{1}{(1 + Ax)(1 + Bx)(1 + Cx)} \tag{10}$$

where A, B and C are constants namely $A = 0.9288$, $B = 0.1596$ and $C = 0.05727$. The Tietz approximation has the same degree of accuracy as the Buchdahl approximation. The Buchdahl approximation is more convenient in practical calculations of the atom form factor. At first we re-write the Buchdahl approximate solution of the Thomas-Fermi equation in the following form

$$\varphi_{Bn}(x) = \frac{\alpha}{1 + Ax} + \frac{\beta}{1 + Bx} + \frac{\gamma}{1 + Cx}\,, \tag{11}$$

where the constants α, β, γ are given by

$$\alpha = \frac{A^2}{(A - B)(A - C)}\,, \quad \beta = \frac{B^2}{(A - B)(C - B)}\,, \quad \gamma = \frac{C^2}{(A - C)(B - C)}\,. \tag{12}$$

A simple calculation shows that the constants α, β, γ fulfil the following relations

[7] K. Umeda, J. Phys. Soc., Japan, **10**, 750, 1955.
[8] T. Tietz, Il Nuovo Cimento, **4**, 1192, 1956.
[9] H. A. Buchdahl, Ann. d. Phys., **17**, 238, 1956.

$$\alpha+\beta+\gamma=1\,,\quad \frac{\alpha}{A}+\frac{\beta}{B}+\frac{\gamma}{C}=0\,,\quad \frac{\alpha}{A^2}+\frac{\beta}{B^2}+\frac{\gamma}{C^2}=0\,. \tag{13}$$

Using eq. (3) and eq. (11) we obtain for the atom form factor $F(s)$ the following expression

$$F(s)=Z\Big[1-s\mu\Big\{\frac{\alpha}{A}\Big(\cos\frac{s\mu}{A}\Big(\frac{\pi}{2}-Si\,\frac{s\mu}{A}\Big)+\sin\frac{s\mu}{A}\,Ci\,\frac{s\mu}{A}\Big)+$$
$$+\frac{\beta}{B}\Big(\cos\frac{s\mu}{B}\Big(\frac{\pi}{2}-Si\,\frac{s\mu}{B}\Big)+\sin\frac{s\mu}{B}\,Ci\,\frac{s\mu}{B}\Big)+$$
$$+\frac{\gamma}{C}\Big(\cos\frac{s\mu}{C}\Big(\frac{\pi}{2}-Si\,\frac{s\mu}{C}\Big)+\sin\frac{s\mu}{C}\,Ci\,\frac{s\mu}{C}\Big)\Big\}\Big], \tag{14}$$

where the symbol $Si(x)$ and $Ci(x)$ have the following meaning

$$Si(x)=\int_0^x\frac{\sin t}{t}\,dt\,;\qquad Ci(x)=-\int_x^\infty\frac{\cos t}{t}\,dt\,. \tag{15}$$

In Table 1 we give a comparison of our results for $f_0(s)$ with the numerical results. The symbol $f_0(s)$ is given by $F(s)=Zf_0(s)$.

Table I

A comparison of our results for $f_0(s)$ with the numerical results of $f_0(s)$ (see reference[4])

$s\mu$	0	0,15	0,31	0,46	0,62	0,77	0,93	1,08	1,24	1,39
Numerical f_0	1,000	0,922	0,796	0,684	0,589	0,522	0,469	0,422	0,378	0,342
Equation (14) f_0	1,000	0,942	0,793	0,693	0,609	0,538	0,469	0,420	0,389	0,348
$s\mu$	1,55	1,70	0,201	2,32	2,63	2,94				
Numerical f_0	0,309	0,284	0,240	0,205	0,175	0,156				
Equation (14) f_0	0,305	0,278	0,234	0,198	0,169	0,149				

Table I shows that our results for $f_0(s)$ are in good agreement with the numerical $f_0(s)$ data. In order to calculate the term $S(s)$ which is responsible for the inelastic scattering we re-write eq. (4) as follows

$$S(s)=1-\int_0^{x_0}\Big[x^{1/2}\varphi_0^{3/2}(x)-\frac{3}{2}\,w\,x\cdot\varphi_0(x)+\frac{1}{2}\,w^3x^2\Big]\,dx. \tag{16}$$

Taking into consideration the Thomas-Fermi equation (7), the boundary conditions for $\varphi_0(x)$ given by eq. (8) and the relation (6), we see that the integration by parts gives us for $S(s)$ the following formula.

$$S(s) = \varphi_0(x) - x_0 \varphi_0'(x) - \frac{1}{6}(w x_0)^3 + \frac{3}{2} w \int_0^{x_0} x \varphi_0(x)\, dx. \tag{17}$$

Substituting for $\varphi_0(x)$ the Buchdahl approximation given by eq. (11) we obtain for $S(s)$ the following expression

$$S(s) = \frac{\alpha(1 + 2A x_0)}{(1 + A x_0)^2} + \frac{\beta(1 + 2B x_0)}{(1 + B x_0)^2} + \frac{\gamma(1 + 2C x_0)}{(1 + C x_0)^2} -$$
$$- \frac{3}{2} w \left[\frac{\alpha}{A^2} \ln(1 + A x_0) + \frac{\beta}{B^2} \ln(1 + B x_0) + \frac{\gamma}{C^2} \ln(1 + C x_0) \right] - \frac{1}{6}(w x_0)^3. \tag{18}$$

In Table II we give a comparison of our results for $S(s)$ with the numerical results for $S(s)$ of BEVILOGUA[10] for several w.

Table II

A comparison of our results* for $S(\omega)$ given by eq. (18) with the numerical results of $S(\omega)$ given by BEVILOGUA

	ω	0	0,001	0.003583	0,025	0,05	0,1	0,2	0,3	0,4	0,6	0,8	∞
Equation (18)	x_0	∞	99,149	49,716	15,751	9,907	5,923	3,352	2,306	1,725	1,103	0,7762	0,000
	$S(\omega)$	0	0,0123	0,0412	0,198	0,321	0,486	0,667	0,783	0,840	0,915	0,964	1
Numerical data	$S(\omega)$	0	—	—	0,199	0,319	0,486	0,674	0,776	0,839	0,909	0,944	1

* $S(\omega)$ has the same meaning as $S(s)$.

Table II shows that our data for $S(s)$ are in good agreement with the numerical data for $S(s)$ of BEVILOGUA.

For small values of s the atom form factor $F(s)$ as given by eq. (14) is quadratic in s, namely

$$F(s << 1) = [1 - \text{const}\, s^2 Z^{-2/3}] \tag{19}$$

and for large values of s the atom form factor $F(s)$ vanishes inversely quadratically in s, namely

[10] L. BEVILOGUA, Phys. Z., **32**, 740, 1931.

$$F(s \gg 1) = \text{Const}\,\frac{Z^{5/3}}{s^2}\,. \tag{20}$$

Relations (13) and (6) show that the term $S(s)$ which is given in our case by eq. (18) has the correct behaviour for $w \to 0$ and $w \to \infty$ as is shown by Table II. The author's point of view is that the approximate analytical formulas, eq. (14) and eq. (18), are the best approximate analytical expressions known hitherto for the atom form factor and the x-ray incoherent scattering function $S(s)$.

Formula (14) for the atom form factor $F(s)$ has a number[11] of less accurate corresponding formulas. Formulae for $S(s)$ given by eq. (18) has been unknown in the physical literature. It is necessary to stress that using the approximate solution for the Thomas-Fermi function (9) proposed by the author one can obtain, using eq. (17), an analytical expression for $S(s)$. The results which will be obtained for $S(s)$ are the same as those given by formula (18).

Formulas (14) and (18) allow the calculation of the scattering intensity when inserted in eq. (1).

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РАССЕЯНИЕ ЭЛЕКТРОНОВ СВОБОДНЫМИ НЕЙТРАЛЬНЫМИ АТОМАМИ ПО МОДЕЛЯМ ТОМАС—ФЕРМИ

Т. ТИТЦ

Р е з ю м е

В работе выведена аналитическая формула для определения рассеянной группой свободных атомов интенсивности, используя приблизительное решение Бухдала для уравнения Томаса—Ферми. Рассеянная интенсивность содержит упругое и неупругое рассеяние электронов, рассеянных один раз свободными атомами модели Томаса—Ферми. Сравнение с нумерическими результатами показывает, что полученная формула рассеянной интенсивности является очень точной.

[11] K. UMEDA, J. Faculty of Science Hokkoido University, VI., 57, 1951 ; T. TIETZ, J. Chem. Phys., **23**, 1965, 1955.