Turkish Computational and Theoretical Chemistry

Turkish Comp Theo Chem (TC&TC)

Volume(Issue): 9(3) – Year: 2025 – Pages: 38-44

e-ISSN: 2602-3237

https://doi.org/10.33435/tcandtc.1451290

Received: 11.03.2024 ***Accepted***: 10.10.2024 *Research Article*

Study of the structure of atomics by the method of electron scattering in the distorted-wave approximation: Atomic energy

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Abstract: Using distorted-wave approximation obtained the differential cross-section (DCS) of elastic scattering at energy of 80 eV of electrons on 49In, 31Ga, 34Se and 70Yb atoms, and calculated accordingly on the proposed mathematical method. The electron density distribution in the atom is chosen as a function calculated in the Dirac-Hartree-Fock-Slater approximation, which is a superposition of the spherically symmetric Yukawa potential. In addition, the DCSs were calculated for the electron density in the 49 In and 20 Ca atoms expressed as a three-parameter Fermi function at incident electron energy of 100 eV. The obtained theoretical calculations of the cross sections were compared with the experimental data. Besides, the proposed mathematical method simplifies the calculation of integral expressions and makes it possible to obtain a convenient and simple expression for the atomic form factor. Data on the scattering cross sections of electrons on atoms are of considerable interest both in the field of fundamental science for in-depth study of interaction processes and in practical applications, and are necessary in many areas of research, such as modeling low-temperature plasma, astrophysics phenomena, laser physics, and atmospheric effects etc. In addition to natural phenomena, the processes of collision of electrons with matter play an essential role in plasma technologies, such as, for example, microelectronics and biomedicine. Atomic physics, plasma physics and optics - fields directly related to electron-atom make a significant contribution to the fundamental understanding of the world. Despite the long study of the effects of electron scattering on atoms, and the results obtained in the physics of atomic collisions, this area still requires theoretical and experimental research, there is a significant lack of data on collision cross sections for their subsequent use in modeling and calculations. In particular, there are no systematized data on the cross sections for elastic scattering of high energy electrons by atomic.

Keywords: scattering, differential section, distribution density, energy, spatial structure of the target atom.

1. Introduction

The study of atoms by electron scattering is one of the effective methods for studying the spatial structure of atoms, since the nature of the electromagnetic interaction of an electron with an atom is well known. To extract important information about the distribution of electrons in atoms from an electron scattering experiment, it is desirable to have as simple expressions as possible for the corresponding form factors or cross sections. This is convenient for carrying out multiple calculations using different test functions of the electron density distribution in atoms.

A clear representation of the properties of electron scattering for the wide energy range [1] can be acquired by investigating the angular position of the minima of the DCSs.

By comparing theoretical calculations with the experiment on electron scattering on atoms obtained the repeated theoretical analysis of the DCSs, and showed that taking into account the distortion in the amplitude and phase of waves. The obtained results from current method in a good agreement with known experimental work [2].

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2. Computational Method

The growth of a novel theoretical method for obtaining the DCS for elastic and inelastic scattering of electrons on atom is the basic arm of current work. The formula for the differential scattering cross section in the standard form [3-5].

$$\frac{d\sigma_{if}}{d\Omega} = \frac{E_i E_f}{(2\pi)^2} \cdot \frac{k_f}{k_i} \frac{1}{2} \cdot \frac{1}{2J_i + 1} \sum_{\sigma_i \sigma_f} \sum_{M_i M_f} \left| T_{if} \right|^2 \quad (1)$$

3.

The matrix element of the transition from the initial state (*i*) of the atom to the final state (*f*) in the high-energy approximation is represented as:

$$T_{if} = \left\langle J_f M_f \left| \int d\mathbf{r} \Psi_f^{(-)+}(\mathbf{r}) V(\mathbf{r}) \Psi_i^{(+)}(\mathbf{r}) \right| J_i M_i \right\rangle \quad (2)$$

The wave functions in (2) of re-scattered electrons in the Coulomb field of the target atom were determined as solutions of the Dirac equation in [6]:

$$\Psi^{(\pm)}(\mathbf{r},\mathbf{k}) = u^{(\pm)}(\mathbf{r},\mathbf{k}) \exp[i\mathbf{kr} - i\frac{E}{k}\int_0^\infty V(\mathbf{r} \mp \hat{k}s)ds] \quad (3)$$

where $\mathbf{u}^{(\pm)}(\mathbf{r},\mathbf{k})$ - spinor functions.

The wave function of the atomic state $\left|\mathrm{JM}\right\rangle$, is determined within the framework of one or another model of the atom. Coulomb interaction of an electron with an atom:

$$V(\mathbf{r}) = -Ze^2 \int \frac{\rho(\mathbf{x})\ d\mathbf{x}}{|\mathbf{r} - \mathbf{x}|} \quad . \quad (4)$$

The product of wave functions of re-scattered electrons is represented as

$$\Psi_f^{(-)^+} \Psi_i^{(+)} = g(\mathbf{r}, \upsilon_f^+ \upsilon_i) \exp[i\mathbf{qr} + i\phi(\mathbf{r})] \quad (5)$$

where

$$\mathrm{g}(\mathbf{r}, \upsilon_\mathrm{f}^+ \upsilon_\mathrm{i}) = \mathrm{u}_\mathrm{f}^+(\mathbf{r}, \upsilon)\mathrm{u}_\mathrm{i}(\mathbf{r}, \upsilon) \quad (6)$$

and the distorting function in phase

$$\phi(\mathbf{r}) = -\frac{E}{k}\int_0^\infty V(r - \hat{k}_i s)ds - \frac{E}{k}\int_0^\infty V(r + \hat{k}_f)ds \quad (7)$$

Now, making a variation of variables $\mathbf{u} = \mathbf{r} - \mathbf{x}$ and applicating expansions, while confining to the first term in the amplitude function, and the first two in the phase function, we can write

$$\phi(\mathbf{u} + \mathbf{x}) = \phi(\mathbf{x}) + \nabla_u \phi(\mathbf{u} + \mathbf{x})_{u=0}$$
$$g(\mathbf{u} + \mathbf{x}, \upsilon_\mathbf{f}^+ \upsilon_i) = g(\mathbf{x}, \upsilon_f^+ \upsilon_i) = g(\mathbf{x})\upsilon_f^+ \upsilon_i \quad (8)$$

For the matrix element of the transition of an atom, we have:
where

$$q_{eff}(\mathbf{x}) = \mathbf{q} + \nabla_u \Phi(\mathbf{u} + \mathbf{x})_{u=0} \quad (10)$$

Now, indicating the cross section in terms of the form factor, we obtain

$$\frac{d\sigma}{d\Omega} = (\frac{d\sigma}{d\Omega})_0 \frac{E_f}{E_i} \frac{k_f}{k_i} \frac{2J_f + 1}{2J_i + 1} \sum_{LM} \frac{1}{2L+1} |F_{LM}|^2 \quad (11)$$

where the equation

$$(\frac{d\sigma}{d\Omega})_0 = (\frac{2Ze^2 k_i}{q^2})^2 \cos^2 \theta/_2$$

Is the cross section of the electron scattering on the point atom. To calculate the cross section for the totality above spinors υ_i and υ_f – the appropriate electron momentum $\mathbf{k}_\mathrm{i}$ and $\mathbf{k}_\mathrm{f}$ for before and after scattering, it was take into consideration that

$$\sum_{\sigma_i \sigma_f} \left| \upsilon_f^+ \upsilon_i \right|^2 = \cos^2(\vartheta/_2) \quad (12)$$

Thus the form factor of an atom in terms of the radial distribution density of electrons in an atom:
Here $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$ is transfer momentum of electron to the target atom.

In order to write the distorting functions $g(\mathbf{x})$ and $\phi(\mathbf{x})$ in explicit form, first of all, it is necessary to express the Coulomb potential (4) for a spherically symmetric electron density distribution $\rho_e(x)$ in the following form:

$$V(r) = -4\pi\gamma\{\frac{1}{r}\int_0^r \rho_e(x)x^2dx + \int_r^\infty \rho_e(x)xdx\} \quad (14)$$

Following [6], we expand this potential in a Taylor series and, confining ourselves to the quadratic term of the expansion, we obtain:

$$V(r) \approx V(0) + \gamma\bar{a}k^3r^2/2 \quad (15)$$

where $\gamma = Ze^2/(\hbar c) = Z/137$ and for potential in the center of the atom

$$\bar{V}(0) = -4\pi\int_0^\infty \rho_e(x)xdx \quad (16)$$

The parameter $\bar{a} = \frac{4\pi}{3k^3}\rho_e(0)$ in the formula (15) defining the radial dependence of the Coulomb potential. The parameter giving the distortion to the wave front of the incident wave has the form $\bar{b} = \frac{\pi}{k^2}\int_0^\infty \rho_e(x)dx$. Expressed the distorting terms in the phase and in the amplitude of the re-scattered waves in terms of these parameters ($\bar{V}(0)$, $\bar{a}$, $\bar{b}$), we obtain:

$$T_{if} = -4\pi Ze^2\left\langle J_f M_f \left| \int d\mathbf{x}\frac{g(\mathbf{x})}{q_{\mathbf{eff}}^2(\mathbf{x})}\exp\{i[\mathbf{qx}+\phi(\mathbf{x})]\}\rho(\mathbf{x})\right| J_i M_i\right\rangle \quad (9)$$

$$F_{LM}(\mathbf{q}) = q^2\int \frac{g(\mathbf{x})d\mathbf{x}}{q_{eff}^2(\mathbf{x})}\exp i[\mathbf{qx}+\phi(\mathbf{x})]\rho_L(x)Y_{LM}^*(\hat{x})d\mathbf{x} \quad (13)$$

$$g(\mathbf{x}) = (1-\frac{V(0)}{k})\{1+\gamma\,\bar{a}((\mathbf{k}_i\mathbf{x})^2-[\mathbf{k}_i\mathbf{x}]^2+(\mathbf{k}_f\mathbf{x})^2-[\mathbf{k}_f\mathbf{x}]^2)+3\gamma\,\bar{b}((\mathbf{k}_i\mathbf{x})-(\mathbf{k}_f\mathbf{x})) \quad (18)$$

Before proceeding to the calculation of the integrals in the form factor (13), let us simplify, i.e. denote

$$I(\mathbf{q},\mathbf{x}) = \exp[i\mathbf{qx}+i\gamma\bar{\phi}(\mathbf{x})] \quad (19)$$

where $\phi(\mathbf{x},\gamma) = \gamma\bar{\phi}(\mathbf{x})$.

Now we expand $I(\mathbf{q},\mathbf{x})$ in a series in powers of a small parameter $\gamma << 1$

$$I(\mathbf{q},\mathbf{x}) = \sum_{n=0}^{\infty}\gamma^n I_n(\mathbf{q},\mathbf{x}) \quad (20)$$

Let us write the derivative of expression (19) with respect to the following form:

$$\frac{\partial I(\mathbf{q},\mathbf{x},\gamma)}{\partial\gamma} = i\bar{\phi}(\mathbf{x})I(\mathbf{q},\mathbf{x},\gamma) \quad (21)$$

On the other hand, expanding (21) in powers into a series and comparing it with the derivative with respect to (20), we obtain the following recurrent formula:

$$(n+1)I_{n+1}(\mathbf{x}) = i\bar{\phi}(\mathbf{x})I_n(\mathbf{x}), n = 0,1,2,3,... \quad (22)$$

$$I_0(\mathbf{q},\mathbf{x}) = \exp(i\mathbf{qx}) \quad (24)$$

The recursive formula (22) allows us to express all terms in (20) through expression (24). And now, limiting ourselves in (20) to the first two terms of the series, we write the form factor (13) in the following simplified form:

$$F_{LM}(\mathbf{q}) = q^2\int G_{LM}(\mathbf{x})\exp(i\mathbf{qx})Y_{LM}^*(\hat{x})\rho_L(x)d\mathbf{x} \quad (25)$$

where amplitude function $G_{LM}(\mathbf{x})$ takes the following form:

$$G_{LM}(\mathbf{x}) = \frac{g(\mathbf{x})\{1+i\phi(\mathbf{x})-\frac{1}{2}\phi^2(\mathbf{x})\}}{q_{eff}^2(\mathbf{x})} \quad (26)$$

Thus, further study of both elastic and inelastic scattering of electrons by atoms reduces to calculating the form factor (25).

To calculate the three-dimensional integral (25), we choose the following coordinate system (Fig. 1).

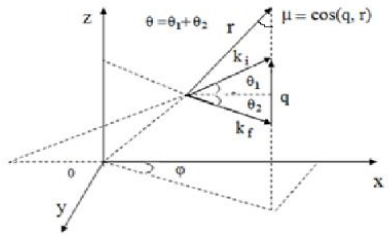

Figure 1. Momentum of incident ($\mathbf{k}_i$) and scattered ($\mathbf{k}_f$) particles in a three-dimensional coordinate system with transfer momentum $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$.

Let choose axe OZ as OZ $\uparrow\uparrow \mathbf{q}$, and denote $\cos(\hat{q}\hat{x}) = \mu$, where $\mathbf{x} = \{x\mu\varphi\}$ and $d\mathbf{x} = x^2 dx d\mu d\varphi$, and neglecting the lost of energy by electron $\Delta E << E_i$ or assuming $|\mathbf{k}_i| = |\mathbf{k}_f| = k$, we obtain:

$$q = 2k\sin\vartheta/2 = 2k\alpha,\ \alpha = \sin\vartheta/2 \qquad (27)$$

$$\cos\hat{x}\hat{k}_i = \mu\alpha + \sqrt{1-\mu^2}\sqrt{1-\alpha^2}\cos\varphi$$

$$\cos\hat{x}\hat{k}_f = -\mu\alpha + \sqrt{1-\mu^2}\sqrt{1-\alpha^2}\cos\varphi \qquad (28)$$

Then the corresponding integral by $d\mu$ from (25) takes the form:

$$I_{LM} = \int_{-1}^{1} G_{LM}(x\mu\varphi) e^{iqx\mu} \rho_L(x) Y^*_{LM}(\mu\varphi) d\mu \qquad (29)$$

After integrating by parts and confining ourselves to the first term, we obtain:

$$I_{LM} = \sum_{\varepsilon=\pm1} \varepsilon \frac{G_{LM}(x\varepsilon)}{iqx} \sum_{\nu=0}^{L} \frac{i^\nu}{(qx)^\nu} \left[\frac{\partial^\nu Y^*_{LM}(\mu\varphi)}{\partial\mu^\nu}\right]_{\mu=\varepsilon} e^{iqx\varepsilon} \qquad (30)$$

$$\phi(x,\varepsilon) = -\varepsilon\ V(0)\,qx/k - b_0(4k^2 - q^2)\,x^2/2 - 3\varepsilon\ a(qk^2 - q^3/12)x^3 \qquad (32)$$

$$q_{eff}(x,\varepsilon) = \varepsilon\ q(1 - V(0)/k) - \varepsilon\ aq(3k^2/2 - q^2/4)x^2 - b_0(4k^2 - q^2)x \qquad (33)$$

$$F_{L0}(q) = 2\pi i q \sum_{\varepsilon=\pm1} \varepsilon \int_0^\infty G_{L0}(x\varepsilon) e^{iqx\varepsilon} \rho_L(x) x dx \qquad (34)$$

In (30), it is taken into account that at the points $\mu = \varepsilon = \pm 1$ the dependence on the azimuth angle in the functions g, ϕ and q^2_{eff} disappears, and they take the following form:

$$g(x,\varepsilon) = (1 - V(0)/k)\{1 + 3\varepsilon b_0 qx + a(q^2 - 2k^2)x^2\} \qquad (31)$$

This allows integration in (25) over $d\varphi$ to be carried out exactly, and as a result, the form factor reduces to the one-dimensional integral:

Here, $G(x,\varepsilon)$ the amplitude function, which has the form:

$$G_{L0} = G_0(x\varepsilon)\left[\frac{\partial\ Y^*(\mu)}{\partial\mu}\right]_{\mu=\varepsilon} \qquad (35)$$

Where

$$G_0(x\varepsilon\ ) = \frac{g(x\varepsilon)(1 + i\phi(x\varepsilon) - \phi^2(x\varepsilon)/2)}{q^2_{eff}(x\varepsilon)} \qquad (36)$$

Having expanded the amplitude functions in a Taylor series and, confining ourselves to the first two terms, we calculate the integral expression (34), which makes it possible for us to express $F_{L=0}(q)$ as a functional of the plane-wave Born form factor:

$$F_{L0}(q)=\frac{2\pi\ i}{q(1-\frac{V(0)}{k})}\{F_B(q)+\zeta\frac{\partial F_B(q)}{\partial q}\}$$

(37)

where

$$\zeta(q)=-3ibq-\frac{q^2}{k}(1-\frac{V(0)}{k})+\frac{2b(4k^2-q^2)}{q(1-\frac{V(0)}{k})} \quad (38)$$

and the Born form factor for a spherical atom is:

$$F_B(q)=\frac{1}{\sqrt{4\pi}}\sum_{\varepsilon=\pm1}\varepsilon\int_0^\infty e^{iqx\varepsilon}\rho_0(x)xdx$$

(39)

3. Results and discussion

Starting theoretical calculations implementing Born form factor (37), we can method of approaching the calculation for the DCS of electrons by atoms. In this case, we need to choose the dispensation function of electron density. For the distribution function, we choose the well-known expression [7], in which, using the property of the electrostatic potential of an individual atom, calculated in the Dirac-Hartree-Fock-Slater approximation, the superposition of the spherical symmetric Yukawa potential:

$$\rho_0(x)=\frac{1}{4\pi}\sum_{\mu=1}^{3}A_\mu\alpha_\mu^2\frac{e^{-\alpha_\mu x}}{x} \quad (40)$$

After taking into account (38) in (37), we obtain the following expression for the Born form factor:

$$F_B(q)=\frac{2i}{4\pi}\sum_{\mu=1}^{3}\frac{A_\mu\alpha_\mu^2}{q^2+\alpha_\mu^2}\left\{qR-\left[qR\cos(qR)+(\alpha_\mu R)\sin(qR)\right]e^{\alpha_\mu R}\right\} \quad (41)$$

$$F(q)=-2\pi(qR)\sum_{n=0}^{2}\beta_n\left[F_B^{(n)}(q)-iF_B^{(n)}(q)\right] \quad (42)$$

$$\frac{d\sigma}{d\Omega}=(\frac{d\sigma}{d\Omega})_{Mott}\left|F_{\mathrm{Re}}(q)\right|^2+\left|F_{\mathrm{Im}}(q)\right|^2 \quad (43)$$

$$F_B(q)=-4\frac{\pi d}{R}\cdot e^{-\pi dq}\left\{[\omega_0+\omega(1-3\pi(\frac{d}{R})^2)]\sin(qR-\frac{\pi d}{R})+\left[\frac{\pi d}{R}(\omega_0+\omega(3-(\frac{\pi d}{R})^2))\right]\cos(qR-\frac{\pi d}{R})\right\}. \quad (45)$$

Thus, the final expression for the atom form factor (40) takes the form:

Here

$$F_B^{(n)}(q)=\frac{\partial^n F_B(q)}{\partial q^n}.$$

The parameters A_μ и α_μ in expression (41), borrowed from [7], in which these parameters were obtained using an analytical fitting procedure to the potential values found by the Dirac-Hartree-Fock-Slater self-consistent field method. Having written the DCS for electron scattering by the formula (43) and have been compared current theoretical calculations with known experimental result

This equation written in the course of the current theoretical studies was applied to calculate the DCS of electrons on $_{49}$In, $_{31}$Ga, $_{34}$Se and $_{70}$Yb atoms at 80 eV.

In current work, the DCS for electron scattering for $_{49}$In and $_{20}$Ca atoms [12] was also obtained at 100 eV. In this case, the three-parameter Fermi function was chosen for the distribution of the electron density in atoms:

$$\rho_e(x)=\rho_0(\omega_0+\omega\frac{x^2}{R^2})(1+\exp(\frac{x-R}{d}))^{-1}$$

(44)

and for Born form factor the following expression:

The results of the dependence of the differential cross section on the scattering angle, obtained from theoretical calculations using formula (43), are compared with known experimental data and are presented in Fig.2. In the figure, the solid line indicates the results of theoretical calculations, and the dots indicate experimental data known from works [8–11].

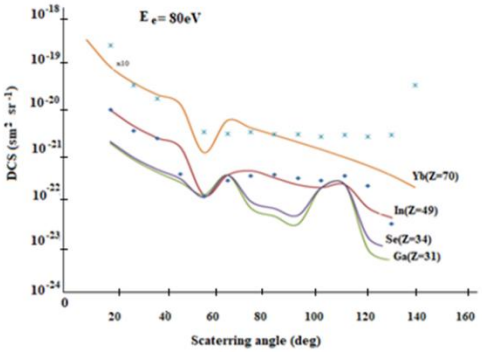

Figure 1. The DCSs for electron scattering by $_{49}$In, $_{31}$Ga, $_{34}$Se, and $_{70}$Yb.

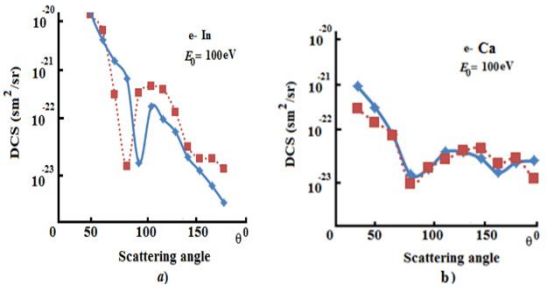

Figure 3. DCS of elastic scattering of electrons from $_{49}$In (*a*) and $_{20}$Ca (*b*) atomics (line) together with experimental results (dots) in Refs. [9, 13].

Fig.2 shows a comparison of known experimental data with the results obtained in the work. As can be seen from Fig.2, the results of theoretical calculations for the $_{49}$In atom show that the first minima are quite deep (within the scattering angle of 60^0) and coincide with experimental data, which cannot be said about the second minimum, which, according to both theoretical and experimental calculations, is somewhat blurred. The same can be said for the $_{70}$Yb atom. As you can see, the first minima practically coincide and occur at a scattering angle of 60^0. Unfortunately, we have no information about experimental results for atoms of other elements. We will take your comment into account and try to find relevant information. As for work 2 in the list of references, it, like several other works, are examples of applications of the new mathematical method we proposed.

From the Figures 2 and 3, the theoretical calculated DCS using the Fermi function are very closer to experimental results. As can be seen from Fig. 2, the results of theoretical calculations for the $_{49}$In atom show that the first minima are quite deep (within a scattering angle of 60^0) and coincide with the experimental data, which cannot be said about the second minimum, which, according to both theoretical and experimental calculations, is somewhat blurred. However, as shown in Fig. 3, at energy of incident electrons of 100 eV, the second minimum is almost imperceptible for the $_{49}$In atom, while for the lighter $_{20}$Ca, the first and second minima, the expressed ones, as well as the theoretical and experimental results, coincide. An interesting case is that the same can be said about the maxima of the $_{20}$Ca atom. It should be noted that taking into account the distortions of both amplitudes and phases of the wave functions of the incident and scattered electrons somewhat complicates the calculations. However, the proposed mathematical method simplifies the calculation of integral expressions and makes it possible to obtain a convenient and simple expression (43) for the atomic form factor.

4. Conclusions

In this work, the differential cross section for elastic electron scattering at an energy of 80 eV of electrons on 49In, 31Ga, 34Se and 70Yb atoms and at an energy of 100 eV on 49In and 20Ca atoms was obtained in analytical form using the distorted wave approximation. In our other works, calculations were carried out for other, lighter and heavier nuclei. The point is that in order to extract important information about the distribution of electrons in atoms from an electron scattering experiment; it is desirable to have the simplest possible expressions for the corresponding form factors or cross sections. This is convenient for performing multiple calculations using various test functions of electron density distribution in atoms. A clear idea of the properties of electron scattering in a wide energy range can be obtained by studying the angular position of the DCS minima, which was done in the work for the corresponding atoms.

By comparing theoretical calculations with experiments on electron scattering on atoms, a repeated theoretical analysis of the DCS was obtained and it was shown that distortions in the amplitude and phase of the waves are taken into account.

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