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INVESTIGATION OF ATOMS BY THE ELECTRON SCATTERING

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Abstract: The expression for differential cross-section of elastic and inelastic scattering of relativistic electrons from atoms has been obtained analytically on the basis of distorted-wave theory. Differential section of elastic scattering of electrons from free gold atom calculated in incident energy of electrons ~ 25 eV has been compared with precise calculation method. Thickness of surface layer and root-mean square radius of density distribution of electron in gold atom have been determined.

Keywords: Distorted electron wave, differential sections, characteristics of atoms.

1. Introduction

At present, there are many experimental and theoretical methods of investigating surfaces and surface area of atoms and solid bodies among which the reactions followed by scattering of electrons should be indicated [1, 2, 3].

Study of atoms by electrons is one of the most effective methods of research of atoms' structure as the character of interaction of electron with nucleus and electrons surrounding nucleus is well-known.

It is important to consider distortion of incident and scattering waves in coulomb field of atom's nucleus and electrons screening this nucleus. However, it complicates the calculation of scattering amplitude.

Differential cross-section of elastic scattering of electron beam from free atom in work [4] has been calculated analytically, considering distortions, only in phase functions of scattered spherical waves which brought to the improvement of the agreement with the results obtained by numerical methods.

Rather precise numerical method to consider distortions in the phase and in the amplitude of scattered electrons in coulomb field was obtained in the frame of highly energetic approximation in the paper [5] by Yennie, Boss and Ravenhall from quasi-classic solution of Dirac equation.

It should be noted that such an approach of calculation of distorted phase function and amplitude of scattered waves depending on distribution density of charges in the target gave satisfactory results that were obtained in a number of calculations of differential sections on elastic and inelastic scattering of high-energetic electrons in nucleus [6].

2. The Proposed Theory

The aim of the work is to get expression in the analytical form for the amplitude of elastic and inelastic scattering of electrons from free atom or from the crystals developing this distorted-wave theory of scattering of electrons.

Moreover, in the frame of terms $kR \gg 1$ and $E \gg V$, where E- is energy of incident particle, V- is atomic potential, R- is area of potential effect; more adequate in the given work is high energetic approximation. These terms allow to develop various approaches in the theory of scattering of electrons.

Differential cross-section of scattering of electrons is determined by standard form [6]:
Now let's indicate the section through the form-factor:

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

where

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

For the form-factor- $F_{LM}(\mathbf{q})$ we get

$$F_{LM}(\boldsymbol{q}) = -\int g_0(\boldsymbol{r}) \frac{e^{i[\boldsymbol{q}\boldsymbol{r}+\phi(\boldsymbol{r})]}}{|\boldsymbol{r}|} d^3r + q^2 \int \frac{g(\boldsymbol{x})}{q_{eff}^2(\boldsymbol{x})} e^{i[\boldsymbol{q}\boldsymbol{x}+\phi(\boldsymbol{x})]} \rho_L(x) Y_{LM}^*(\hat{x}) d^3\boldsymbol{x} \quad (3)$$

Here $\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$ is the impulse of electron transfer to the target atom and $\rho_L(x)$ –is radial transition density of an atom.

For spherical symmetric distribution of electron density *ρ(x)* and to present it in the form of

$$V_e(r) = -4\pi\gamma \ \left\{ \frac{1}{r} \int_0^r \rho(x) x^2 dx + \int_r^\infty \rho(x) x dx \ \right\} \quad (4)$$

Here, $\gamma = e^2/\hbar c) = 1/137$

Distorting terms expressing in the phase and amplitude of scattered waves through these parameters we get:

$$\phi(\mathbf{x}, \gamma) = -(\mathbf{qx}) \frac{V(0)}{k} + a(3/2\, k^2 x^2 \mathbf{qx} - (\mathbf{k}_i \mathbf{x})^3 + (\mathbf{k}_f \mathbf{x})^3) - b([\mathbf{x}\mathbf{k}_i]^2 + [\mathbf{x}\mathbf{k}_f]^2) \quad (5)$$

$$g(\mathbf{x}) = (1 - \frac{V(0)}{k})\{1 + a((\mathbf{k}_i \mathbf{x})^2 - [\mathbf{k}_i \mathbf{x}]^2 + (\mathbf{k}_f \mathbf{x})^2 - [\mathbf{k}_f \mathbf{x}]^2) + 3b((\mathbf{k}_i \mathbf{x}) - (\mathbf{k}_f \mathbf{x})) \quad (6)$$

Here parameter *a*, describing radial dependence of coulomb potential in the atom's center is proportional to the charge density

$$a = -4\pi\gamma + \frac{4\pi\gamma}{3k^3} \rho(0), \quad (7)$$

parameter *b*- giving curviness to wave front of the incident wave has the form

$$b = \frac{\pi\gamma}{k^2} \int_0^\infty \rho(x) dx, \quad (8)$$

but for potential in the center of the atom we have

$$V(0) = -4\pi\gamma + 4\pi\gamma \int_0^\infty \rho(x) x dx \tag{9}$$

For the form-factor of atoms we get the following expression, which is the functional of Born form-factor

$$F_{L=0}(q) = 2\pi i \frac{R^3}{(1 - \frac{V(0)}{k})} \{F_B(q) - \frac{V(0)}{kR} \frac{\partial F_B(q)}{\partial q} - i \; 3b[1 + \frac{2(4k^2 - q^2)}{3q^2 R(1 - \frac{V(0)}{k})}] \frac{\partial F_B(q)}{\partial q}\} \tag{10}$$

However, in calculating Born form-factor - $F_B(q)$, it is necessary to choose the function of electrons' density distribution in the atom.

It is known that scattered electrons on the atom's surface "feel" thin structure well. Thin structure in the distribution of electrons density is revealed in three-parametric Fermi-functions with the help of parameter- ω

$$\rho_e(x) = \rho_0(\omega_0 + \omega \frac{x^2}{R^2})(1 + \exp(\frac{x-R}{d})^{-1} \tag{11}$$

Pole method is used for calculation of the radial integral –

$$F_B(q) = \frac{3}{4\pi R^5 [1 + (\frac{\pi d}{R})^2]} \sum_{\varepsilon = \pm 1} \varepsilon \int_0^\infty \ell^{iqx\varepsilon} \frac{\omega_0 + \omega \frac{x^2}{R^2}}{1 + e^{\frac{x-R}{d}}} x dx \tag{12}$$

which is shown in [8] :

$$F_B(q) = -4\frac{\pi d}{R} \cdot e^{-\pi d q} \left\{ [\omega_0 + \omega(1 - 3\pi(\frac{d}{R})^2)] \sin(qR - \frac{\pi d}{R}) + \left[\frac{\pi d}{R}(\omega_0 + \omega(3 - (\frac{\pi d}{R})^2 \right] \cos(qR - \frac{\pi d}{R} \right\} \tag{13}$$

After determining the evident expression of the form-factor and elastic scattering of electrons from free atoms, let's calculate the differential cross-section.

3. Results and Discussions

Compactness of the obtained analytic expression of differential cross-section allows to check the above-developed theory on a level of high accuracy.

Such examination has been carried out on the example of elastic scattering of electrons from atom of $_{79}$Au in the energy of incident electrons - 25 eV.

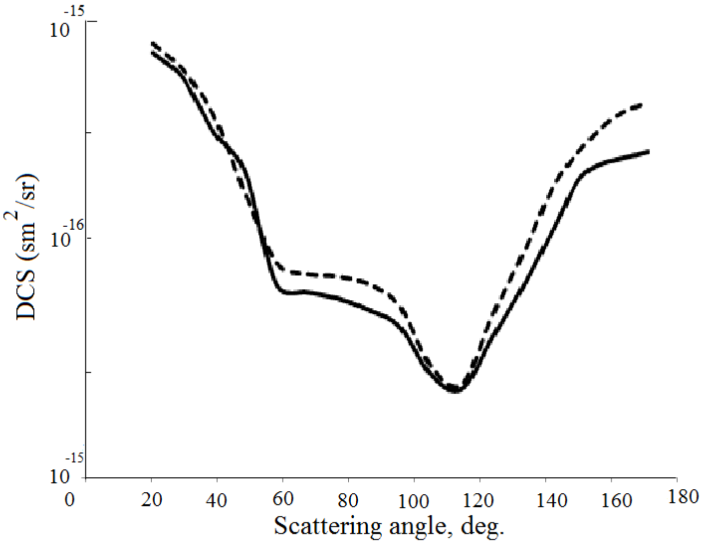

Fig.1. Differential cross-section (DCS) of elastic scattering of electrons with 25 eV energy on gold atom: Full line-the result of the given work. Points-Mott calculations [9].

In fig.1 comparison has been shown, calculated differential section with the data has been taken from [11-7] where calculation has been carried out based on Mott's scattering theory in Dirac-Hartree-Fock-Slater's approximation by spherical symmetric potential of Yukava type. As it is seen from this figure, although in these calculations various approaches have been made while choosing potentials (in this case function of electrons' density distribution in the atom according to Fermi-Dirac statistics has been chosen in the form of (Fermi function) movement of curved differential cross sections is in a good agreement.

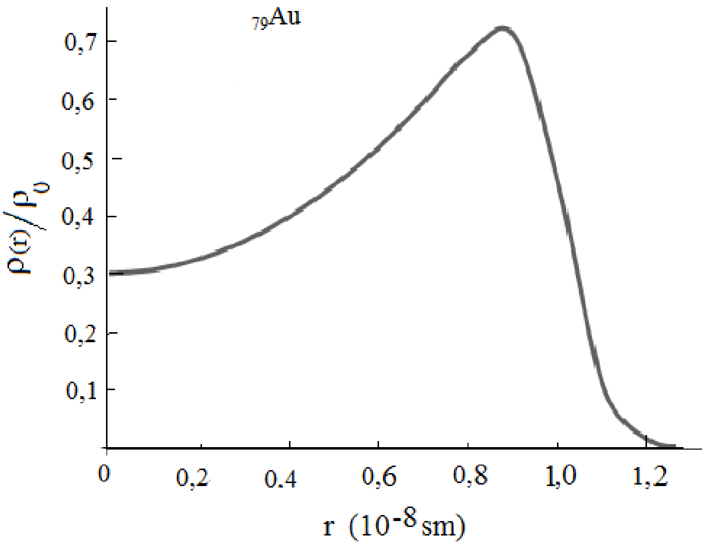

Fig 2.Distribution of electrons density on atom $_{79}Au$.
$d=0,1\cdot10^{-8}$sm, $R=1,37\cdot10^{-8}$sm (from the eksp.).

The curve describing the distribution function of radial density of electrons in gold atom in various values of parameters ω_0 =0.3, ω =0,6has been shown in fig.2 Thickness of surface layer of distribution of electrons density in the atom is determined with the help of the expression

$\Delta r = r_2(0{,}1\rho_{max}) - r_1(0{,}9\rho_{max})$ =0,167·10^{-8} sm. For the radius of root-mean-square distribution of electrons density in gold atom - $< r >^{1/2} = 0{,}19 \cdot 10^{-8}\ sm$ has been found in atom radius $R = 1{,}37 \cdot 10^{-8}\ sm$.

4. Conclusion

Thus, carried-out calculations and comparisons of charged atoms form-factors with the results obtained by precise numerical methods show that calculation of amplitude of elastic scattering process of electrons obtained in distorted wave high energy approximation is both a convenient and a precise method.

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ИССЛЕДОВАНИЕ АТОМОВ РАССЕЯНИЕМ ЭЛЕКТРОНОВ

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Резюме: На основе искаженно-волновой теории в аналитическом виде получено выражение для дифференциального сечения упругого и неупругого рассеяние электронов на атомах. Дифференциальное сечение упругого рассеяние электронов на свободном атоме золота вычисленный при падающей энергии электронов ~ 25 эВ сопоставлено с точным метода расчета. Определены толщины поверхностного слоя и среднеквадратичный радиус распределения плотности электронов в атоме золота.

Ключевые слова: искаженная электронная волна, дифференциальные сечения, характеристики атомов.

ELEKTRONLARIN SƏPİLMƏSİLƏ ATOMLARIN TƏDQİQİ

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Xülasə: Təhrif olunmuş dalğalar nəzəriyyəsi əsasında elektronların atomdan elastiki və qeyri-elastiki səpilməsinin diferensial effektiv kəsiyinin ifadəsi analitik şəkildə alınmışdır. Enerjisi ~ 25 eV olan elektronların qızıl atomundan elastiki səpilməsinin diferensial effektiv kəsiyi hesablanmaqla bu atomda elektronların sıxlığının paylanma funksiyası, elektronların paylanmasının orta kvadratik radiusu və atomun səth təbəqəsinin qalınlığı hesablanmışdır.

Açar sözlər: əyri elektron dalğası, diferensial kəsiklər, atomların xüsusiyyətləri.