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DISTORTED-WAVE APPROXIMATION THEORY FOR ELECTRON SCATTERING FROM ATOMIC

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Abstract

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 atoms $_{49}$In and $_{20}$Ca calculated in incident energy of electrons ~ 100 eV has been compared with experiments. Thickness of surface layer and root-mean square radius of density distribution of electron in that atoms have been determined.

Key words: Distorted Electron Wave, Differential sections, Atomic Structure

1. Introduction

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

Analyses of a number of experimental data of differential cross-section of on atom nuclear showed that good conformation is obtained in the cases, when wave functions of scattered electrons are distorted both on the phase and amplitude.

These effects bring to the displacement of diffraction minimums to the side of small angles and partially fill these minimums.

Apparently these phenomena are conditioned with that distorted functions are the functions of the distribution of charges density in the nuclear [4,5,6,7].

At present for modeling of the processes of electrons scattering from free atom or atomic crystallic lattice various set up models of calculation based on Monte-Carlo method are widely used [4].

Another widely used calculation method of differential cross section of elastic and inelastic electrons scattering is Mott's method of partial waves with screened atom potential of Dirac-Hartree-Fock where phase shift of scattered waves is determined from the number integration of differential equation [5]. Application of these calculation methods in analyzing of scattering from free atoms or the atoms in crystals in big energy of incident electrons is rather labour-consuming.

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

Differential cross section of elastic scattering of electron beam from free atom in work [6] 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 high energetic approximation in work [7] by Yennie, Boss and Ravenhall from quasi-classic solution of Dirac equation.

It should be noted that such approach of calculation of distorted phase function and amplitude of scattered waves depending on distribution density of charges in the target gave satisfactory results obtained in a number of calculations of differential sections on elastic and inelastic scattering of high-energetic electrons in nuclear [8].

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 electrons scattering.

Moreover in the frame of terms kR>>1 and E>>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 developing various approaches in the theory of electrons scattering.

Differential cross section of electrons scattering is determined by standard form [8]:

$$\frac{d\sigma_{if}}{d\Omega}=\frac{E_iE_f}{(2\pi)^2}\cdot\frac{k_f}{k_i}\frac{1}{2}\cdot\frac{1}{2J_i+1}\sum_{\sigma_i\sigma_f}\sum_{M_iM_f}\left|\;T_{if}\right|^2 \qquad (1)$$

Matrix element of atom transition from initial state (i) into final (f) in distorted-wave high energetic approximation is presented in the form

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

For wave functions of incident and scattered electrons the following expression has been obtained

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

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

Wave function of atomic state $|\mathrm{JM}\rangle$ is determined in the frame of this or that atom model. Coulomb interaction of incident electron with point nuclear and atom electrons with distribution density $\rho(r)$ is chosen in the form [9]:

$$V(\mathbf{r}) = -\frac{Ze^2}{\hbar c}\frac{1}{|\mathbf{r}|} + \frac{Ze^2}{\hbar c}\int \frac{\rho(\mathbf{x})\ d^3\mathbf{x}}{|\mathbf{r}-\mathbf{x}|} \qquad (4)$$

Product of wave functions of scattered electrons is presented as

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

Thus, for matrix element get

$$T_{if} = \langle J_f M_f \left| -\frac{Ze^2}{\hbar c}\int d^3r g(\boldsymbol{r})\frac{e^{i[qr+\phi(r)]}}{|r|} + \frac{4\pi Ze^2}{\hbar}\int dx \frac{g(x)e^{i[qx+\phi(x)]}}{q_{eff}^2(x)}\rho(x)\right| J_i M_i\rangle \qquad (6)$$

where

$$q_{eff}(\mathbf{x}) = \mathbf{q} + \nabla_u \phi(\mathbf{u}+\mathbf{x})_{u=0}.$$

Let's indicate function of electrons density distribution in the atom through radial transition density

$$< J_f M_f |\rho(\mathbf{x})| J_i M_i > = \sum_{LM} \rho_L(x) Y_{LM}^*(\hat{x}) \ (J_i L M_i M | J_f M_f)$$

$\rho_L(x)$ –is called radial transition density of atom.Now let's indicate section through form factor

$$\frac{d\sigma}{d\Omega} = (\frac{d\sigma}{d\Omega})_0 \frac{E_f}{E_i}\frac{k_f}{k_i}\frac{2J_f+1}{2J_i+1}\sum_{LM}\frac{1}{2L+1}|F_{LM}|^2 \qquad (7)$$

Where

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

for form-factor - $F_{LM}(\mathbf{q})$ get

$$F_{LM} = -\int g_0(\boldsymbol{r})\frac{e^{i[qr+\phi(r)]}}{|r|}d^3r + +q^2\int\frac{g(x)}{q_{eff}^2(x)}e^{i[qx+\phi(x)]}\rho_L(x)Y_{LM}^*(\hat{x})d^3 \qquad (8)$$

Here $\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$ is the impulse of electrons transfer to the target atom.

Let's write evident expression for distorting functions g(**x**) and ϕ(**x**). First of all let's write coulomb potential (4) for spherical symmetric distribution of electrons density $\rho(x)$ and present it in the form of

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

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

Now, expressing distorting terms in the phase and amplitude of scattered waves through these parameters one can get:

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

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

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

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

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

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

but potential in the centre of the atom have the form:

$$V(0) = -4\pi\gamma + 4\pi\gamma\int_0^\infty \rho(x)xdx$$

Before calculating integrals in form-factor (8), after applying the mathematical method of calculating the distorted-wave form-factor proposed by us in [8], then form-factor takes the following expression

$$F_{LM}(q) = -\int G_0(r)e^{iqr}d^3r + q^2\int G_{LM}(x)e^{iqx}\rho_L(x)Y^*_{LM}d^3x, \quad (9)$$

where amplitude functions $G_0(\mathbf{r})$ and $G_{LM}(\mathbf{x})$ accept the following form

$$G_0(r) = \left(1 - \frac{V(0)}{k}\right)\{1 + a((k_ir)^2 - [k_ir]^2 + \left((k_fr)^2 - [k_fr]^2\right) + \\ + b((k_ir) - -(k_fr))\},$$

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

Thus further research both elastic and inelastic scattering of electrons from the free atom brings to the calculation of form-factor.

3. Application of the theory

As the form-factor of the atom is experimentally measured value in elastic scattering of electrons, then its theoretical calculation with the help of obtained analytical expression by these or other methods is of great significance.

With this purpose let's choose the following coordinate system in calculating three-dimensional integral (9). Choosing axis $oz \uparrow\uparrow \mathbf{q}$ and indicating, $\cos(\hat{q}\hat{x}) = \mu$, where $\mathbf{x} = \{x\mu\varphi\}$ and $d\mathbf{x} = -x^2dxd\mu d\varphi$ disregarding loss of electron energy $\Delta E << E_i$, that is $|\mathbf{k}_i| = |\mathbf{k}_f| = k$ supposing that for impulse of transfer of scattered electrons we get $q = 2k\sin\theta/2 = 2k\alpha$

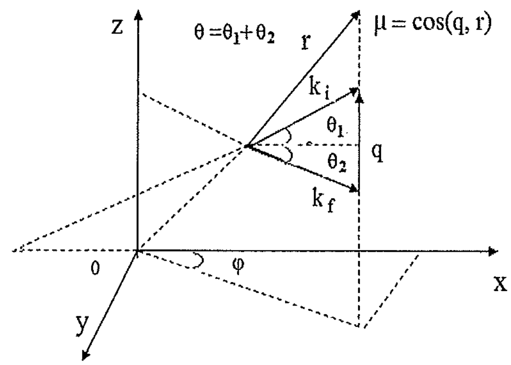

Fig.1. Impulse of incident ($\mathbf{k}_i$)and scattered ($\mathbf{k}_f$) electrons in three-dimension Decart coordinate system with transfer impulse $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$

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

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

After integration into (9) on the angles, the obtained form-factor for elastic scattering (*L=0*) can be brought to one-dimensional integral, which is the functional of Born form-factor

$$F_{L=0}(q) = \frac{2\pi i R^3}{(1-\frac{V(0)}{k})}\{F_B(q) - \frac{V(0)}{kR}\frac{\partial F_B(q)}{\partial q} -$$

$$- i3b\ [1 + \frac{2(4k^2-q^2)}{3q^2R(1-\frac{V(0)}{k})}]\frac{\partial F_B(q)}{\partial q}\}.$$

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 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

$$\rho_e(x) = \rho_0(\omega_0 + \omega\frac{x^2}{R^2})(1+\exp(\frac{x-R}{d}))^{-1} \qquad (10)$$

Pole method is used for calculation of radial integral-

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

which is shown in [8].

Final expression of differential cross section of elastic scattering of electrons from free atom has the following form:

$$\frac{d\sigma}{d\Omega} = (\frac{d\sigma}{d\Omega})_0\{|\mathrm{Re}\,F_0(q)|^2 + |\mathrm{Im}\,F_0(q)|^2\} \qquad (11)$$

where

$$\operatorname{Re} F_0(q) = F_B(q) - \frac{V(0)}{kR}\frac{\partial F_B(q)}{\partial q}$$

$$\operatorname{Im} F_0(q) = -3b\ [1+\frac{2(4k^2-q^2)}{3q^2R(1-\frac{V(0)}{k})}]\ \frac{\partial F_B(q)}{\partial q}$$

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

$$\left.\left[\frac{\pi d}{R}(\omega_0+\omega(3-(\frac{\pi d}{R})^2))\right]\cos(qR-\frac{\pi d}{R})\right\}$$

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

4. Results and discussions

Compactness of the obtained analytic expression of differential cross section (11) allows checking above developed theory in high accuracy level. Such examination has been carried out on the example of elastic scattering of electrons from atomics of ${}_{49}In$ and ${}_{20}Ca$ in the energy of incident electrons ~100 eV.

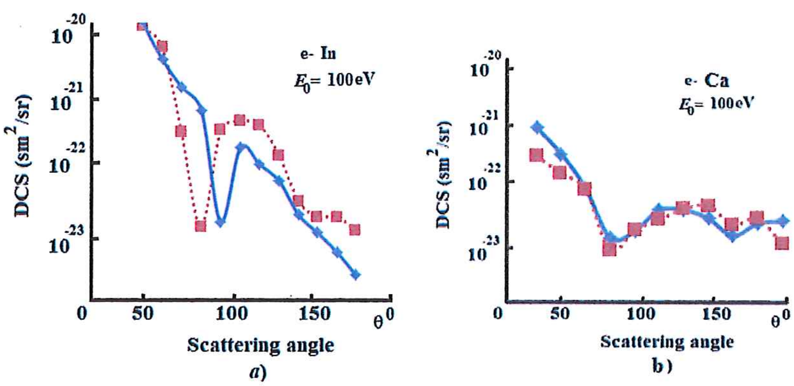

Fig.2. Differential cross section(DCS) of elastic scattering of electrons from ${}_{49}$In (a) and ${}_{20}$Ca (b) atomics by the comparison with experiments [12,13].

In fig. 2 comparison has been shown, calculated differential section with the data experiment. As it is seen from this figure-2 though 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.

Thickness of surface layer of distribution of electrons density in the atom is determined with the help of the expression

$$\Delta r = r_2(0{,}1\ \rho_{max}) - r_1(0{,}9\ \rho_{max}) = 0{,}167\cdot 10^{-8}\text{sm}$$

For radius of root-mean-square distribution of electrons density in atom ${}_{49}In$ - $< r >^{1/2} = 0{,}12\cdot 10^{-8}\ sm$ has been found in atom radius

$R = 1{,}27\cdot 10^{-8}\ sm$, also for atom ${}_{20}Ca$- $< r >^{1/2} = 0{,}12\cdot 10^{-8}\ sm$, $R = 1{,}16\cdot 10^{-8}\ sm$, (ω_0 =0,3; ω =0,6).

5. Conclusion

Thus carried out calculations and comparisons of charged atoms form-factors with the results obtained by experiments show that calculation of amplitude of elastic scattering process of electrons obtained in distorted wave high energy approximation is both convenient and precise method. This makes possibility to apply this theory to study the electronic structure of crystals by means elastic and inelastic electron scattering.

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