# Analytic Distorted-Wave Approximation for Electron Scattering from Atomic Calculations

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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, 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].

Study of atomic by electrons is one of the effective methods of research of atoms structure as the character of interaction of electron with nuclear and electrons surrounding nuclear is well known.

When studying surface structure of atoms with the help of scattered electrons physics-theoretic have two main tasks: to have more precise wave function of incident particles from atom and possibility of choice of more real test functions of electrons density distribution and also transition density. Besides it is advisable also to have maximum simple expressions for corresponding form-factors or sections in order to extract important information from the experiment on electrons scattering. It will allow carrying out repeated calculations using various test functions chosen for comparison with the experiment.

In this case the plain wave Born approach is considered the simplest one. This method can be used for atoms in all accessible modern experiments of the transmitted impulses excluding points of minimum sections. However, as the experience of practice shows values of average characteristic

atom parameters obtained by this method are some more excessive than the values of precise calculations. This difference affects especially in the case of average and heavy atoms.

As it is generally known from elastic scattering of electrons angular positions of minimums of differential cross section are one of the fundamental properties of scattering in the wide sphere of energies [3].

Energetic dependences of positions of differential cross sections minimums measured or calculated by various method are much better conformed with each other than values of cross sections in minimums [4].

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 nuclears [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]:

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

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

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

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

Wave function of atomic state $\varphi(\mathbf{x})$ 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 [10]:

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

Product of wave functions of scattered electrons is presented as

$$\Psi_f^{(-)*} \Psi_i^{(+)} = g(\mathbf{r}, v_f^+ v_i) \exp[i\mathbf{q}\mathbf{r} + i\varphi(\mathbf{r})] \qquad (5)$$

where

$$g(\mathbf{r}, v_f^+ v_i) = u_f^+(\mathbf{r}, v) u_i(\mathbf{r}, v) \qquad (6)$$

But distorted function in phase-is

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

Now substituting variables u=r-x and using expansion, limiting with the first term in amplitude function and with first two ones in the phase function write

$$\varphi(\mathbf{u}+\mathbf{x}) = \varphi(\mathbf{x}) + \nabla_u \varphi(\mathbf{u}+\mathbf{x})_{u=0}$$
$$g(\mathbf{u}+\mathbf{x}, v_f^+ v_i) = g(\mathbf{x}, v_f^+ v_i) = g(\mathbf{x}) v_f^+ v_i \qquad (8)$$

Thus, for matrix element get

$$T_{if} = \langle J_f M_f \left| -\frac{Ze^2}{\hbar c} \int d^3 r g(\mathbf{r}) \frac{e^{i[qr+\phi(r)]}}{|r|} + \frac{4\pi Ze^2}{\hbar} \int dx \frac{g(x)e^{i[qx+\phi(x)]}}{q_{eff}^2(x)} \rho(\mathbf{x}) \right| J_i M_i \rangle \qquad (9)$$

where

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

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

$$< J_f M_f |\rho(\mathbf{x})| J_i M_i > = \sum_{LM} \rho_L(x) Y_{LM}^*(\hat{x}) \; \left( J_i L M_i M | J_f M_f \right),$$ (11)

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

$$\frac{d\sigma}{d\Omega} = (\frac{d\sigma}{d\Omega})_0 \frac{E_f}{E_i} \frac{k_f}{k_i} \frac{2J_f+1}{2J_i+1} \sum_{LM} \frac{1}{2L+1} |F_{LM}|^2$$ (12)

where

$$(\frac{d\sigma}{d\Omega})_0 = (\frac{2Ze^2 k_i}{q^2})^2 \cos^2 \theta/_2$$ (13)

$$\sum_{\sigma_i \sigma_f} \left| \upsilon_f^+ \upsilon_i \right|^2 = \cos^2(\vartheta/_2)$$ (14)

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

$$F_{LM}(\boldsymbol{q}) = - \int g_0(\boldsymbol{r}) \frac{e^{i[qr+\phi(r)]}}{|r|} d^3r + q^2 \int \frac{g(x)}{q_{eff}^2(x)} e^{i[qx+\phi(x)]} \rho_L(x) Y_{LM}^*(\hat{x}) d^3x$$ (15)

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

$$V_e(r) = -4\pi\gamma \{\frac{1}{r} \int_0^r \rho(x)x^2 dx + \int_r^\infty \rho(x)x dx \}$$ (16)

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:

$$\varphi(\mathbf{x}, \gamma) = -(\mathbf{qx}) \frac{V(0)}{k} + a(3/_2 k^2 x^2 \mathbf{qx} -$$
$$- (\mathbf{k}_i \mathbf{x})^3 + (\mathbf{k}_f \mathbf{x})^3) - b([\mathbf{xk}_i]^2 + [\mathbf{xk}_f]^2)$$ (17)

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

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

$$a = -4\pi\gamma + \frac{4\pi\gamma}{3k^3} \rho(0),$$ (19)

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

$$b = \frac{\pi\gamma}{k^2} \int_0^\infty \rho(x)dx$$ (20)

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

$$V(0) = -4\pi\gamma + 4\pi\gamma \int_0^\infty \rho(x)x dx$$ (21)

before calculating integrals in form factor (15), let's do simplification that's indicate

$$I(\mathbf{x}, \gamma) = e^{i[\mathbf{qx}+\varphi(\mathbf{x}, \gamma)]}$$ (22)

and expand it into a power series of small parameter $\gamma \ll 1$,

$$I(\mathbf{x}, \gamma) = \sum_{n=0}^\infty \gamma^n I_n(\mathbf{x})$$ (23)

For determining the terms of this series $I_n(\mathbf{x})$, let's write product expression (22) on $\gamma$ in the following form

$$\frac{\partial I(\mathbf{q}, \mathbf{x})}{\partial \gamma} = i\bar{\varphi}(\mathbf{x}) \cdot I(\mathbf{q}, \mathbf{x})$$ (24)

where

$$\varphi(\mathbf{x}, \gamma) = \gamma \bar{\varphi}(\mathbf{x})$$ (25)

From the other side expanding (24) in a power series of $\gamma$ and comparing it with the product on from (23), we get the following recurrent formula

$$I_{n+1}(\mathbf{x}) = \frac{i\varphi(\mathbf{x})}{\gamma(n+1)} I_n(\mathbf{x}), \qquad n = 0,1,2,3,...., \qquad (26)$$

Here

$$I_0(\mathbf{x}) = e^{i\mathbf{q}\mathbf{x}} \qquad (27)$$

then form-factor takes the following expression

$$F_{LM}(\mathbf{q}) = - \int G_0(r)e^{iqr}\,d^3r + q^2 \int G_{LM}(\mathbf{x})e^{iqx}\rho_L(x)Y_{LM}^*(\hat{x})d^3x, \qquad (28)$$

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

$$G_0(\mathbf{r}) = \left(1 - \frac{V(0)}{k}\right)\left\{1 + a((\mathbf{k}_i\mathbf{r})^2 - [\mathbf{k}_i\mathbf{r}]^2 + \left((\mathbf{k}_f\mathbf{r})^2 - [\mathbf{k}_f\mathbf{r}]^2\right) + b((\mathbf{k}_i\mathbf{r}) - (\mathbf{k}_f\mathbf{r}))\right\} \qquad (29)$$

$$G_{LM}(\mathbf{x}) = \frac{g(\mathbf{x})\{1 + i\varphi(\mathbf{x}) - \frac{1}{2}\varphi^2(\mathbf{x})\}}{q_{eff}^2(\mathbf{x})} \qquad (30)$$

$$\cos\hat{x}\hat{k}_f = -\mu\alpha + \sqrt{1-\mu^2}\sqrt{1-\alpha^2}\cos\phi \qquad (32)$$

Thus further research both elastic and inelastic scattering of electrons from the free atom brings to the calculation of form-factor (28).

## 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 (28). Choosing axis $oz \uparrow\uparrow \mathbf{q}$ and indicating, $\cos(\hat{q}\hat{x}) = \mu$, where $\mathbf{x} = \{x\mu\phi\}$ and $d\mathbf{x} = -x^2 dx\,d\mu\,d\phi$ disregarding loss of electron energy $\Delta E \ll E_i$, that is $|\mathbf{k}_i| = |\mathbf{k}_f| = k$ supposing that for impulse of transfer of scattered electrons we get $q = 2k\sin\frac{\vartheta}{2} = 2k\alpha$, $\alpha = \sin\frac{\vartheta}{2}$,

$$\cos\hat{x}\hat{k}_i = \mu\alpha + \sqrt{1-\mu^2}\sqrt{1-\alpha^2}\cos\phi \qquad (31)$$
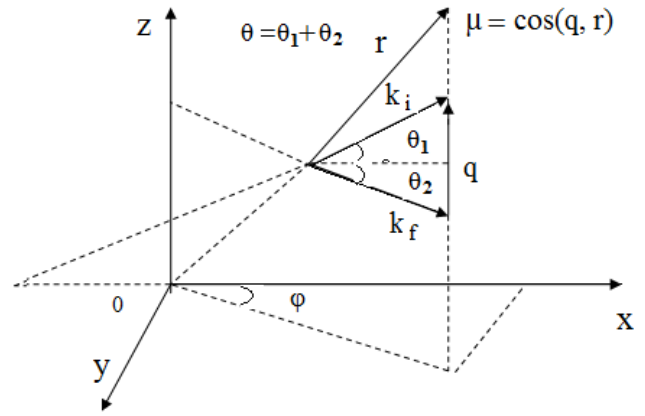


**Figure 1.** *Impulse of incident ($\mathbf{k}_i$) and scattered ($\mathbf{k}_f$) electrons in three-dimension Decart coordinate system with transfer impulse $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$*

After integration into (28) 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

$$F_{L=0}(q) = 2\pi i \frac{R^3}{(1-\frac{V(0)}{k})}\left\{F_B(q) - \frac{V(0)}{kR}\frac{\partial F_B(q)}{\partial q} - i\ 3b[1 + \frac{2(4k^2 - q^2)}{3q^2 R(1-\frac{V(0)}{k})}]\frac{\partial F_B(q)}{\partial q}\right\} \qquad (33)$$

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- $\omega$

$$\rho_e(x) = \rho_0(\omega_0 + \omega\frac{x^2}{R^2})(1 + \exp(\frac{x-R}{d}))^{-1} \qquad (34)$$

Pole method is used for calculation of radial integral -

$$F_B(q) = \frac{3}{4\pi R^5[1 + (\frac{\pi d}{R})^2]}\sum_{\varepsilon=\pm 1}\varepsilon\int_0^\infty \ell^{iqx\varepsilon}\frac{\omega_0 + \omega\frac{x^2}{R^2}}{1 + e^{\frac{x-R}{d}}}x\,dx, \quad (35)$$

which is shown in [8].

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

$$\frac{d\sigma}{d\Omega} = (\frac{d\sigma}{d\Omega})_0\{|\text{Re}\,F_0(q)|^2 + |\text{Im}\,F_0(q)|^2\} \qquad (36)$$

where

$$\mathrm{Re}\,F_0(q) = F_B(q) - \frac{V(0)}{kR}\frac{\partial F_B(q)}{\partial q} \qquad (37)$$

$$\mathrm{Im}\,F_0(q) = -3b\,\left[1 + \frac{2(4k^2 - q^2)}{3q^2 R(1 - \frac{V(0)}{k})}\right]\frac{\partial F_B(q)}{\partial q} \qquad (38)$$

$$F_B(q) = -4\frac{\pi d}{R}\cdot e^{-\pi dq}\left\{[\omega_0 + \omega(1 - 3\pi(\frac{d}{R})^2)]\sin(qR - \frac{\pi d}{R}) + \left[\frac{\pi d}{R}(\omega_0 + \omega(3 - (\frac{\pi d}{R})^2))\right]\cos(qR - \frac{\pi d}{R})\right\} \qquad (39)$$

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 (35) allows checking above developed theory in high accuracy level.

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.
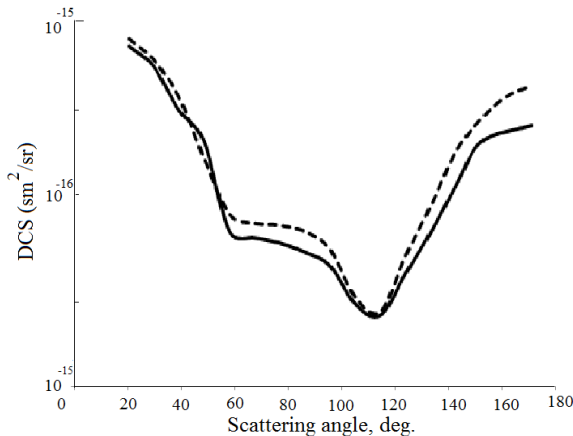
**Figure 2.** *Differential cross section (DCS) of elastic scattering of electrons with 25 eV energy on gold atom: Full line-the result of the given work. Points-Mott calculations [11].*

In Figure 2 comparison has been shown, calculated differential section with the data has been taken from [11] where calculation has been carried out 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 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.

d=0,1·10$^{-8}$sm, R=1,37·10$^{-8}$sm (from the eksp.)

The curve describing the distribution function of radial density of electrons in gold atom in various values of parameters $\omega_0 = 0,3; \omega = 0,6$ has been shown in Figure 3. Thickness of surface layer of distribution of electrons density in the atom is determined with the help of the expression $\Delta r = r_2(0,1\rho_{max}) - r_1(0,9\rho_{max}) = 0,167\cdot 10^{-8}$ sm. For radius of root-mean-square distribution of electrons density

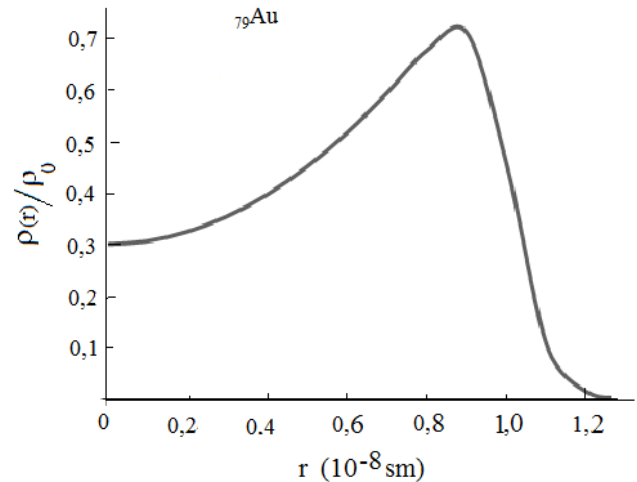in gold atom - $< r >^{1/2} = 0,19\cdot 10^{-8}$ sm has been found in atom radius $R = 1,37\cdot 10^{-8}$ sm.

**Figure 3.** *Distribution of electrons density on atom $_{79}$Au.*

## 5. 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 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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