

SURFACE SCATTERING POTENTIAL FOR ELECTRON DIFFRACTION*

K. STACHULEC

*Technical University,
25-314 Kielce, Poland*

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A simple dynamical scattering potential for electron diffraction by a free surface of a solid state sample is proposed. A few monoatomic layers parallel to the surface of the scattering sample are treated as a thin film while the other part of the sample is considered as a substrate. The scattering potential of the sample is expressed in terms of the mean square displacement of atoms and the electron density distribution at a scattering surface of the thin film sample. The obtained formula for the scattering potential in special cases leads to results of Dvoriankin's paper [3]. The proposed surface scattering potential can be used to describe low energy electron diffraction (LEED) as well as high energy electron diffraction (HEED) experiments.

1. Introduction

In the present paper we propose a simple dynamical scattering potential for electron diffraction by a solid state sample with a free surface. The sample is treated as a thin film evaporated on a substrate. We regard a thin film as a system of a few monoatomic layers parallel to the surface of the sample, while the other part of the sample is considered as the substrate.

For such samples we have calculated a scattering potential including the exchange of the incident electrons with the electrons of the sample. Including the exchange part of the scattering potential gives a possibility to use of the scattering potential to describe a polarized electron diffraction experiment in the cases of low energy electron diffraction (LEED) as well as of high energy electron diffraction (HEED).

The proposed surface scattering potential in its analytical form is a temperature and thickness dependent quantity and it is expressed in terms of the mean square displacement of atoms and the electron density distribution of the thin film. The division of the scattering film into the thin film and the substrate allows one to compute the dynamical parameters of the scattering potential by means of the field theories developed for thin films [2].

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2. The scattering potential for electron diffraction by a sample with free surface

We shall assume that a spin polarized electron beam is incident on a perfectly clean, well ordered surface of a sample. Our interest will focus on the elastically scattering electrons, because they produce almost all the structure in the diffraction patterns.

To construct the scattering potential we divide the scattering sample into a thin film and a substrate. By the thin film we understand n monoatomic layers parallel to the surface. They are numbered by ν , starting with $\nu = 1$ for the free surface of the film and finishing with $\nu = n$ for the atomic layer evaporated directly on the substrate. Any monoatomic layer ν we divide into two-dimensional elementary cells and the position of any cell inside the ν -th atomic layer related to the cell chosen as the origin of the coordinate system is given by a two-dimensional vector $\mathbf{j}_\nu = \mathbf{a}j'_x + \mathbf{b}j'_y$, where \mathbf{a} and \mathbf{b} are lattice vectors and j'_x, j'_y denote integer numbers.

Let the z -axis of the coordinate system be perpendicular to the surface and directed into the inside of the film. A position of any atom in the film can be described by the vector

$$\mathbf{R}_{\nu\mathbf{j}_\nu s} = \mathbf{j}_\nu + \hat{e}_z c_\nu \nu + \rho'_s = \mathbf{R}_{\nu\mathbf{j}_\nu} + \rho'_s, \quad (1)$$

where ρ'_s describes the position of an s -th atom belonging to the $(\nu\mathbf{j}_\nu)$ -th cell related to the origin of the local coordinate system bounded with the $(\nu\mathbf{j}_\nu)$ -th cell inside the film.

From the point of view of the diffraction problem the thin film is regarded as a system of $n \cdot N^2$ bounded atoms, where N^2 denotes the number of atoms in any ν -th layer parallel to the surface.

Such a system produces a suitable effective scattering potential localized round about each lattice node of the film. In general case, the scattering potential of the $(\nu\mathbf{j}_\nu s)$ -th atom of the thin film depends on the position $(\mathbf{r} - \mathbf{R}_{\nu\mathbf{j}_\nu s})$ and spin coordinates s_0 of the diffracted electrons. Denoting this potential by $V(\mathbf{r} - \mathbf{R}_{\nu\mathbf{j}_\nu s}, s_0)$, a total scattering potential on the position \mathbf{r} inside the film and spin s_0 $V(\mathbf{r}, s_0)$ can be treated in a first approximation as the superposition of the effective potentials of the individual atoms from which the film is built:

$$V(\mathbf{r}, s_0) = \sum_{\nu\mathbf{j}_\nu s} V(\mathbf{r} - \mathbf{R}_{\nu\mathbf{j}_\nu s}, s_0). \quad (2)$$

By the effective potential of the individual atom we understand the potential produced by a given atom in the presence of other atoms of the thin film and the substrate on which the film is evaporated. This potential can be constructed by a modification of the scattering potential of a free atom.

Now, let us consider the scattering of an electron by free atom. Denoting by \mathbf{r}_0 and s_0 the position and spin coordinates of the incident electron, and by $\mathbf{r}_1 s_1$,

$\mathbf{r}_2 s_2, \dots, \mathbf{r}_N s_N$, the position and spin coordinates of the atomic electrons, where N denotes the total number of electrons in the atom, we should describe the scattering problem by means of a wave function $\Phi = \Phi(\mathbf{r}_0 s_0, \mathbf{r}_1 s_1, \dots, \mathbf{r}_N s_N)$ which depends on all coordinates of the $(N + 1)$ electrons.

The many body function Φ has to satisfy an equation which we write in the form:

$$\left[\sum_{j=0}^N \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{Z e^2}{r_j} \right) + \sum_{j=0}^N \sum_{i=j+1}^N \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right] \Phi = E_i \Phi, \quad (3)$$

where $(-\hbar^2 \nabla^2 / 2m)$ is the operator of the kinetic energy of the j -th electron, so that $\sum (-\hbar^2 \nabla^2 / 2m)$ describes the kinetic energy of the system of N atomic electrons plus an incident electron. The term $\sum (-Z e^2 / r_j)$ is the potential energy of all the electrons in the field of nucleus, the third term in Eq. (3) stands for the Coulomb interaction between electrons. E_i denotes the total energy of the system and Z_e the nuclear charge while j numbers the electrons of the system.

The difficulty in Eq. (3) is that electrons influence one another via Coulomb repulsion and the incident electron may distort wave functions of the atomic electrons by its own electrostatic field correlating their motion with its own and changing the potential seen by the incident electron itself.

If the free atom wave function is known, we can express the many body function by means of the free atom functions $\psi_1(\mathbf{r}_1 s_1) \psi_2(\mathbf{r}_2 s_2) \dots \psi_N(\mathbf{r}_N s_N)$ as follows [1]

$$\Phi = \sum_p \varepsilon_p \phi(\mathbf{r}_0 s_0) \psi_1(\mathbf{r}_1 s_1) \dots \psi_N(\mathbf{r}_N s_N), \quad (4)$$

where $\phi(\mathbf{r}_0 s_0)$ is the incident electron's function.

The sum is over permutations of the particle coordinates and ε_p takes the value of $+1$ if permutation p can be achieved by exchanging an even number of particle coordinates, -1 for an odd number. There are $(N + 1)!$ possible permutations.

Since the atom state part of Φ is known, we want to eliminate this part from our equations and concentrate on $\phi(\mathbf{r}_0 s_0)$ being the incident electron wave function.

Multiplying Eq. (3) by

$$\chi^* = \psi_1^*(\mathbf{r}_1 s_1) \psi_2^*(\mathbf{r}_2 s_2) \dots \psi_N^*(\mathbf{r}_N s_N), \quad (5)$$

integrating over space, and summing over spin coordinates of χ we obtain the equation for $\phi(\mathbf{r}_0 s_0)$

$$\left[-\frac{\hbar^2}{2m} \nabla_0^2 - \frac{Z e^2}{r_0} + \sum_j \int \sum_{s_j} \frac{|\psi_j(\mathbf{r}_j s_j)|^2}{|\mathbf{r}_0 - \mathbf{r}_j|} d^3 r_j \right] \phi(\mathbf{r}_0 s_0) - e^2 \sum_j \int \sum_{s_j} \frac{\psi_j^*(\mathbf{r}_j s_j) \phi(\mathbf{r}_j s_j)}{|\mathbf{r}_0 - \mathbf{r}_j|} d^3 r_j \psi_j(\mathbf{r}_0 s_0) = E_0 \phi(\mathbf{r}_0 s_0), \quad (6)$$

where E_0 denotes the energy of the incident electron.

The last equation is a one-electron equation for the wave function of the incident electron and it defines the effective scattering potential of the free atom $V_0(\mathbf{r}_0 s_0)$

$$V_0(\mathbf{r}_0 s_0) = \frac{Ze}{r_0} - e \sum_j \int \sum_{s_j} \frac{|\psi_j^*(\mathbf{r}_j s_j)|^2}{|\mathbf{r}_0 - \mathbf{r}_j|} d^3 r + V_{\text{exc}}(\mathbf{r}_0 s_0), \quad (7)$$

where by $V_{\text{exc}}(\mathbf{r}_0 s_0)$ we denote the so called exchange potential, which is defined by the equation:

$$V_{\text{exc}}(\mathbf{r}_0 s_0) \phi(\mathbf{r}_0 s_0) = \sum_j \sum_{s_j} \int d^3 r_j \frac{\psi^*(\mathbf{r}_j s_j) \phi(\mathbf{r}_j s_j)}{|\mathbf{r}_0 - \mathbf{r}_j|} \psi_j(\mathbf{r}_0 s_0). \quad (8)$$

The two first terms on the right hand side of the equation (7) have a simple interpretation as the electrostatic potentials produced by the nucleus and the electron density distribution of the atom, respectively. The exchange potential defined by (8) is non-local potential and it arises out of considerations of antisymmetry of the wave function under exchange of particle coordinates, because no two electrons can be in the same place at the same time, hence each electron is surrounded by a region depleted of other electrons and hence lower potential.

Writing the one-electron wave function $\psi_j(\mathbf{r}_j s_j)$ as $\psi_j(\mathbf{r}_j s_j) = \psi_j(\mathbf{r}_j) \chi_j(s_j)$, where $\chi_j(s_j)$ is the spin coordinate dependent part of the wave function of the j -th atomic electron while $\psi_j(\mathbf{r}_j)$ is space coordinate dependent only, we can express the electrostatic potential of atomic electrons by means of the electron distribution in the atom $\rho_j(\mathbf{r})$ as:

$$e \sum_j \sum_{s_j} \int d^3 r_j \frac{|\psi_j(\mathbf{r}_j s_j)|^2}{|\mathbf{r}_0 - \mathbf{r}_j|} = -e \sum_j \int d^3 r \frac{\rho_j(\mathbf{r})}{|\mathbf{r}_0 - \mathbf{r}|}. \quad (9)$$

Analogically, writing $\phi(\mathbf{r}_0 s_0) = \phi(\mathbf{r}_0) \eta(s_0)$, where $\eta(s_0)$ is the spin wave function of an incident electron, the exchange potential can be written as

$$V_{\text{exc}}(\mathbf{r}_0 s_0) = \sum_j \sum_{s_j} \frac{\chi_j^*(s_j) \eta(s_j) \chi_j(s_0) \eta^*(s_0)}{|\eta(s_0)|^2} \cdot I_j(\mathbf{r}_0) = \sum_j \delta_{s_0, s_j} I_j(\mathbf{r}_0), \quad (10)$$

where

$$I_j(\mathbf{r}_0) = \frac{\psi_j(\mathbf{r}_0) \phi^*(\mathbf{r}_0)}{|\phi(\mathbf{r}_0)|^2} \int d^3 r_j \frac{\psi^*(\mathbf{r}_j) \phi(\mathbf{r}_j)}{|\mathbf{r}_0 - \mathbf{r}_j|} \quad (11)$$

and the sum is over the atomic electrons which have the same spin as the incident electron.

In this way a full scattering potential of a free atom takes the form:

$$V_{\text{at}}(\mathbf{r}_0 s_0) = \frac{eZ}{r_0} - e \sum_j \int \frac{\rho_j(\mathbf{r})}{|\mathbf{r}_0 - \mathbf{r}|} d^3 r + \sum_j \delta_{s_0, s_j} I_j(\mathbf{r}_0). \quad (12)$$

The above formula will be a basis to construct the scattering potential for the electrons scattered by thin films.

It is known that crystal lattice atoms at a given temperature take part in the temperature vibrations around their equilibrium position and the influence of the temperature on the scattering potential must be taken into consideration defining a dynamic scattering potential for an atom as [3, 7]

$$V_T(\mathbf{r}, s_0) = \int V_{\text{at}}(\mathbf{r}', s'_0) T(\mathbf{r} - \mathbf{r}') d^3 r', \quad (13)$$

where $T(\mathbf{r})$ describes a distribution of the mass centre of an atom in its vibrations around the equilibrium position. For the atom bounded in crystal $T(\mathbf{r})$ is determined by the lattice dynamics.

Other thing we would like to stress is that placing an atom in a lattice site of an infinite size sample does not change the mean square displacement which characterizes the dynamics of the atom in the sample and it is the same for every atom. However, in the thin film crystal case the surface atoms of any solid body are in a situation which is different from that of atoms situated in the inside of the film. The surface atoms feel the changes in the geometry of the neighbours surrounding them caused by the missing neighbours, by the spontaneous deformation of the lattice near the surface. As a result, the scattering potential near the surface must be different from that inside of a bulk material. It is to be expected that the changes of the electronic structure near the surface must cause some changes of the physical properties related to the surface.

To take above into consideration we introduce the effective numbers of electrons per j -th orbital of the $(\nu j_\nu s)$ atom in the film $\langle n_{\nu j_\nu s} \rangle$ which are the same for the atoms in the ν -th monoatomic layer but they create a distribution in the direction perpendicular to the surface. The redistribution of the electronic charge in the film creates some new boundary conditions for lattice vibrations which must influence the temperature dependence of the mean square displacements of the atoms in other atomic layers parallel to the surface. Denoting the mean square displacement of the $(\nu j_\nu s)$ -th atom in the film by $B_{\nu j_\nu s}$ we can write

$$B_{\nu j_\nu s} \equiv \langle (\delta \mathbf{R}_{\nu j_\nu s})^2 \rangle = B_{\nu s}, \quad (14)$$

as well as for the electron density distribution of the j -th orbital

$$\langle n_{\nu j_\nu s}^j \rangle = \langle n_{\nu s}^j \rangle, \quad (15)$$

where the symbol $\langle \dots \rangle$ stands for the thermodynamical average, and the above relations are the consequence of the translation symmetry of the film.

By means of the above dynamical parameters $B_{\nu s}$ and $\langle n_{\nu s}^j \rangle$ we propose the following modification of the scattering potential of the atom in the $(\nu j_\nu s)$ -th site of the film:

$$V_T(\mathbf{r}_0 - \mathbf{R}_{\nu j_\nu s}, s_0) = (2\pi B_{\nu s})^{-\frac{3}{2}} \int d^3 r' V_{\text{at}}(\mathbf{r}' - \mathbf{R}_{\nu j_\nu s}, s_0) e^{-\frac{|\mathbf{r}_0 - \mathbf{R}_{\nu j_\nu s} - \mathbf{r}'|^2}{2B_{\nu s}}}, \quad (16)$$

where $T(\mathbf{r}') = (2\pi B_{\nu s})^{-\frac{3}{2}} \exp(-|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s} - \mathbf{r}'|^2 / 2B_{\nu s})$ describes the distribution of the mass centre of the $(\nu j \nu s)$ -th atom in its temperature vibrations [3] and in place of the free atom potential V_{at} given by (12) we take \tilde{V}_{at} which we define as

$$\begin{aligned} \tilde{V}_{\text{at}}(\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}, s_0) = & \frac{Ze}{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|} - e \sum_j \langle n_{\nu s}^j \rangle \int \frac{\rho_j(\mathbf{r}_j - \mathbf{R}_{\nu j \nu s})}{|\mathbf{r}_0 - \mathbf{r}_j|^0} d^3 r_j + \\ & + e \sum_j \langle n_{\nu s}^j \rangle I_j(\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}) \delta_{s_0 s_j}. \end{aligned} \quad (17)$$

To obtain an analytic formula for the scattering potential of the spin polarized electrons scattered by thin films using the formulae (2), (16) and (17) we have to know the atomic orbitals of a free atom. By means of these orbitals the quantities ρ_j and I_j in formula (17) are expressed. For that we restrict our next considerations to the case when the free atom orbitals are spherically symmetric and we take them in the Slater form [1, 4]:

$$\psi_j(r) = A_j r^{\mu_j} \exp(\lambda_j r), \quad (18)$$

where μ_j, λ_j are the numerical parameters given for all free atoms in [4], and A_j is the normalization constant. If we now write the incident electron wave function in the form of the plane wave:

$$\phi(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (19)$$

where \mathbf{k} is the wave vector of the incident electron, we can insert expressions (18) and (19) into the equation (17) and calculate the static scattering potential of $(\nu j \nu s)$ atom $\tilde{V}_{\text{at}}(\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}, s_0)$ of the film. We have:

$$\begin{aligned} \tilde{V}_{\text{at}}((\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}), s_0) = & \frac{Ze}{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|} - \\ -4\pi e \sum_j A_j^2 \langle n_{\nu s}^j \rangle & \left[\frac{1}{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|} \int_0^{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|} |\mathbf{r}_j - \mathbf{R}_{\nu j \nu s}|^{2\mu_j + 2} e^{-2\lambda_j |\mathbf{r}_j - \mathbf{R}_{\nu j \nu s}|} d r_j + \right. \\ & + \int_{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|}^{\infty} |\mathbf{r}_j - \mathbf{R}_{\nu j \nu s}|^{2\mu_j + 1} e^{-2\lambda_j |\mathbf{r}_j - \mathbf{R}_{\nu j \nu s}|} d r_j \left. \right] + \\ + 4\pi e \sum_j A_j^2 \langle n_{\nu s}^j \rangle & |\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|^{\mu_j} e^{-(\lambda_j + i\mathbf{k}') \cdot |\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|} * \\ * \left[\frac{1}{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|} \int_0^{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|} & |\mathbf{r}_j - \mathbf{R}_{\nu j \nu s}|^{\mu_j + 2} e^{-(\lambda_j - i\mathbf{k}') \cdot |\mathbf{r}_j - \mathbf{R}_{\nu j \nu s}|} d r_j + \right. \\ & + \int_{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|}^{\infty} |\mathbf{r} - \mathbf{R}_{\nu j \nu s}|^{\mu_j + 1} e^{-(\lambda_j - i\mathbf{k}') \cdot |\mathbf{r}_j - \mathbf{R}_{\nu j \nu s}|} d r_j \left. \right]. \end{aligned} \quad (20)$$

Integrating over r_j by means of the standard formulae [5]:

$$\int_0^u x^{\nu-1} \exp(-\mu x) dx = \mu^{-\nu} \gamma(\nu, \mu u),$$

$$\int_u^\infty x^{\nu-1} \exp(-\mu x) dx = \mu^{-\nu} \Gamma(\nu, \mu u),$$

where $\gamma(\nu, \mu u)$ and $\Gamma(\nu, \mu u)$ are so-called incomplete gamma functions, as the result we obtain

$$\begin{aligned} \tilde{V}_{at} = & \frac{Ze}{|\mathbf{r} - \mathbf{R}_{\nu j \nu s}|} - 4\pi e \sum_j A_j^2 \frac{\langle n_{\nu s}^j \rangle}{(2\lambda_j)^{2\mu_j+2}} * \\ & * \left[\frac{\gamma(\mu_j + 3, |\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}| 2\lambda_j)}{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}| 2\lambda_j} + \Gamma(\mu_j + 2, |\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}| 2\lambda_j) \right] + \\ & + 4\pi e \sum_j A_j^2 \delta_{s_0 s_j} \langle n_{\nu s}^j \rangle e^{-(\lambda_j + ik')|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|} \cdot |\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|^{\mu_j} (\lambda_j - ik')^{(\mu_j+2)} * \\ & * \left[\frac{\gamma(\mu_j + 3, (\lambda_j - ik')|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|)}{|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}| (\lambda_j - ik')} + \Gamma(\mu_j + 2, (\lambda_j - ik')|\mathbf{r}_0 - \mathbf{R}_{\nu j \nu s}|) \right]. \end{aligned} \tag{21}$$

Next, the calculation for the dynamical scattering potential by means of the formula (16) and explicit form of \tilde{V}_{at} given by (21) leads to the expression

$$V_T(\mathbf{r} - \mathbf{R}_{\nu j \nu s}, s_0) = e^{-\frac{|\mathbf{r} - \mathbf{R}_{\nu j \nu s}|^2}{2B_{\nu s}}} \sum_{k=0}^\infty \frac{(1/B_{\nu s})^{2k}}{(2k+1)!} \tilde{V}_T^{(k)}(B_{\nu s}, s_0), \tag{22}$$

where

$$\begin{aligned} \tilde{V}_T^{(k)}(B_{\nu s}, s_0) = & (2\pi B_{\nu s})^{-\frac{3}{2}} \int_0^\infty 4\pi r'^{2k+2} e^{-\frac{r'^2}{2B_{\nu s}}} \cdot \tilde{V}_{at}(\mathbf{r}', s_0) dr' = \\ = & Ze \langle F_{0,-1} \rangle_k - 4\pi e \sum_j A_j^2 \langle n_{\nu s}^j \rangle \frac{(2\mu_j + 1)!}{(2\lambda_j)^{2\mu_j+2}} * \\ & * \left[\frac{2\mu_j + 2}{2\lambda_j} \langle F_{0,-1} \rangle_k - (2\mu_j + 2) \sum_{m=0}^{2\mu_j+2} \frac{(2\lambda_j)^{m-1}}{m!} \langle F_{2\lambda_j, m-1} \rangle_k + \right. \\ & + \sum_{m=0}^{2\mu_j+1} \frac{(2\lambda_j)^m}{m!} \langle F_{2\lambda_j, m} \rangle_k \left. \right] + 4\pi e \sum_j A_j^2 \langle n_{\nu s}^j \rangle \delta_{s_0 s_j} \frac{(2\mu_j + 1)!}{\beta_j^{\mu_j+2}} * \\ & * \left[(\mu_j + 2) \left\langle F_{\beta_j', \mu_j-1} \right\rangle_k \frac{1}{\beta_j} - \sum_{m=0}^{\mu_j+2} \frac{\beta_j^{m-1}}{m!} \langle F_{\beta_j', m+\mu_j-1} \rangle_k \right] + \sum_{m=0}^{\mu_j+1} \frac{\beta_j^m}{m!} \langle F_{\beta_j', m+\mu_j} \rangle_k \end{aligned} \tag{23}$$

where $F_{xn} = r^n e^{-xr}$ and $\langle F_{x,n} \rangle$ stands for the following integral for the $(\nu j_\nu s)$ - site of the lattice

$$\begin{aligned} \langle F_{x,n} \rangle_k &= (2\pi B_{\nu s})^{-\frac{3}{2}} \int 4\pi r^{2k+2} \exp(-r^2/2B_{\nu s}) F_{xn}(r) dr = \\ &= 4(2\pi B_{\nu s})^{-\frac{3}{2}} (B_{\nu s})^{\frac{2k+n+3}{2}} (2k+n+2)! e^{\frac{1}{2} B_{\nu s} x^2} D_{-(2k+n+3)} \left(x \sqrt{B_{\nu s}} \right). \end{aligned} \quad (24)$$

In the last expression $D_n(x)$ denotes the standard function of the parabolic cylinder [5], while the quantity β'_j which appears in (23) is defined as

$$\beta'_j = 2\lambda_j - ik(1 - \cos \Theta) = 2 \left(\lambda_j - ik \sin^2 \left(\frac{\Theta}{2} \right) \right), \quad (25)$$

where Θ is the scattering angle of the electrons and $\beta_j = \lambda_j - ik$.

The final result for the total scattering potential produced by thin films for the spin polarized electrons takes the form

$$V_T(\mathbf{r}, s_0) = \sum_{\nu j_\nu s} e^{-\frac{|\mathbf{r} - \mathbf{R}_{\nu j_\nu s}|^2}{2B_{\nu s}}} \sum_{k=0}^{\infty} \frac{(1/b_{\nu s})^2}{(2k+1)!} \tilde{V}_T^{(k)}(B_{\nu s}, s_0) \quad (26)$$

and $\tilde{V}_T^{(k)}(B_{\nu s}, s_0)$ is given by expressions (23,24) and (25).

3. Conclusions

The formulae obtained for the scattering potential have interesting properties. At first this potential is finite at every lattice point $\mathbf{R}_{\nu j_\nu s}$ contrary to the effective potential of the free atom which is infinite at the middle of the atom. Another thing we point out is that one can obtain from it the forms used in literature [3,7]. Namely, if we ignore the exchange part of this potential and restrict a consideration to the high temperature limit, which means the high values of $B_{\nu s}$, the formula (26) can be approximated and for simple cubic lattice it takes the form:

$$V_T(\mathbf{r}) \cong \sum_{\nu j_\nu} e^{-\frac{|\mathbf{r} - \mathbf{R}_{\nu j_\nu}|^2}{B_\nu}} V_T^{(0)}(B_\nu) \quad (27)$$

where $V_T^{(0)}(B_\nu)$ is given by

$$\begin{aligned} V_T^{(0)}(B_\nu) &= Ze \langle F_{0,-1} \rangle_0 - 4\pi \sum_j e A_j^2 \langle n_{\nu s}^j \rangle \frac{(2\mu_j + 1)!}{(2\lambda_j)^{2\mu_j+2}} \left[\frac{2\mu_j + 2}{2\lambda_j} \langle F_{0,-1} \rangle_0 - \right. \\ &\quad \left. - (2\mu_j + 2) \sum_{m=0}^{2\mu_j+2} \frac{(2\lambda_j)^{m-1}}{m!} \langle F_{2\lambda_j, m-1} \rangle_0 + \sum_{m=0}^{2\mu_j+1} \frac{(2\lambda_j)^m}{m!} \langle F_{2\lambda_j, m} \rangle_0 \right] = \end{aligned}$$

$$= 4\pi e \sum_j A_j^2 \langle n_\nu^j \rangle \frac{(2\mu_j + 1)!}{(2\lambda_j)^{2\mu_j + 2}} * \\ * \left[(2\mu_j + 2) \sum_{m=0}^{2\mu_j + 2} \frac{(2\lambda_j)^{m-1}}{m!} \langle F_{2\lambda_j, m-1} \rangle_0 + \sum_{m=0}^{2\mu_j + 1} \frac{(2\lambda_j)^m}{m!} \langle F_{2\lambda_j, m} \rangle_0 \right]$$

and

$$\langle F_{2\lambda_j, n} \rangle_0 = 4\pi (2\pi B_\nu)^{-\frac{3}{2}} (B)^{\frac{n+3}{2}} (n+2)! e^{B_\nu \lambda_j^2} D_{-(n+3)}(2\lambda_j \sqrt{B_\nu}). \quad (28)$$

The last two formulae in the hydrogen atom case, for which the wave function has the simplest form lead to the result of Dworjankin [3]. Instead of the Slater type of function by means of which the electrostatic potential of free atoms is calculated one can use the electrostatic potential of a free atom in the Strand and Tietz form [6]:

$$V(r) = \frac{Ze}{r} \left[\frac{Zp(r)}{Z} \right] = \frac{Ze}{r} \sum_\lambda a_\lambda e^{-b_\lambda r}, \quad (29)$$

where a_λ and b_λ are numerical parameters given in [6]. In this case the formulae (27-29) give the results we have obtained in the papers [7, 8].

Let us remark that the surface scattering potential given by the formulae (26, 23-25) due to its general and analytical form can be very useful for the description of the LEED as well as of the HIED experiments. Due to including the exchange part of the scattering potential it can be used to search the magnetic sample surfaces by means of the spin polarized low energy electron diffraction, which introduces a new dimension to surface physics. The last problem is presented in our recent paper [9].

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