# INVESTIGATION OF THE INFLUENCE OF EXTERNAL ELECTRIC FIELD ON THE ELECTRON DENSITY OF SEMI-BOUNDED METAL

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The influence of an external uniform electric field on the electron subsystem of a semi-bounded metal in the "jellium" model is investigated. It is discovered that the applied field results in a change of the effective interelectron interaction even in the direction normal to the field. The influence of the intensity of the external electric field on the electron density of a semi-bounded metal is studied.

Due to the intensive experimental investigations of surfaces by means of scanning tunneling microscopy, scanning tunneling spectroscopy, field-ion microscopy, and their modifications [1–4], the problem of investigating the electron density of a metal under the action of an external electric field takes on the special actuality.

Solving these and many other problems of condensed systems, one widely uses the density functional theory (DFT). The DFT allows one to calculate, to a high accuracy, the characteristics of the ground state of a system which are determined by the behavior of the electron density. Historically, the DFT was first developed for the description of complex atoms and molecules and afterwards adopted for the description of electron liquids with strong nonuniformity. However, all the approximations of exchange-correlation effects that should be considered in order to construct an effective one-particle potential generally use the local density approximation (LDA) based on the results obtained for a uniform electron liquid. Due to this fact, the DFT-LDA doesn't allow one to obtain the proper behavior of the one-electron potential far from the metal surface [5] or to correctly describe the phenomena conditioned by Van der Waals forces [6]. These effects are many-particle and can't be taken into account in DFT.

The cycle of works [7–11] deals with the development of a technique that takes into consideration many-particle effects when investigating the electron structure of a semi-bounded metal described in the framework of the "jellium" model. In these papers, the dominant problem lies in the choice of a one-particle surface potential that should, on the one hand, adequately describe the real electric field acting on electrons and, on the other, be simple enough for analytically solving the corresponding Schrödinger equation. As a rule, one chooses such a potential in the form of an infinitely high potential wall, a rectangular barrier of finite height [12], or a linear potential [13–16]. The given paper is devoted to the investigation of the semi-bounded metal ("jellium" model) subjected to an external uniform electric field applied along the normal to the metal surface. As real characteristic physical fields are not weak, they can't be considered small disturbances; instead, it is necessary to take them into account along with the spatial nonuniformity in the Hamiltonian of non-interacting electrons.

In order to calculate the electron density distribution in the presence of a uniform external electric field, let's use a linear potential as a model surface one. In this case, after the external field is turned on, the electron appears to be under the action of the potential

$$V(z) = \frac{\hbar^2}{2m} k_0 z\,\theta(z) + \frac{\hbar^2}{2m} k_1 z\,\theta(z), \tag{1}$$

where $\hbar = h/(2\pi)$, $h$ is the Planck constant, and $m$ is the electron mass. The first term represents the surface potential without external electric field (the parameter $k_0$ is chosen by using the condition of the minimal surface energy of the semi-bounded "jellium" without external field), while the second term is the potential of the external electric field. Moreover, the coefficient $k_1$ can be both positive and negative depending on the direction of the applied electric field with the intensity $\frac{\hbar^2}{2me} k_1$, where $-e$ is the electron charge.

The solutions of the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + V(z)\right]\varphi(z) = E\varphi(z) \tag{2}$$

are the following wave functions and energy values:

$$\varphi_\alpha(z)=\begin{cases}\dfrac{2}{\sqrt{L}}\sin(\alpha z+\gamma_\alpha), & z<0,\\ \dfrac{2}{\sqrt{L}}\dfrac{\sin\gamma_\alpha}{\mathrm{Ai}\left(-\frac{\alpha^2}{k^{2/3}}\right)}\mathrm{Ai}\left(k^{1/3}z-\dfrac{\alpha^2}{k^{2/3}}\right), & z>0,\end{cases} \tag{3}$$

$$E_\alpha=\frac{\hbar^2\alpha^2}{2m}. \tag{4}$$

Here, $\alpha$ is the quantum number that satisfies the equation

$$\alpha=\frac{2\pi}{L}n+\gamma_\alpha,\quad n\in\mathbb{N}, \tag{5}$$

$\mathrm{Ai}(x)$ is the Airy function,

$$\gamma_\alpha=\mathrm{arctg}\left[\frac{\alpha}{k^{1/3}}\frac{\mathrm{Ai}\left(-\dfrac{\alpha^2}{k^{2/3}}\right)}{\mathrm{Ai}'\left(-\dfrac{\alpha^2}{k^{2/3}}\right)}\right],\ k=k_0+k_1, \tag{6}$$

and the range of variation of the normal coordinate $z$ lies in the interval $[-L/2,+\infty)$, moreover, $L\to\infty$.

In order to calculate the electron density, we use the expression obtained in papers [7,8,10] for $n(z)$ in the case of low temperatures ($\beta\mu\gg1$, where $\beta$ is the reciprocal thermodynamic temperature, $\mu$ is the chemical potential of the semi-bounded "jellium"):

$$n(z)=n_0(z)\exp\left\{-\frac{f_0(z)}{n_0(z)}\frac{1}{S}{\sum_{\mathbf{q}}}'\tilde{g}(q|z,z)\right\}. \tag{7}$$

Here, $S$ denotes the area of the metal surface, ($S\to\infty$), $\mathbf{q}=(q_x,q_y)$, $q_{x,y}=\frac{2\pi}{\sqrt{S}}m_{x,y}$, $m_{x,y}=0,\pm1,\pm2,\ldots$, $\tilde{g}(q|z,z)$ stands for the effective potential of the interelectron interaction $g(q|z,z)$ with no regard for self-action. The prime near the summation sign indicates the absence of the term with $\mathbf{q}=0$,

$$n_0(z)=\frac{1}{S}\sum_{\mathbf{p},\alpha}|\varphi_\alpha(z)|^2\,\theta\left(p_\mathrm{F}^2-(p^2+\alpha^2)\right) \tag{8}$$

is the electron density in the ideal exchange approximation, $\mathbf{p}$ denotes the two-dimensional momentum of an electron in the division plane (the motion of an electron in parallel to the division plane is described by plane waves), $p_\mathrm{F}=\sqrt{2m\mu/\hbar^2}$ is the Fermi momentum, and

$$f_0(z)=\frac{\partial}{\partial\mu}n_0(z). \tag{9}$$

The effective potential of the interelectron interaction $g(q|z_1,z_2)$ represents the solution of the integral equation

$$g(q|z_1,z_2)=\nu(q|z_1-z_2)+$$

$$+\frac{\beta}{SL^2}\int\limits_{-\infty}^{+\infty}\mathrm{d}z\int\limits_{-\infty}^{+\infty}\mathrm{d}z'\nu(q|z_1-z)\mathfrak{M}(q|z,z')g(q|z',z_2), \tag{10}$$

where

$$\mathfrak{M}(q|z,z')=\sum_{k',k}\mathfrak{M}_{k,k'}(\mathbf{q},-\mathbf{q})\mathrm{e}^{\mathrm{i}kz+\mathrm{i}k'z'}, \tag{11}$$

$$\mathfrak{M}_{k,k'}(\mathbf{q},-\mathbf{q})=\mathrm{i}^2\langle\mathrm{T}\rho_k(\mathbf{q})\rho_{k'}(-\mathbf{q})\rangle_0 \tag{12}$$

stands for the two-particle correlation function "density-density" in the ideal exchange approximation in the case of low temperatures; $k=\frac{2\pi}{L}n$, $n=0,\pm1,\pm2,\ldots$, $\rho_k(\mathbf{q})$ is the mixed Fourier transform of the local electron density,

$$\rho_k(\mathbf{q})=\sum_{\mathbf{p},\alpha,\alpha'}\langle\alpha|\mathrm{e}^{-ikz}|\alpha'\rangle a_\alpha^\dagger(\mathbf{p})a_{\alpha'}(\mathbf{p}-\mathbf{q}), \tag{13}$$

$$\langle\alpha|\ldots|\alpha'\rangle=\int\limits_{-\infty}^{+\infty}\mathrm{d}z\,\varphi_\alpha^*(z)\ldots\varphi_\alpha(z),$$

$a_\alpha^\dagger(\mathbf{p})$, $a_\alpha(\mathbf{p})$ denote the operators of creation and annihilation of an electron in the $(\mathbf{p},\alpha)$ state, correspondingly; moreover, the standard commutation relations are satisfied:

$$\left\{a_{\alpha_1}(\mathbf{p}_1),a_{\alpha_2}^\dagger(\mathbf{p}_2)\right\}=\delta_{\mathbf{p}_1,\mathbf{p}_2}\delta_{\alpha_1,\alpha_2}. \tag{14}$$

In order to solve the integral equation (10), let's use the approach proposed in papers [7, 9–11], which allows one to find the analytical solution $g(q|z_1,z_2)$ with regard for the electron scattering in the division plane [17]. As a result, we obtain

at $z_1,\ z_2\leqslant0$,

$$g(q|z_1,z_2)=\tfrac{2\pi e^2}{Q_1}\left[\mathrm{e}^{-Q_1|z_1-z_2|}+\tfrac{Q_1-Q_2}{Q_1+Q_2}\mathrm{e}^{Q_1(z_1+z_2)}\right], \tag{15}$$

at $z_1,\ z_2\geqslant0$,

$$g(q|z_1,z_2)=\tfrac{2\pi e^2}{Q_2}\left[\mathrm{e}^{-Q_2|z_1-z_2|}-\tfrac{Q_1-Q_2}{Q_1+Q_2}\mathrm{e}^{-Q_2(z_1+z_2)}\right], \tag{16}$$

at $z_1\leqslant0,\ z_2\geqslant0$,

$$g(q|z_1,z_2)=\tfrac{4\pi e^2}{Q_1+Q_2}\mathrm{e}^{Q_1z_1-Q_2z_2}, \tag{17}$$

at $z_1 \geqslant 0,\ z_2 \leqslant 0$,

$$g(q|z_1, z_2) = \frac{4\pi e^2}{Q_1 + Q_2} \mathrm{e}^{Q_1 z_2 - Q_2 z_1}, \tag{18}$$

where $\varkappa_{\mathrm{TF}}$ denotes the Thomas—Fermi reciprocal screening radius;

$$\mathrm{L}(x) = \frac{1}{2} + \frac{1 - x^2}{4x} \ln \left| \frac{1 + x}{1 - x} \right|$$

is the Lindhard function, $p_{\mathrm{F}}$ is the Fermi momentum, $a_{\mathrm{B}}$ is the Bohr radius,

$$Q_1 = \sqrt{q^2 + \varkappa_{\mathrm{TF}}^2 \left( \mathrm{L}\Big(\frac{q}{2p_{\mathrm{F}}}\Big) + \Delta(q) \right)},$$

$$Q_2 = \sqrt{q^2 - \varkappa_{\mathrm{TF}}^2 \Delta(q)},$$

$$\Delta(q) = \frac{1}{p_{\mathrm{F}}} \int\limits_0^{p_{\mathrm{F}}} \mathrm{d}\alpha \sin(2\gamma_\alpha) \times$$

$$\times \left[ 1 - \sqrt{1 - 4\frac{p_{\mathrm{F}}^2 - \alpha^2}{q^2}}\, \theta \left( 1 - 4\frac{p_{\mathrm{F}}^2 - \alpha^2}{q^2} \right) \right].$$

In Fig. 1, we present the results of calculations of the effective potential of the interelectron interaction,

$$g(r, z_1, z_2) = \frac{1}{S} \sum_{\mathbf{q}} \mathrm{e}^{i\,\mathbf{q}\,\mathbf{r}} g(q|z_1, z_2),$$

as a function of the distance $r$ between the electrons in the division plane in the presence of an external electric field (dashed curve) and without it (solid curve) at $r_{\mathrm{S}} = 2$ ($r_{\mathrm{S}}$ is the Wigner—Seitz radius in units of the Bohr radius $a_{\mathrm{B}}$).

The given picture indicates that the electric field normal to the division plane results in the strengthening (Fig. 1,*a,b*) or weakening (Fig. 1,*c*) of the effective repulsion between electrons even in the direction normal to the field. The strengthening of repulsion takes place for electrons being inside the region with a positive charge and the weakening — for those being out of it. This testifies to the fact that two-particle effects are important and should be taken into account when calculating the variation of the electron density $n(z)$ conditioned by the application of an external electric field.

Knowing the electron density (7), one can find the electrostatic potential $\varphi(z)$ that represents the solution of the Poisson equation

$$\varphi(z) = \varphi(-\infty) + 4\pi e \int\limits_{-\infty}^{z} \mathrm{d}z'(z' - z)\big(n(z') - n_+(z')\big), \tag{19}$$

**a**

**b**

**c**

Fig. 1. Effective potential of the interelectron interaction as a function of the distance between electrons in the division plane for the following coordinates of electrons normal to the division plane: $z_1 = z_2 = -10\,a_{\mathrm{B}}$ (*a*), $z_1 = z_2 = -1\,a_{\mathrm{B}}$ (*b*), and $z_1 = z_2 = 1\,a_{\mathrm{B}}$ (*c*). The solid curve corresponds to the case of the absence of an external field, the dashed curve — the external uniform electric field with an intensity of 40 V/nm is applied

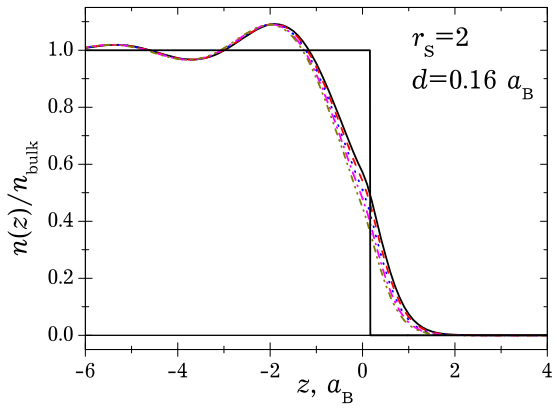


Fig. 2. Electron density distributions in the absence of an external electric field (solid curve) and in the presence of the external field of various intensities $E_0$, V/nm: 10 (dashed curve), 20 (dots), 30 (dash dot), 40 (dash dot dot). The positive charge is located at $z \leqslant 0.16\, a_B$

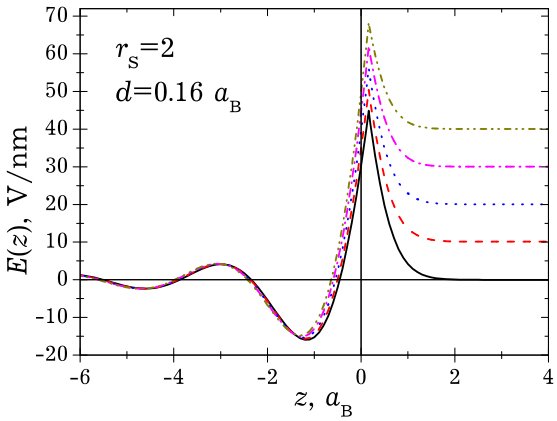


Fig. 3. The same as in Fig.2 for the distribution of the electric field intensity

where $n_+(z) = n_{\rm bulk}\theta(-d-z)$, $d > 0$, $n_{\rm bulk} = 3/(4\pi r_S^3)$. The parameter $d$ can be found in the self-consistent way from the electroneutrality condition

$$\int\limits_{-\infty}^{+\infty} {\rm d}z\big(n(z) - n_+(z)\big) = 0.$$

The intensity of the electric field will have the form

$$E(z) = -\frac{{\rm d}\varphi(z)}{{\rm d}z} = 4\pi\, e \int\limits_{-\infty}^{z} {\rm d}z'\Big(n(z') - n_+(z')\Big). \qquad (20)$$

Figure 2 presents the result of numerical calculations of the electron density for the surface potentials (1) at $r_S = 2$. As one can see from the figure, the switching-on of the external uniform electric field results in a shift of

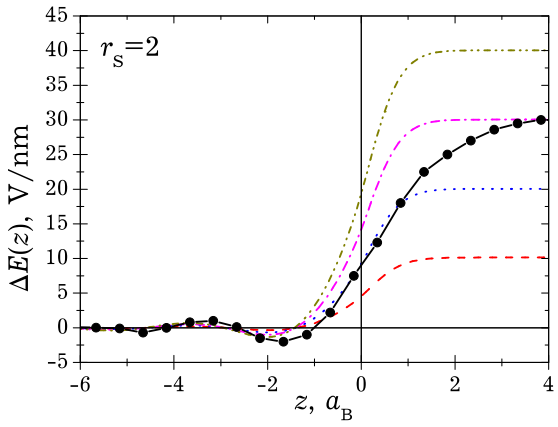


Fig. 4. Distribution of the electric field intensity $\Delta E(z) = E(z, E_0) - E(z, E_0 = 0)$. The notations are the same as in Fig.3. The solid curve with dots presents the data from papers [18–21]

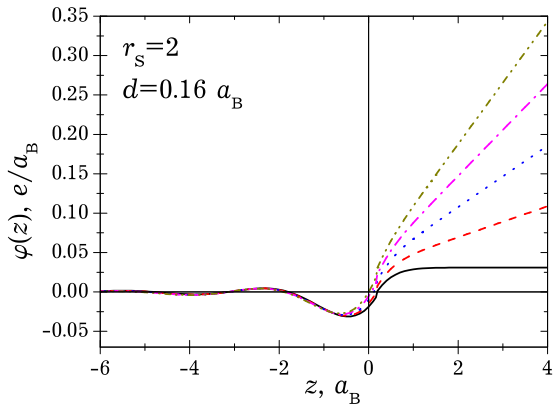


Fig. 5. The same as in Fig.3 for the electrostatic potential distribution.

the electron density inside the metal and an increase of the potential barrier, so that it becomes more difficult for an electron to leave the metal. Figures 3 and 4 depict the results of calculations of the electric field intensity according to (20) and the distribution of the difference of the electric field intensity $\Delta E(z)$ in the presence of an external electric field and without it. Figure 5 shows the distribution of the electrostatic potential near the metal surface. In Fig. 4, we present our results together with the data from papers [18–21] obtained by means of DFT. The comparison of the results demonstrates that, in our calculations, a more rapid increase of the electric field intensity $E(z)$ is observed, and its rise depends on the applied external electric field $E_0$; in the region

$\sim 0.5$ Å near the "jellium" surface, the intensity $E(z)$ increases by a factor of 1.5–4 depending on the applied field.


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ДОСЛІДЖЕННЯ ВПЛИВУ ЗОВНІШНЬОГО ЕЛЕКТРИЧНОГО ПОЛЯ НА ЕЛЕКТРОННУ ГУСТИНУ НАПІВОБМЕЖЕНОГО МЕТАЛУ

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Р е з ю м е

Досліджується вплив зовнішнього однорідного електричного поля на електронну підсистему напівобмеженого металу в моделі "желе". Виявлено, що прикладене поле спричинює зміну ефективної міжелектронної взаємодії навіть в перпендикулярному до поля напрямку. Досліджено вплив напруженості зовнішнього електричного поля на електронну густину напівобмеженого металу.