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Effective inter-electron interaction for metallic slab

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A system of electrons in a metal slab, which is described by the jellium model, is considered. The potential that forms a surface of the slab is modeled by the infinite square well potential. By using some approximations, the analytical expressions for effective inter-electron interaction inside the slab and outside it are obtained.

Keywords: *slab, effective interaction, correlator*
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1. Introduction

The development of nanotechnologies involving deposition of metals on substrates requires further theoretical development and understanding of effects related to the electronic structure of nanoclusters and nanofilms. If the size of nanostructure is comparable with the corresponding electron Fermi wavelength, various physical properties are size dependence [1–3]. For metal nanofilms, many physical quantities, such as thermodynamic stability, electrical resistivity, superconducting critical temperature, the perpendicular upper critical field, surface adhesion, thermal-expansion coefficient, surface free energy, surface diffusion barriers, surface adsorption energy, work function, etc., oscillate as a function of film thickness [4].

The main problem of the statistical theory of such systems is the calculation of thermodynamic and statistical distribution functions. Using the functional integration method for such calculations allows us to get expansions for these characteristics, the basis for the construction of which is the effective interaction potential [5,6]. This potential satisfies the integral equation of convolution, analytical solving of which is a difficult problem [7].

In Refs. [8–10], the problem of determining screened potentials of electron interaction in such thin films is considered. This problem is solved with neglecting of frequency dispersion [8] or spatial dispersion [9] of screened potential. In Ref. [10], analytical expressions for the screened potentials of classic systems such as thin films are found within constant density approximation.

In this paper, the problem of determining the effective inter-electron interaction for metal slab in the quantum case is considered. The analytical expressions for this interaction both in the slab and, in contrast to Ref. [7], beyond it. In the case of increasing of the slab thickness, obtained results go over to results of Ref. [12].

2. Model

We consider a metal slab with the thickness L, which is laid along the z axis, and two sides with the area S ($S \to \infty$) are parallel to the xy plane. We consider that one side of slab coincides with the xy plane, i.e., is specified by the equation $z = 0$, and the other parallel side is described by the equation $z = L$.

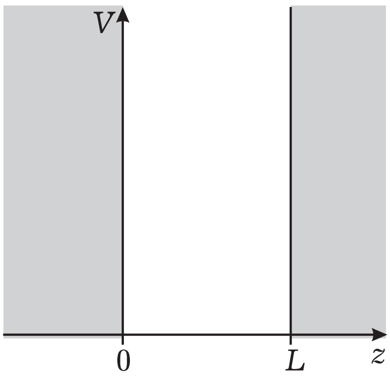

Fig. 1.

This slab is considered within the jellium model. Then the electron motion in a plane that is parallel to the xy plane is free, and the motion along the z axis is determined by the potential $V(z)$, which depends on the normal to the slab sides coordinate of the electron only. This potential is modelled by the infinite square well potential (see Fig. 1):

$$V(z) = \begin{cases} 0, & 0 < z < L, \\ \infty, & z \leqslant 0,\ z \geqslant L. \end{cases} \tag{1}$$

The single-particle wave functions and the corresponding energies of the electron in the field of this potential can be written as

$$\Psi_{\mathbf{k}_{||},\alpha}(\mathbf{r}_{||}, z) = \frac{1}{\sqrt{S}} \mathrm{e}^{\mathrm{i}\mathbf{k}_{||}\mathbf{r}_{||}} \varphi_\alpha(z), \quad E_\alpha(\mathbf{k}_{||}) = \frac{\hbar^2 k_{||}^2}{2m} + \varepsilon_\alpha, \tag{2}$$

where $\mathbf{r}_{||}$ is the two-dimensional coordinate of the electron in the xy plane, $\mathbf{k}_{||}$ is the wave vector of the electron in the xy plane. The functions $\varphi_\alpha(z)$ satisfy the one-dimensional stationary Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + V(z)\right] \varphi_\alpha(z) = \varepsilon_\alpha \varphi_\alpha(z)$$

and have the form

$$\varphi_\alpha(z) = \sqrt{\frac{2}{L}} \sin(\alpha z)\, \theta(z)\, \theta(L - z), \tag{3}$$

where m is the electron mass, $\theta(z)$ is the Heaviside step function, $\varepsilon_\alpha = \frac{\hbar^2\alpha^2}{2m}$, $\alpha = \frac{\pi n}{L}$, $n = 1, 2, \ldots$.

3. Effective inter-electron interaction

3.1. Integral equation for effective inter-electron interaction

In the case of low temperatures, the two-dimensional Fourier transform of the effective inter-electron interaction is a solution of the integral equation [11,12]

$$g(q|z_1, z_2) = \nu(q|z_1 - z_2) + \frac{\beta}{SL^2} \int_{-\infty}^{+\infty} \mathrm{d}z \int_{-\infty}^{+\infty} \mathrm{d}z' \nu(q|z_1 - z) \mathfrak{M}(q|z, z') g(q|z', z_2), \tag{4}$$

where β is the reciprocal of the thermodynamic temperature, $\nu(q|z_1 - z_2) = \frac{2\pi e^2}{q} \mathrm{e}^{-q|z_1 - z_2|}$ is the two-dimensional Fourier transform of the Coulomb interaction, $\mathfrak{M}(q|z, z')$ is the two-particle correlator in the case of low temperatures,

$$\mathfrak{M}(q|z, z') = \frac{L^2}{\beta} \sum_{\alpha_1, \alpha_2} \Lambda_{\alpha_1,\alpha_2}(q) \varphi^*_{\alpha_1}(z) \varphi_{\alpha_2}(z) \varphi^*_{\alpha_2}(z') \varphi_{\alpha_1}(z'), \tag{5}$$

$$\Lambda_{\alpha_1,\alpha_2}(q) = \sum_{\mathbf{k}_{||}} \Pi_{\alpha_1,\alpha_2}(\mathbf{k}_{||}, \mathbf{q}),$$

$$\Pi_{\alpha_1,\alpha_2}(\mathbf{k}_{||}, \mathbf{q}) = \frac{\theta\big(\mu - E_{\alpha_1}(\mathbf{k}_{||})\big) - \theta\big(\mu - E_{\alpha_2}(\mathbf{k}_{||} - \mathbf{q})\big)}{E_{\alpha_1}(\mathbf{k}_{||}) - E_{\alpha_2}(\mathbf{k}_{||} - \mathbf{q})},$$

μ is the chemical potential.

In the mirror electron scattering approximation [12] $\Lambda_{\alpha_1,\alpha_2}(q) \approx \Lambda_{\alpha_1,\alpha_1}(q)$, taking the summation over α_2 we get

$$\mathfrak{M}(q|z,z') = -\frac{L^2}{\beta}\frac{2m}{\hbar^2}\frac{S}{2\pi}\sum_{\alpha}|\varphi_\alpha(z)|^2 \times \left[1-\sqrt{1-4\frac{k_{\mathrm{F}}^2-\alpha^2}{q^2}}\,\theta\left(1-4\frac{k_{\mathrm{F}}^2-\alpha^2}{q^2}\right)\right]\theta(k_{\mathrm{F}}-\alpha)\,\delta(z-z'), \tag{6}$$

where k_{F} is the magnitude of the Fermi wave vector, $k_{\mathrm{F}} = \frac{\sqrt{2m\mu}}{\hbar}$.

For further simplify the expression (6), we use the constant density approach [12]. Then the integral equation (4) is greatly simplified,

$$g(q|z_1,z_2) = \nu(q|z_1-z_2) - \frac{\varkappa^2(q)}{4\pi e^2}\int_0^L \mathrm{d}z\,\nu(q|z_1-z)g(q|z,z_2), \tag{7}$$

where

$$\varkappa^2(q) = 4\pi e^2\frac{2m}{\hbar^2}\frac{1}{2\pi L}\sum_{\alpha}\left[1-\sqrt{1-4\frac{k_{\mathrm{F}}^2-\alpha^2}{q^2}}\,\theta\left(1-4\frac{k_{\mathrm{F}}^2-\alpha^2}{q^2}\right)\right]\theta(k_{\mathrm{F}}-\alpha).$$

3.2. Analytical solution of integral equation for effective inter-electron interaction

The integral equation (7) can be solved analytically. For this purpose, we reduce this integral equation to a boundary value problem. Let us differentiate twice this integral equation with respect to variable z_1. Taking into account that

$$\frac{\mathrm{d}\nu(q|z_1-z_2)}{\mathrm{d}z_1} = -q\,\nu(q|z_1-z_2)\,\mathrm{sign}(z_1-z_2),$$
$$\frac{\mathrm{d}^2\nu(q|z_1-z_2)}{\mathrm{d}z_1^2} = q^2\,\nu(q|z_1-z_2) - 4\pi e^2\delta(z_1-z_2),$$

we get

$$\frac{\mathrm{d}g(q|z_1,z_2)}{\mathrm{d}z_1} = -q\,\nu(q|z_1-z_2)\,\mathrm{sign}(z_1-z_2) + \frac{\varkappa^2(q)}{4\pi e^2}q\int_0^L \mathrm{d}z\,\nu(q|z_1-z)\,\mathrm{sign}(z_1-z)\,g(q|z,z_2), \tag{8}$$

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - q^2 - \varkappa^2(q)\theta(z_1)\theta(L-z_1)\right]g(q|z_1,z_2) = -4\pi e^2\delta(z_1-z_2). \tag{9}$$

For solving the differential equation (9), we divide the domain of normal coordinates of two electrons z_1z_2 into nine domains, as it is shown in Fig. 2, and consistently we find solution in the each domain.

In the domain I, the differential equations (9) takes the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - Q^2\right)g(q|z_1,z_2) = -4\pi e^2\delta(z_1-z_2), \quad 0 < z_1 < L,\ 0 \leqslant z_2 \leqslant L, \tag{10}$$

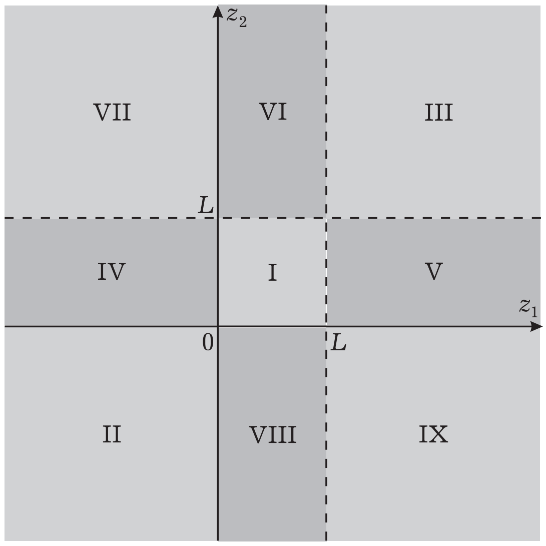

Fig. 2.

where $Q^2 = q^2 + \varkappa^2(q)$. From Eq. (8) we obtain two following boundary conditions

$$\left(\frac{\mathrm{d}}{\mathrm{d}z_1} - q\right) g(q|z_1, z_2)\bigg|_{z_1=0} = 0, \quad 0 \leqslant z_2 \leqslant L, \tag{11}$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}z_1} + q\right) g(q|z_1, z_2)\bigg|_{z_1=L} = 0, \quad 0 \leqslant z_2 \leqslant L. \tag{12}$$

A solution of the boundary value problem (10)–(12) is found analytically and it has the form

$$g(q|z_1, z_2) = \frac{2\pi e^2}{Q} \frac{1}{1 - \left(\frac{Q-q}{Q+q}\right)^2 \mathrm{e}^{-2QL}} \left[\mathrm{e}^{-Q|z_1-z_2|} + \left(\frac{Q-q}{Q+q}\right)^2 \mathrm{e}^{-Q(2L-|z_1-z_2|)} \right.$$
$$\left. + \frac{Q-q}{Q+q}\left(\mathrm{e}^{-Q(z_1+z_2)} + \mathrm{e}^{-Q(2L-z_1-z_2)}\right) \right]. \tag{13}$$

In the domain II, the differential equation (9) has the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - q^2\right) g(q|z_1, z_2) = -4\pi e^2 \delta(z_1 - z_2), \quad z_1 < 0,\ z_2 \leqslant 0. \tag{14}$$

From Eq. (8) we get the boundary condition

$$\left(\frac{\mathrm{d}}{\mathrm{d}z_1} - q\right) g(q|z_1, z_2)\bigg|_{z_1=0} = -4\pi e^2 \mathrm{e}^{q z_2}, \quad z_2 \leqslant 0. \tag{15}$$

With this condition, the finiteness condition of solution, and the continuity condition of solution at the origin, the solution of the boundary value problem (14), (15) is found analytically,

$$g(q|z_1, z_2) = \frac{2\pi e^2}{q}\left(\mathrm{e}^{-q|z_1-z_2|} - \mathrm{e}^{q(z_1+z_2)}\right) +$$
$$+ \frac{4\pi e^2}{Q+q} \frac{1 + \frac{Q-q}{Q+q}\mathrm{e}^{-2QL}}{1 - \left(\frac{Q-q}{Q+q}\right)^2 \mathrm{e}^{-2QL}} \mathrm{e}^{q(z_1+z_2)}. \tag{16}$$

In the domain III, the differential equations (9) takes the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - q^2\right) g(q|z_1, z_2) = -4\pi e^2 \delta(z_1 - z_2), \quad z_1 > L,\ z_2 \geqslant L. \tag{17}$$

From Eq. (8) we obtain the boundary condition

$$\left(\frac{\mathrm{d}}{\mathrm{d}z_1} + q\right) g(q|z_1, z_2)\Big|_{z_1 = L} = -4\pi e^2 \mathrm{e}^{q(L - z_2)}, \quad z_2 \geqslant L. \tag{18}$$

With this condition, the finiteness condition of solution, and the continuity condition of solution at the point (L, L), the solution of the boundary value problem (17), (18) is found analytically,

$$g(q|z_1, z_2) = \frac{2\pi e^2}{q}\left(\mathrm{e}^{-q|z_1 - z_2|} - \mathrm{e}^{-q(z_1 + z_2 - 2L)}\right) + \\ + \frac{4\pi e^2}{Q + q}\frac{1 + \frac{Q-q}{Q+q}\mathrm{e}^{-2QL}}{1 - \left(\frac{Q-q}{Q+q}\right)^2 \mathrm{e}^{-2QL}}\mathrm{e}^{-q(z_1 + z_2 - 2L)}. \tag{19}$$

In the domain IV, the differential equation (9) has the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - q^2\right) g(q|z_1, z_2) = 0, \quad z_1 < 0,\ 0 \leqslant z_2 \leqslant L. \tag{20}$$

From Eq. (8) we get the boundary condition

$$\left(\frac{\mathrm{d}}{\mathrm{d}z_1} - q\right) g(q|z_1, z_2)\Big|_{z_1 = 0} = 0, \quad 0 \leqslant z_2 \leqslant L, \tag{21}$$

which is satisfied automatically for all solutions of the differential equations (20). With the finiteness condition of solution, and the continuity condition of solution at $z_1 = 0$, the solution of Eq. (20) is found analytically,

$$g(q|z_1, z_2) = \frac{4\pi e^2}{Q + q}\frac{1}{1 - \left(\frac{Q-q}{Q+q}\right)^2 \mathrm{e}^{-2QL}}\left[\mathrm{e}^{qz_1 - Qz_2} + \frac{Q - q}{Q + q}\mathrm{e}^{qz_1 - Q(2L - z_2)}\right]. \tag{22}$$

In the domain V, the differential equations (9) takes the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - q^2\right) g(q|z_1, z_2) = 0, \quad z_1 > L,\ 0 \leqslant z_2 \leqslant L. \tag{23}$$

From Eq. (8) we obtain the boundary condition

$$\left(\frac{\mathrm{d}}{\mathrm{d}z_1} + q\right) g(q|z_1, z_2)\Big|_{z_1 = L} = 0, \quad 0 \leqslant z_2 \leqslant L, \tag{24}$$

which is satisfied automatically for all solutions of the differential equations (23). With the finiteness condition of solution, and the continuity condition of solution at $z_1 = L$, the solution of Eq. (23) is found analytically,

$$g(q|z_1, z_2) = \frac{4\pi e^2}{Q + q}\frac{1}{1 - \left(\frac{Q-q}{Q+q}\right)^2 \mathrm{e}^{-2QL}}\left[\mathrm{e}^{-q(z_1 - L) - Q(L - z_2)} + \frac{Q - q}{Q + q}\mathrm{e}^{-q(z_1 - L) - Q(L + z_2)}\right]. \tag{25}$$

In the domain VI, the differential equation (9) has the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2}-Q^2\right)g(q|z_1,z_2)=0,\quad 0<z_1<L,\ z_2\geqslant L. \tag{26}$$

From Eq. (8) we get two following boundary conditions

$$\left.\left(\frac{\mathrm{d}}{\mathrm{d}z_1}-q\right)g(q|z_1,z_2)\right|_{z_1=0}=0,\quad z_2\geqslant L, \tag{27}$$

$$\left.\left(\frac{\mathrm{d}}{\mathrm{d}z_1}+q\right)g(q|z_1,z_2)\right|_{z_1=L}=2q\,\nu(q|L-z_2),\quad z_2\geqslant L. \tag{28}$$

A solution of the boundary value problem (26)–(28) is found analytically and it has the form

$$g(q|z_1,z_2)=\frac{4\pi e^2}{Q+q}\frac{1}{1-\left(\frac{Q-q}{Q+q}\right)^2\mathrm{e}^{-2QL}}\left[\mathrm{e}^{-Q(L-z_1)-q(z_2-L)}+\frac{Q-q}{Q+q}\mathrm{e}^{-Q(L+z_1)-q(z_2-L)}\right], \tag{29}$$

and it is continuous at the point $z_1=L$.

In the domain VII, the differential equations (9) takes the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2}-q^2\right)g(q|z_1,z_2)=0,\quad z_1<0,\ z_2\geqslant L. \tag{30}$$

From Eq. (8) we obtain the boundary condition

$$\left.\left(\frac{\mathrm{d}}{\mathrm{d}z_1}-q\right)g(q|z_1,z_2)\right|_{z_1=0}=0,\quad z_2\geqslant L, \tag{31}$$

which is satisfied automatically for all solutions of the differential equations (30). With the finiteness condition of solution, and the continuity condition of solution at $z_1=0$, the solution of Eq. (30) is found analytically,

$$g(q|z_1,z_2)=\frac{4\pi e^2}{Q+q}\frac{\frac{2Q}{Q+q}\mathrm{e}^{-QL}}{1-\left(\frac{Q-q}{Q+q}\right)^2\mathrm{e}^{-2QL}}\mathrm{e}^{qz_1-q(z_2-L)}. \tag{32}$$

In the domain VIII, the differential equation (9) has the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2}-Q^2\right)g(q|z_1,z_2)=0,\quad 0<z_1<L,\ z_2\leqslant 0. \tag{33}$$

From Eq. (8) we get the boundary condition

$$\left.\left(\frac{\mathrm{d}}{\mathrm{d}z_1}-q\right)g(q|z_1,z_2)\right|_{z_1=0}=-2q\,\nu(q|-z_2),\quad z_2\leqslant 0, \tag{34}$$

$$\left.\left(\frac{\mathrm{d}}{\mathrm{d}z_1}+q\right)g(q|z_1,z_2)\right|_{z_1=L}=0,\quad z_2\leqslant 0. \tag{35}$$

A solution of the boundary value problem (33)–(35) is found analytically and it has the form

$$g(q|z_1,z_2)=\frac{4\pi e^2}{Q+q}\frac{1}{1-\left(\frac{Q-q}{Q+q}\right)^2\mathrm{e}^{-2QL}}\left[\mathrm{e}^{-Qz_1+qz_2}+\frac{Q-q}{Q+q}\mathrm{e}^{Q(z_1-2L)+qz_2}\right], \tag{36}$$

and it is continuous at the point $z_1 = 0$.

In the domain IX, the differential equations (9) takes the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - q^2\right) g(q|z_1, z_2) = 0, \quad z_1 > L,\ z_2 \leqslant 0. \tag{37}$$

From Eq. (8) we obtain the boundary condition

$$\left(\frac{\mathrm{d}}{\mathrm{d}z_1} + q\right) g(q|z_1, z_2)\Big|_{z_1=L} = 0, \quad z_2 \leqslant 0, \tag{38}$$

which is satisfied automatically for all solutions of the differential equations (37). With the finiteness condition of solution, and the continuity condition of solution at $z_1 = L$, the solution of Eq. (37) is found analytically,

$$g(q|z_1, z_2) = \frac{4\pi e^2}{Q+q} \frac{\frac{2Q}{Q+q}\mathrm{e}^{-QL}}{1 - \left(\frac{Q-q}{Q+q}\right)^2 \mathrm{e}^{-2QL}} \mathrm{e}^{-q(z_1-L)+qz_2}. \tag{39}$$

It should be noted that increasing the thickness of the slab to infinity leads to disappearance of the domains III, V, VI, VII, and IX, and the effective inter-electron interaction in the domains I, II, IV, and VIII are transformed to the well-known expressions [12],

$$g(q|z_1 \geqslant 0, z_2 \geqslant 0) = \frac{2\pi e^2}{Q}\left[\mathrm{e}^{-Q|z_1-z_2|} + \frac{Q-q}{Q+q}\mathrm{e}^{-Q(z_1+z_2)}\right],$$

$$g(q|z_1 \leqslant 0, z_2 \leqslant 0) = \frac{2\pi e^2}{q}\left[\mathrm{e}^{-q|z_1-z_2|} - \frac{Q-q}{Q+q}\mathrm{e}^{q(z_1+z_2)}\right],$$

$$g(q|z_1 \leqslant 0, z_2 \geqslant 0) = \frac{4\pi e^2}{Q+q}\mathrm{e}^{qz_1-Qz_2},$$

$$g(q|z_1 \geqslant 0, z_2 \leqslant 0) = \frac{4\pi e^2}{Q+q}\mathrm{e}^{-Qz_1+qz_2}.$$

4. Conclusion

The problem of finding of the effective inter-electron interaction for the metallic slab is considered. This interaction is a solution of the integral equation, which in general should be solved numerically. However, by using the constant density approach for $|\varphi_\alpha(z)|^2$, the integral equation can be reduced to nine boundary value problems that can be solved analytically. In the paper, these boundary value problems are solved analytically, and the obtained solutions are continuous at the boundary edges of the domains. Forms of these solutions shows that the image forces relative the planes, which limit the metallic slab, $z = 0$, and $z = L$, are taken into account in the effective inter-electron interaction.

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Ефективний потенціал міжелектронної взаємодії для металевої плівки

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Розглянуто систему електронів у металевій плівці, яка описується моделлю «желе». Потенціал, який формує поверхні плівки, змодельовано безмежно високою прямокутною потенціальною ямою. Використовуючи деякі наближення, отримано аналітичні вирази для ефективного потенціалу міжелектронної взаємодії як всередині плівки, так і поза нею.

Ключові слова: *плівка, ефективний потенціал, кореляційна функція*

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