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An effective potential of electron-electron interaction in semi-infinite jellium

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An effective potential of electron-electron interaction and a two-particle "density-density" correlator are calculated for semi-infinite jellium. Their asymptotics at large distances between electrons are studied in a plane parallel to the surface.

Key words: *semi-infinite jellium, "density-density" electron correlator, pair effective electron-electron interaction*

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1. Introduction

At present one of the basic methods for investigating properties of semirestricted systems is the density-functional theory (DFT) [1,2], which is inherently a one-particle approach. Nevertheless modifications are possible (LDA, GGA and others). Therefore it is impossible to correctly allow for collective phenomena in the DFT (i. e., lack of image forces, weak coupling and so on) [3,4].

The first attempt to construct the many-body theory of inhomogeneous electron gas was the paper [5], where the set of five equations (GWA-approximation) was formulated. Conjunction of GWA approach with DFT by way of taking into account many-body effects for correcting the DFT imperfections was considered in [6]. However, this approach calls for numerous uncontrolled simplifications at carrying out numerical calculations that appear in the absence of oscillations of effective pair electron interaction potential.

The authors developed the approach for calculating Gibbs potential and distribution functions of inhomogeneous electron gas using the method of functional integration presented in the works [7–9]. These characteristics are represented as expansions by effective potential of electron-electron interaction that takes into account both availability of image forces and collective effects (screening). This paper investigates an effective potential of electron-electron interaction and a two-particle correlator "density-density". Approximations are proposed for finding the correlator "density-density" and the effective potential of electron-electron interaction in analytical form as well as determinating their asymptotics. Robastness of these approximations is studied by comparison with results of numerical calculations.

2. The model

The semi-infinite jellium is a neutral system of dynamical electrons in a background of uniform positive ionic charge density ϱ_+ restricted division plane (surface) $z = -d$:

$$\varrho_+(x, y, z) \equiv \varrho_+(z) = n\,\theta(-d - z), \tag{1}$$

where $\theta(t)$ is Heaviside function:

$$\theta(t) = \begin{cases} 1, & t > 0, \\ 0, & t < 0, \end{cases}$$

n is uniform electron density, $n = (4\pi r_{\mathrm{S}}^3/3)^{-1}$, r_{S} is the radius in atomic units of the sphere which encloses one unit of electron charge; $d > 0$ is a parameter self-consistently defined from the condition of electrical neutrality

$$\int\limits_{-\infty}^{+\infty} \mathrm{d}z \Big(\varrho(z) - \varrho_+(z) \Big) = 0, \tag{2}$$

where $\varrho(z)$ is an electron density.

We suppose that the ionic system forms a surface potential for electrons which does not allow them to abandon the surface. This surface potential is modelled as follows:

$$V(z) = \begin{cases} \infty, & z \geqslant 0, \\ 0, & z < 0. \end{cases} \tag{3}$$

Such a model correctly represents a real situation from physical viewpoint and it admits analytical solutions of the corresponding Schrödinger equation.

Eigenfunctions and eigenvalues of this potential are

$$\varphi_\alpha(z) = \frac{2}{\sqrt{L}} \sin(\alpha z)\theta(-z), \qquad \varepsilon_\alpha = \frac{\hbar^2\alpha^2}{2m}, \qquad \alpha = \frac{2\pi k}{L}, \qquad k = 1, 2, \ldots, \tag{4}$$

where L determines the area of the change of the electron coordinate normal to the surface $z \in [-L/2, +\infty)$, and $L \to \infty$ so that a thermodynamical boundary takes place. Allowing for this, the surface potential $V(z)$ is the following function:

$$\Psi_{\mathbf{p},\alpha}(\mathbf{r}, z) = \frac{1}{\sqrt{S}} \mathrm{e}^{\mathrm{i}\mathbf{pr}} \varphi_\alpha(z), \qquad E_\alpha(\mathbf{p}) = \frac{\hbar^2(p^2 + \alpha^2)}{2m}, \tag{5}$$

where $\hbar\mathbf{p}$ is a two-dimensional wave-vector of electron in the plane parallel to the surface.

In the secondary quantization representation constructed on the wave function (5), Hamiltonian of the system is as follows:

$$H = H_0 - \frac{1}{2S} N \sum_{\mathbf{q}}{}' \nu(\mathbf{q}|0) + \frac{1}{2SL} \sum_{\mathbf{q}}{}' \sum_{k} \nu_k(\mathbf{q}) \rho_k(\mathbf{q}) \rho_{-k}(-\mathbf{q}), \tag{6}$$

where

$$H_0 = \sum_{\mathbf{p},\alpha} E_\alpha(\mathbf{p}) a_\alpha^\dagger(\mathbf{p}) a_\alpha(\mathbf{p}) \tag{7}$$

is Hamiltonian of the system without reference to Coulomb interaction between electrons,

$$\nu\left(\mathbf{q}|z - z'\right) = \frac{2\pi e^2}{q} \mathrm{e}^{-q|z-z'|}$$

is a two-dimensional Fourier-image of Coulomb interaction, $\mathbf{q} = (q_x, q_y)$, $q_{x,y} = \frac{2\pi}{\sqrt{S}} m_{x,y}$, $m_{x,y} = 0, \pm 1, \pm 2, \ldots$, $\nu_k(\mathbf{q}) = 4\pi e^2/(\mathbf{q}^2 + k^2)$ is Fourier-image of Coulomb interaction, $k = \frac{2\pi}{L} n$, $n = 0, \pm 1, \pm 2, \ldots$, $\rho_k(\mathbf{q})$ is a mixed Fourier-representation of local density of electrons:

$$\rho_k(\mathbf{q}) = \sum_{\mathbf{p},\alpha,\alpha'} \langle \alpha | \mathrm{e}^{-\mathrm{i}kz} | \alpha' \rangle a_\alpha^\dagger(\mathbf{p}) a_{\alpha'}(\mathbf{p} - \mathbf{q}), \tag{8}$$

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

$a_\alpha^\dagger(\mathbf{p})$, $a_\alpha(\mathbf{p})$ are operators of electron creation and destruction in the state $(\mathbf{p}, \alpha)$ such that the standard commutation relationships take place

$$\left\{ a_{\alpha_1}(\mathbf{p}_1), a_{\alpha_2}^\dagger(\mathbf{p}_2) \right\} = \delta_{\mathbf{p}_1,\mathbf{p}_2} \delta_{\alpha_1,\alpha_2}; \tag{9}$$

$N = \sum\limits_{\mathbf{p},\alpha} a^{\dagger}_{\alpha}(\mathbf{p})a_{\alpha}(\mathbf{p})$ is the operator of particle quantity; the prime on the sum in the formula (6) denotes the absence of summands at $\mathbf{q} = 0$ which is caused by the condition of electrical neutrality (2).

3. Effective potential of electron-electron interaction

Effective potential of electron-electron interaction is a solution of the integral equation (see, for example, [6,7])

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

where

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

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

is a two-particle "density-density" correlator in the approach of ideal exchange in the case of low temperatures ($\beta\mu \gg 1$, where β is a reciprocal thermodynamical temperature, μ is a chemical potential of electron),

$$\langle\cdots\rangle_0 = \frac{\mathrm{Sp}\,\left(\mathrm{e}^{-\beta(H_0-\mu N)}\cdots\right)}{\mathrm{Sp}\,\mathrm{e}^{-\beta(H_0-\mu N)}}\,.$$

3.1. Calculation of $\mathfrak{M}(q|z, z')$

Consider the coordinate representation of the correlator

$$\mathfrak{M}(r, z, z') = \frac{1}{S}\sum_{\mathbf{q}}\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}}\mathfrak{M}(q|z, z') = \frac{1}{2\pi}\int\limits_0^{\infty}\mathrm{d}q\,q\mathrm{J}_0(qr)\mathfrak{M}(q|z, z'),$$

where $\mathrm{J}_0(x)$ is a cylindrical Bessel function, r is the distance between electrons in the plane parallel to the surface, $\mathfrak{M}(q|z, z')$ is the correlator in $(\mathbf{q}, z)$-representation and according to [8] it takes the following form

$$\mathfrak{M}(q|z, z') = \frac{L^2}{\beta}\sum_{\alpha_1,\alpha_2}\Lambda_{\alpha_1,\alpha_2}(\mathbf{q})\varphi^*_{\alpha_1}(z)\varphi_{\alpha_2}(z)\varphi^*_{\alpha_2}(z')\varphi_{\alpha_1}(z'), \tag{13}$$

where

$$\Lambda_{\alpha_1,\alpha_2}(\mathbf{q}) = \sum_{\mathbf{p}}\Pi_{\alpha_1,\alpha_2}(\mathbf{p}, \mathbf{q}), \tag{14}$$

$$\Pi_{\alpha_1,\alpha_2}(\mathbf{p}, \mathbf{q}) = \frac{\theta(\mu - E_{\alpha_1}(\mathbf{p})) - \theta(\mu - E_{\alpha_2}(\mathbf{p}-\mathbf{q}))}{E_{\alpha_1}(\mathbf{p}) - E_{\alpha_2}(\mathbf{p}-\mathbf{q}))} \tag{15}$$

is the polarization operator.

Taking the summation with respect to $\mathbf{p}$ in (14) we obtain the following expression for $\Lambda_{\alpha_1,\alpha_2}(\mathbf{q})$

$$\begin{aligned}\Lambda_{\alpha_1,\alpha_2}(\mathbf{q}) \;&=\; \frac{2m}{\hbar^2}\frac{S}{2\pi}\frac{\alpha_1^2 - \alpha_2^2 - q^2}{q^2}\left[1 - \sqrt{1 - 4q^2\frac{p_{\mathrm{F}}^2 - \alpha_1^2}{(\alpha_1^2 - \alpha_2^2 - q^2)^2}}\,\theta\left(1 - 4q^2\frac{p_{\mathrm{F}}^2 - \alpha_1^2}{(\alpha_1^2 - \alpha_2^2 - q^2)^2}\right)\right]\\ &\times\theta(p_{\mathrm{F}} - \alpha_1),\end{aligned} \tag{16}$$

where p_{F} is Fermi wave-vector, $p_{\mathrm{F}} = \sqrt{2m\mu}/\hbar$.

Consider some approximation allowing us to obtain analytical expressions for the two-particle correlator $\mathfrak{M}(q|z, z')$.

3.1.1. A mirror electron scattering approximation

Regard that the polarization operator is diagonal, i.e.

$$\Lambda_{\alpha_1,\alpha_2}(\mathbf{q}) \approx \Lambda_{\alpha_1,\alpha_1}(\mathbf{q}). \tag{17}$$

Physically it means that we take into account only the mirror electron scattering normal to the surface. Then the correlator (13) takes the following form

$$\begin{aligned}\mathfrak{M}(q|z,z') \;=\; & -\frac{L^2}{\beta}\frac{2m}{\hbar^2}\frac{S}{2\pi}\sum_{\alpha}|\varphi_\alpha(z)|^2\delta(z-z')\left[1-\sqrt{1-4\frac{p_{\mathrm{F}}^2-\alpha^2}{q^2}}\,\theta\left(1-4\frac{p_{\mathrm{F}}^2-\alpha^2}{q^2}\right)\right] \\ & \times\theta(p_{\mathrm{F}}-\alpha).\end{aligned} \tag{18}$$

In the expression (18) we use the approach of "constant density" [7,8], i.e. we regard

$$|\varphi_\alpha(z)|^2 \approx \frac{2}{L}\theta(-z).$$

Then the summation over α in the expression (18) can be done analytically. And thus we get for $\mathfrak{M}(q|z,z')$:

$$\mathfrak{M}(q|z,z') = -\frac{SL^2}{\beta}\frac{2m}{\hbar^2}\frac{1}{\pi^2}\frac{p_{\mathrm{F}}}{2}\mathrm{L}\left(\frac{q}{2p_{\mathrm{F}}}\right)\theta(-z)\delta(z-z'), \tag{19}$$

where $\mathrm{L}(x) = \dfrac{1}{2} + \dfrac{1-x^2}{4x}\ln\left|\dfrac{1+x}{1-x}\right|$ is Lindhard function [10].

3.1.2. Nonmirror electron scattering

Let the condition be satisfied

$$4q^2\frac{p_{\mathrm{F}}^2-\alpha_1^2}{\left(q^2-\alpha_1^2+\alpha_2^2\right)^2} \ll 1 \tag{20}$$

that takes place in the case of large q (small distances between electrons on the surface) or in the case of small q under the condition $\alpha_1^2-\alpha_2^2 \neq 0$. Then the correlator takes the following form

$$\begin{aligned}\mathfrak{M}(q|z,z') &= -\frac{SL^2}{\beta}\frac{2m}{\hbar^2}\frac{1}{\pi}\sum_{\alpha_1,\alpha_2}\varphi^*_{\alpha_1}(z)\varphi_{\alpha_2}(z)\varphi^*_{\alpha_2}(z')\varphi_{\alpha_1}(z')\frac{p_{\mathrm{F}}^2-\alpha_1^2}{q^2-\alpha_1^2+\alpha_2^2}\theta\left(p_{\mathrm{F}}-\alpha_1\right) \\ &\approx -\tfrac{SL^2}{\beta}\tfrac{2m}{\hbar^2}\tfrac{1}{\pi}\sum_{\alpha_1}\theta\left(p_{\mathrm{F}}-\alpha_1\right)\left(p_{\mathrm{F}}^2-\alpha_1^2\right)\varphi^*_{\alpha_1}(z)\varphi_{\alpha_1}(z')\sum_{\alpha_2}\tfrac{\varphi_{\alpha_2}(z)\varphi^*_{\alpha_2}(z')}{q^2+\alpha_2^2},\end{aligned} \tag{21}$$

where we have done the approximation $q^2-\alpha_1^2+\alpha_2^2 \approx q^2+\alpha_2^2$ using $\alpha_1 \in [0,p_{\mathrm{F}}]$ and $\alpha_2 \in [0,\infty)$.

Taking the summation over α_1 and α_2 in the expression (21) we get

$$\begin{aligned}\mathfrak{M}(q|z,z') \;=\; & -\frac{SL^2}{\beta}\frac{2m}{\hbar^2}\frac{1}{\pi^2}\frac{1}{q}\left(\mathrm{e}^{-q|z-z'|}-\mathrm{e}^{-q|z+z'|}\right)\theta(-z)\theta(-z') \\ & \times\left[\tfrac{p_{\mathrm{F}}\cos(p_{\mathrm{F}}(z+z'))}{(z+z')^2}-\tfrac{p_{\mathrm{F}}\cos(p_{\mathrm{F}}(z-z'))}{(z-z')^2}+\tfrac{\sin(p_{\mathrm{F}}(z-z'))}{(z-z')^3}-\tfrac{\sin(p_{\mathrm{F}}(z+z'))}{(z+z')^3}\right].\end{aligned} \tag{22}$$

Carrying out the inverse Fourier-transform and allowing for [11]

$$\int\limits_0^\infty \mathrm{d}q\,\mathrm{e}^{-q|z-z'|}\mathrm{J}_0(qr) = \frac{1}{\sqrt{r^2+(z-z')^2}}\,,$$

we get the correlator in the coordinate representation

$$\mathfrak{M}(r,z,z') = -\frac{SL^2}{\beta}\frac{m}{\hbar^2}\frac{1}{\pi^3}\left(\frac{1}{\sqrt{r^2+(z-z')^2}} - \frac{1}{\sqrt{r^2+(z+z')^2}}\right)\theta(-z)\theta(-z') \times\left[p_{\mathrm{F}}\frac{\cos(p_{\mathrm{F}}(z+z'))}{(z+z')^2} - p_{\mathrm{F}}\frac{\cos(p_{\mathrm{F}}(z-z'))}{(z-z')^2} + \frac{\sin(p_{\mathrm{F}}(z-z'))}{(z-z')^3} - \frac{\sin(p_{\mathrm{F}}(z+z'))}{(z+z')^3}\right]. \tag{23}$$

The obtained expression (23) shows that the approximation (20) leads to a physically correct result, namely, the image forces and collective effects (the analogue of Friedel oscillations for homogeneous electron gas) are taken into account.

In figure 1 and figure 2 the results of numerical calculations of the correlator are presented in a dimensionless form:

$$\widetilde{\mathfrak{M}}(r,z,z') = \mathfrak{M}(r,z,z')/\left(-\frac{SL^2}{\beta}\frac{m}{\hbar^2 a_{\mathrm{B}}^4}10^{-3}\right).$$

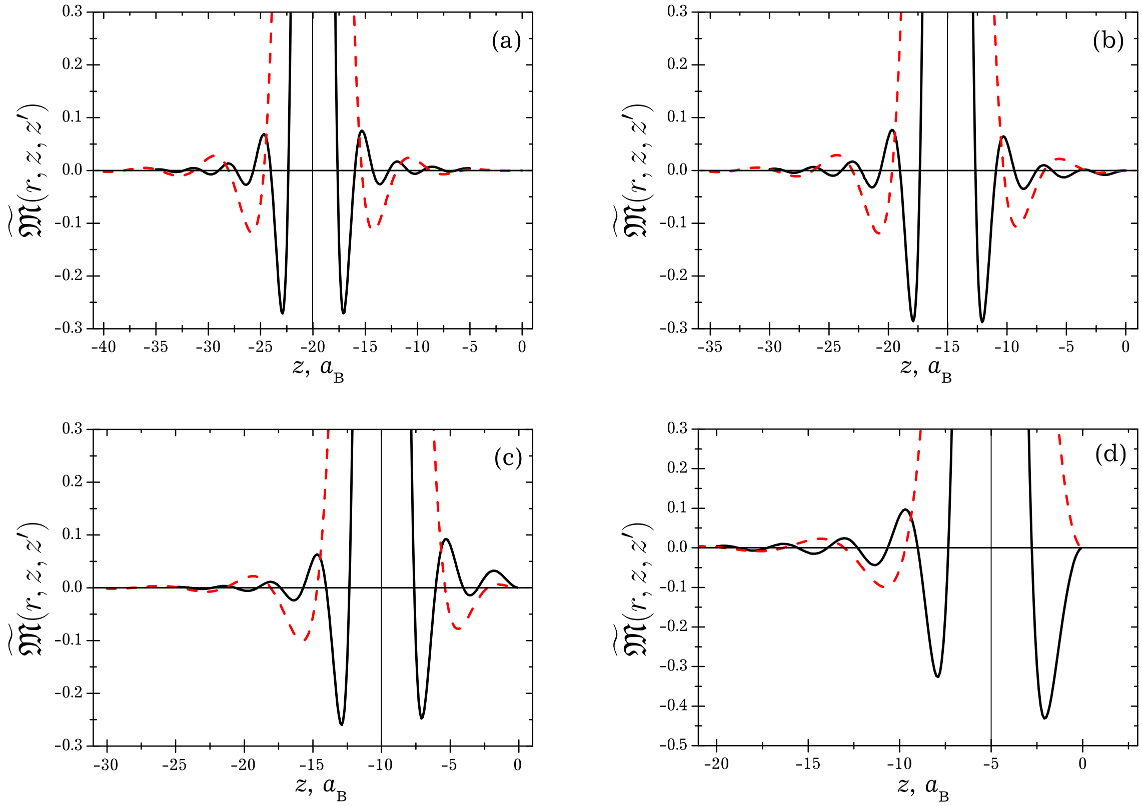

Figure 1. The correlator under $r=0$ in such cases: a) $z'=-20a_{\mathrm{B}}$, b) $z'=-15a_{\mathrm{B}}$, c) $z'=-10a_{\mathrm{B}}$, d) $z'=-5a_{\mathrm{B}}$. A solid line marks the data of numerical calculation of the formula (13) and a dash line corresponds to the tabulated function (23).

In figure 1 the approximation (20) proposed herein leads to a qualitatively correct dependence of the correlator on normal coordinates of electrons. However, there is disagreement with data of numerical calculations, namely, lesser amplitudes of oscillations and stronger repulsion of electrons. We can see in figure 2 that the approximation (20) does not allow for oscillations in the coordinate r. Near the surface (see figure 2a) there is a good agreement of numerical calculation data with the analytical expression (23) and at the removal from the surface (see figure 2b) there is observed a major departure because the expression (23) gives too strong repulsion of electrons.

Figure 2c and figure 2d present the tabulated correlator (23) and data of its numerical calculations. Calculations show that the shorter the distance between the electrons and the surface is, the lesser is the correlation between them. This is clear from the physical viewpoint since that electron density near the surface is smaller in average.

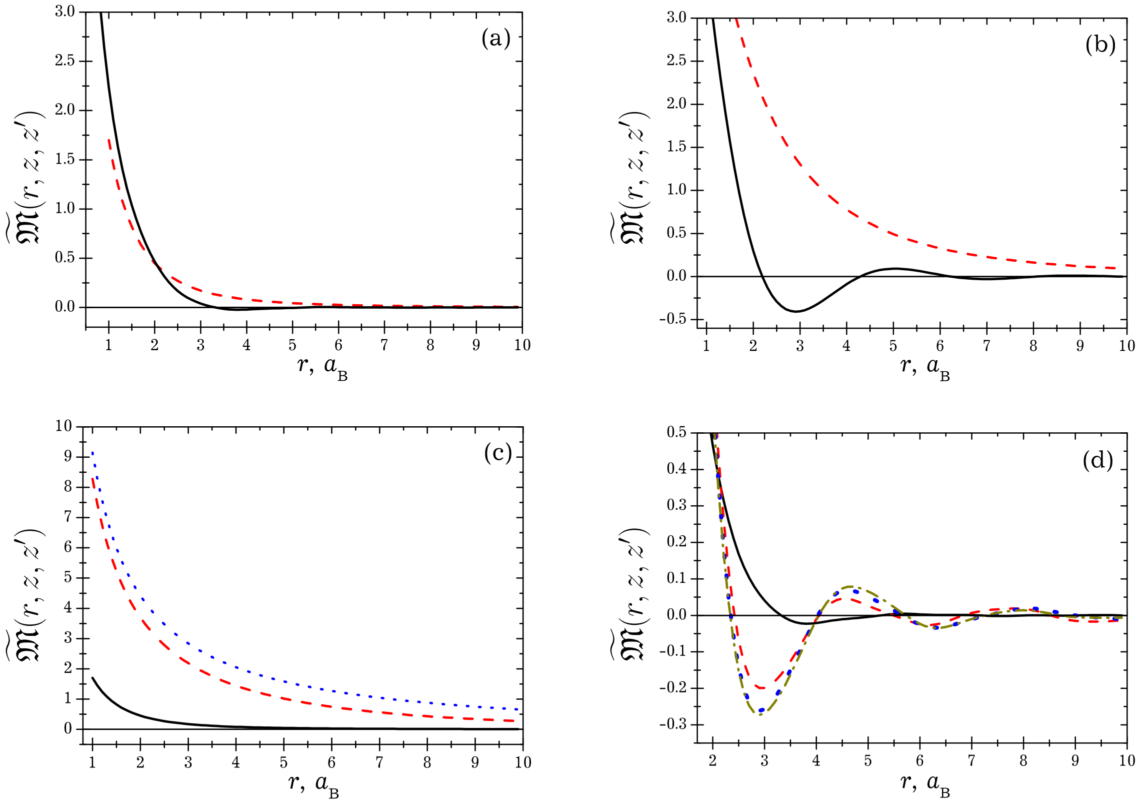

Figure 2. The correlator in the following case:
(a) $z = z' = -1a_{\rm B}$, b) $z = -2a_{\rm B}$, $z' = -3a_{\rm B}$ (A solid line marks data of numerical calculation of the formula (13) and a dash line corresponds to the tabulated function (23));
c) the tabulated function (23) at $z = z' = -1a_{\rm B}$ (a solid line, at $z = z' = -5a_{\rm B}$ (a dash line), at $z = z' = -15a_{\rm B}$ (a point line);
d) data of numerical calculation of the formula (13) under $z = z' = -1a_{\rm B}$ (a solid line), $z = z' = -5a_{\rm B}$ (a dash line), $z = z' = -15a_{\rm B}$ (a point line), $z = z' = -20a_{\rm B}$ (a dash-dotted line).

3.2. Calculation of the effective potential of electron-electron interaction

Consider the case corresponding only to mirror electron scattering in the two-particle "density-density" correlator (19). Then equation (10) takes the form

$$g(q|z_1,z_2) = \frac{2\pi e^2}{q}\mathrm{e}^{-q|z_1-z_2|} - \frac{\varkappa_{\rm TF}^2}{2q}\mathrm{L}\left(\frac{q}{2p_{\rm F}}\right)\theta(-z_1)\int\limits_{-\infty}^{0}\mathrm{d}z\,\mathrm{e}^{-q|z_1-z|}g(q|z,z_2), \tag{24}$$

where $\varkappa_{\rm TF}$ is an inverse Thomas-Fermi radius of screening, $\varkappa_{\rm TF}^2 = 4p_{\rm F}/(\pi a_{\rm B})$.

Such type of equation is solved analytically (see, for example, [8]) and its solution is as follows

$$g(q|z_1,z_2) = \begin{cases} \frac{2\pi e^2}{Q}\left(\mathrm{e}^{-Q|z_1-z_2|} + \frac{Q-q}{Q+q}\mathrm{e}^{Q(z_1+z_2)}\right), & z_1 \leqslant 0,\ z_2 \leqslant 0, \\ \frac{2\pi e^2}{q}\left(\mathrm{e}^{-q|z_1-z_2|} - \frac{Q-q}{Q+q}\mathrm{e}^{-q(z_1+z_2)}\right), & z_1 \geqslant 0,\ z_2 \geqslant 0, \\ \frac{4\pi e^2}{Q+q}\mathrm{e}^{Qz_1-qz_2}, & z_1 \leqslant 0,\ z_2 \geqslant 0, \\ \frac{4\pi e^2}{Q+q}\mathrm{e}^{Qz_2-qz_1}, & z_1 \geqslant 0,\ z_2 \leqslant 0, \end{cases} \tag{25}$$

where $Q=\sqrt{q^2+\varkappa_{\mathrm{TF}}^2\mathrm{L}\left(\frac{q}{2p_{\mathrm{F}}}\right)}$. If we pass to the limit $q\to 0$ in Lindhard function $\mathrm{L}\left(q/(2p_{\mathrm{F}})\right)$ then the solution (25) agrees with the effective potential of electron interaction $g_{\mathrm{TF}}(q|z_1,z_2)$ obtained in the works [7,8] in Thomas-Fermi approximation.

Take the inverse Fourier transform of the effective potential of electron interaction

$$g(r,z_1,z_2)=\frac{1}{S}\sum_{\mathbf{q}}\mathrm{e}^{\mathrm{i}\mathbf{qr}}g(q|z_1,z_2)=\frac{1}{2\pi}\int\limits_0^\infty \mathrm{d}q\,q\mathrm{J}_0(qr)g(q|z_1,z_2), \tag{26}$$

where r is the distance between electrons. Asymptotics of the effective potential of electron-electron interaction $g(r,z_1,z_2)$ under $r\to\infty$ is

$$g(r,z_1,z_2)\approx\frac{\sqrt{\pi}}{4}e^2\frac{\varkappa_{\mathrm{TF}}^2}{\sqrt{p_{\mathrm{F}}}}\phi(2p_{\mathrm{F}}|z_1,z_2)\frac{\sin(2p_{\mathrm{F}}r-\pi/4)}{r^{5/2}}, \tag{27}$$

where

$$\begin{aligned}\phi(q|z_1,z_2) &= \frac{1}{Q}\left[-\frac{1+Q|z_1-z_2|}{Q^2}\mathrm{e}^{-Q|z_1-z_2|}+\frac{1}{Q}\frac{1}{Q+q}\left(\frac{q}{Q}-\frac{Q-q}{Q+q}\right.\right.\\ &\quad \left.\left.+\ (Q-q)(z_1+z_2)\right)\mathrm{e}^{Q(z_1+z_2)}\right],\quad z_1\leqslant 0,\ z_2\leqslant 0, \qquad (28)\\ \phi(q|z_1,z_2) &= -\frac{2}{Q(Q+q)^2}\mathrm{e}^{-q(z_1+z_2)},\quad z_1\geqslant 0,\ z_2\geqslant 0, \qquad (29)\\ \phi(q|z_1,z_2) &= -\frac{2}{Q}\frac{1-(Q+q)z_1}{(Q+q)^2}\mathrm{e}^{Qz_1-qz_2},\quad z_1\leqslant 0,\ z_2\geqslant 0, \qquad (30)\\ \phi(q|z_1,z_2) &= -\frac{2}{Q}\frac{1-(Q+q)z_2}{(Q+q)^2}\mathrm{e}^{Qz_2-qz_1},\quad z_1\geqslant 0,\ z_2\leqslant 0. \qquad (31)\end{aligned}$$

The found expression (27) agrees in form with the result of the work [12]. However, the expression for function ϕ has been obtained first.

The asymptotics of the effective potential (27) is presented in figure 3 as well as the results of numerical calculation of the formula (26), where the expressions (25) and (25) in Thomas-Fermi approximation are taken as an effective potential $g(q|z_1,z_2)$. It is shown in figure 3 that in Thomas-Fermi approximation the oscillations vanish but it corresponds to the qualitatively correct behaviour of the effective potential. For $z_1,z_2\ll 0$ (occurring far from the surface in jellium, see figure 3b) the asymptotics presents well the potential behaviour under $r>5a_{\mathrm{B}}$. The effective potential for electrons occurring outside the near-surface area has a strongly repulsive character (see figure 3c,d) and the oscillations vanish (see figure 3d). This is physically clear because electron density is lesser than the one outside the near-surface area. So the collective effects are weak and the electrons interact according to the law similar to the Coulomb law. This fact is represented in figure 4, where Fourier-image of the effective potential (25) is illustrated as well as its Thomas-Fermi approximation at $r=0$.

In figure 4a and figure 4b the effective potential of electron-electron interaction is shown as the function of the normal coordinate of one of electrons and another one occurs at $z_2=-5a_{\mathrm{B}}$ (figure 4a) and $z_2=0$ (figure 4b). These figures show that the effective potential obtained by numerical solution of the integral equation (10) oscillates (solid line) and the neglect of electron scattering along the normal to the surface leads to the absence of the effective potential oscillations along the normal while there are oscillations in the plane parallel to the surface (see figures 3a,b,d).

Figure 5 presents a comparison of the numerical solution of the integral equation (10), the results of the work [6] and Coulomb potential. As follows from this figure, there is observed a qualitative agreement between the results of our calculations and the results of the work [6]. However, the effective potential in the work [6] decreases faster to zero and there is no oscillation. In our opinion, the collective effects being insufficiently taken into account are responsible for this situation.

All the calculations in the paper have been made for $r_{\mathrm{S}}=2a_{\mathrm{B}}$.

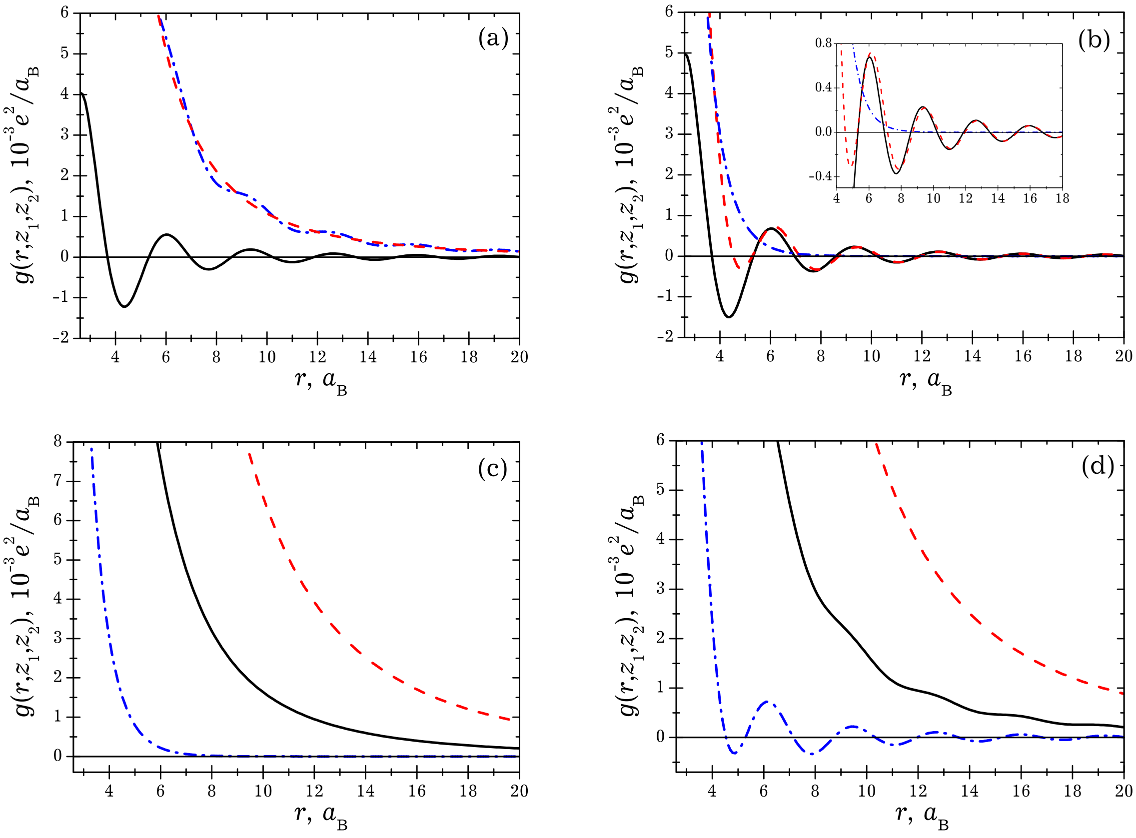

Figure 3. The effective potential of electron interaction $g(r, z_1, z_2)$ in such cases:
a) $z_1 = z_2 = -0.2a_B$, b) $z_1 = z_2 = -5a_B$ (a solid line marks the asymptotic $g(r, z_1, z_2)$ (27), a dash line corresponds to Fourier-image of the function (25), a dash-dotted line marks Fourier-image of the effective potential (25) in the Thomas-Fermi approximation);
c) Fourier-image of the effective potential (25) in the Thomas-Fermi approximation at $z_1 = z_2 = 0$ (a solid line), $z_1 = z_2 = 1a_B$ (a dash line), $z_1 = z_2 = -10a_B$ (a dash-dotted line);
d) Fourier-image of the effective potential (25) at $z_1 = z_2 = 0$ (a solid line), $z_1 = z_2 = 1a_B$ (a dash line), $z_1 = z_2 = -10a_B$ (a dash-dotted-line).

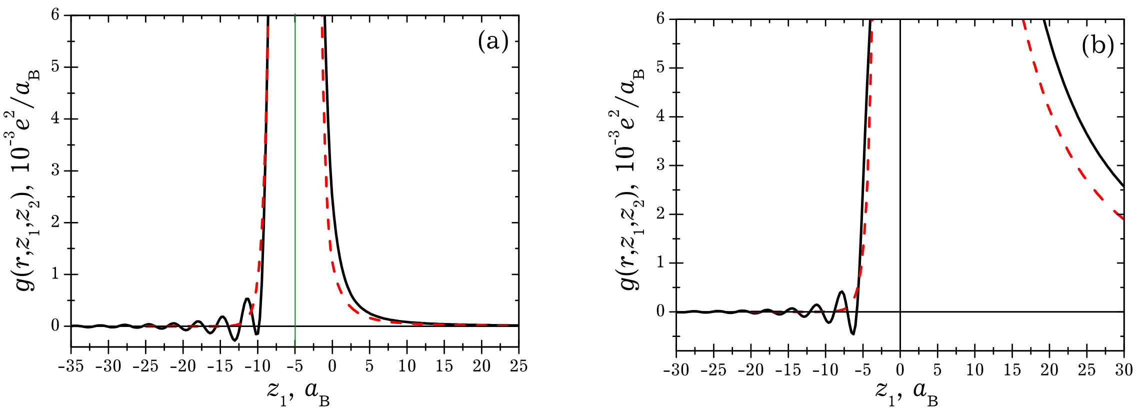

Figure 4. The effective potential of electron interaction $g(r, z_1, z_2)$ at $r = 0$ in such cases: a) $z_2 = -5a_B$, b) $z_2 = 0$ (a solid line marks the numerical solution of the integral equation (10), a dash line corresponds to the effective potential (25)).

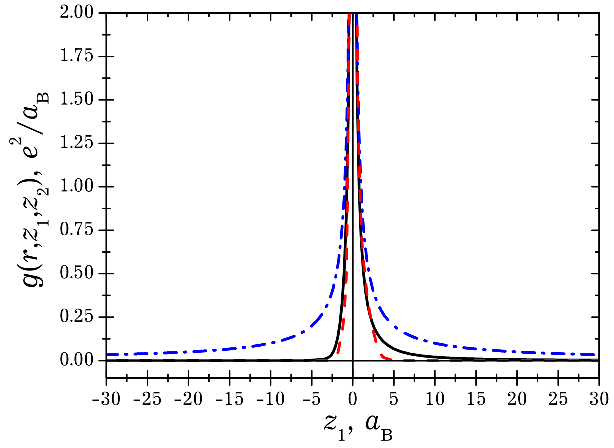

Figure 5. A solid line marks the effective potential of electron interaction $g(r = 0, z_1, z_2 = 0)$ as a numerical solution of the integral equation (10), a dash line corresponds to the effective potential of electron interaction $g(r = 0, z_1, z_2 = 0)$ by the data of the work [6], a dash-dotted line marks Coulomb potential.

4. Conclusion

In the work numerical calculations have been carried out for the two-particle "density-density" correlator $\mathfrak{M}$ and analytical approximating expressions have been proposed for $\mathfrak{M}$ which agree well with the results of numerical calculations.

The obtained analytical expressions allow us to investigate the asymptotic behaviour for both $\mathfrak{M}$ at large distances between electrons ($r \to \infty$):

$$\mathfrak{M}(r, z, z') \sim \frac{\sin(2p_{\mathrm{F}}r - \pi/4)}{r^{5/2}}$$

and the effective potential of electron-electron interaction g:

$$g(r, z_1, z_2) \approx \frac{\sqrt{\pi}}{4} e^2 \frac{\varkappa_{\mathrm{TF}}^2}{\sqrt{p_{\mathrm{F}}}} \phi(2p_{\mathrm{F}}|z_1, z_2) \frac{\sin(2p_{\mathrm{F}}r - \pi/4)}{r^{5/2}}, \qquad r \to \infty.$$

The obtained analytical expression for $\mathfrak{M}$ in the case of the mirror electron scattering approximation makes it possible to analytically solve the integral equation for the effective potential of electron-electron interaction g taking into account both the effects of image forces and screening.

For the first time it is shown that the collective effects being correctly taken into account at numerically solving the integral equation for the effective potential of electron-electron interaction lead to the oscillations of the effective potential. It is shown that numerical results for g [6] correspond to the mirror electron scattering approximation for g (25).

References

1. Hohenberg P., Konh W., Phys. Rev. B, 1964, **136**, No. 3, 864.
2. Jones R.O., Gunnarsson O., Rev. Mod. Phys., 1989, **61**, No. 3, 689.
3. Mattsson A.E., Kohn W., J. Chem. Phys., 2001, **115**, No. 8, 3441.
4. Eguiluz A.G., Heinrichsmeier M., Fleszar A., Hanke W., Phys. Rev. Lett., 1992, **68**, No. 9, 1359.
5. Hedin L., Phys. Rev., 1965, **139**, No. 3A, A796.
6. Fratesi G., Brivio G.P., Molinari L.G. Preprint arXiv: cond–mat/0305344, 2003.
7. Kostrobij P.P., Markovych B.M., Condens. Matter Phys., 2003, **6**, No. 2(34), 347.
8. Kostrobij P.P., Markovych B.M., Journ. Phys. Stud., 2003, **7**, No. 2, 195 (in Ukrainian).
9. Kostrobij P.P., Markovych B.M., Journ. Phys. Stud., 2003, **7**, No. 3, 298 (in Ukrainian).
10. Harrison W.A., Solid state theory. New York-London-Toronto, 1970.

11. Gradshtein I.S., Ryzhyk I.M., Tables of intergals, sums, series and products. Nauka, Moscow, 1971 (in Russian).
12. Gabovich A.M., Pashytsky E.A., Fiz. Tverd. Tela, 1976, **18**, No. 2, 377 (in Russian).

Ефективний потенціал міжелектронної взаємодії для напівобмеженого електронного газу

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Розраховано ефективний потенціал міжелектронної взаємодії та двочастинкову електронну кореляційну функцію “густина-густина” для напівобмеженого металу в моделі “желе” та досліджено їх асимптотичні поведінки при великих віддалях між електронами в площині поверхні.

Ключові слова: *напівобмежена модель “желе”, електронна кореляційна функція “густина-густина”, ефективний потенціал парної міжелектронної взаємодії*

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