UDC 53.043:621.315.5, PACS 21.60.Jz, 73.20.Dx

ON SCREENING IN SOME LOW-DIMENSIONAL CRYSTALS

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Received April 22, 1996

On the basis of the proposed diagram technique in quantizing magnetic field, two problems of interelecteren screening are investigated. In the first one in the RPA framework the Fourier-transformation of Coulomb interactions is analysed. It is obtained to have an oscillating character with respect magnetic field and band filling. In ultraquantum magnetic field the polarization loop which is diagonal over Landau numbers formally coincides with that in the one-dimensional case. In the second problem in RPA the renormalization of the interelectron potential in a one-dimensional crystal with the narrow band is studied. It is shown, that at some conditions such potential is an oscillating sign-variable function on an interelectron distance.

1. Introduction

One-dimensional (1D) model is not only simple and convenient for calculations. There is a number of objects described by such a model: a class of anisotropic conductors whose structures consist of parallel linear chains, along which conduction electrons propagate essentially in one dimension (such as TTF-TCNQ, inorganic salts such as the "mixed-valence" platinocyanides).

Recently this model was widely used for the description of stage ordering phenomenon i.e. a periodic sequence of layers intercalated in the host crystal matrix [1]. In the frame of 1D model the average layer occupancies of the intercalant sites were analysed, ignoring the electron subsystem. Particularly, for better understanding of the electron subsystem influence on, for instance, the stage ordering in a layer crystal the studying of screening effects is necessary. However, actuality of such problems is much wider.

Some problems of screening are solved below i) in crystal placed into external magnetic field ii) renormalization of the interelectron interaction potential.

2. Crystal in the external magnetic field

Before studying of 1D problem let's consider 3D-crystal placed in the magnetic field. Results of such problem, as it will be shown below, can be used in 1D-case.

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For better understanding of physical processes in solid state it is necessary to analyse many-body effects. In spite of the essential improvements of such type analysis for an ideal crystal, they are more modest when external magnetic field is applied. It means impossibility of the straight usage of many-body investigation methods, suited for the ideal crystal without field, to the case for the ideal crystal in the field. Really for the ideal crystal without field diagram technique is usually based on the Fourier transformations of Green's functions taking into account the space homogeneity, that occurs in this case [2]. For the crystal placed in the field, studied system becomes unhomogeneous because of vector potential dependence on coordinate, that significantly complicates this problem from the mathematical point of view.

Let's introduce the diagram technique for the description of the electrons in the magnetic field [3], based on the Landau functions which form orthonormal full set [4]. In this basis the Hamiltonian of interacted electrons in the field $\mathcal{H}$, directed along OZ, has a form

$$H = H_0 + H_{int}, \tag{2.1}$$

where

$$H_0 = \sum_{\alpha} \varepsilon_{\alpha}\ a^{+}_{\alpha} a_{\alpha} \tag{2.2}$$

with

$$\varepsilon_{\alpha} = \varepsilon(k_z) + \omega_c \left(n + \frac{1}{2}\right), \quad \omega_c = \frac{e\mathcal{H}}{mc}. \tag{2.3}$$

$\alpha = \{n, k_x, k_z\}$ - quantum numbers set in the Landau representation, $\varepsilon(k_z)$ is electron dispersion law along OZ, $\hbar = 1$.

$$H_{int} = \tfrac{1}{2} \sum_{\alpha_i} B_{\alpha_1\alpha_2\alpha_3\alpha_4} a^{+}_{\alpha_1} a^{+}_{\alpha_2} a_{\alpha_3} a_{\alpha_4}, \tag{2.4}$$

where $B_{\alpha_1\alpha_2\alpha_3\alpha_4}$ is the matrix element of the Coulomb interaction between electrons, found on the Landau functions:

$$\begin{gathered} B_{\alpha_1\alpha_2\alpha_3\alpha_4} = \tfrac{\bar{n}!\bar{n}'!}{\sqrt{n_1!n_2!n_3!n_4!}} \sum U(\vec{q}) \delta\left(k_x^{(1)} - k_x^{(4)} - q_x\right) \times \\ \delta\left(k_z^{(1)} - k_z^{(4)} - q_z\right) \delta\left(k_x^{(2)} - k_x^{(3)} + q_x\right) \delta\left(k_z^{(2)} - k_z^{(3)} + q_z\right) \times \\ X^{|n_1 - n_4|} \times X'^{|n_2 - n_3|} \times L_{\bar{n}}^{|n_1 - n_4|}(|X|^2) \times L_{\bar{n}}^{|n_2 - n_3|}(|X'|^2) \\ \exp\left[\tfrac{i}{2} q_y \left(y_0^{(1)} + y_0^{(4)}\right) - \tfrac{i}{2} q_y \left(y_0^{(2)} + y_0^{(3)}\right) - \tfrac{|X|^2}{2} - \tfrac{|X'|^2}{2}\right] \end{gathered} \tag{2.5}$$

with

$$U(q) = \frac{1}{\lambda^2} \frac{4\pi e^2}{q^2},\ \bar{n} = \min(n_1, n_4),\ \bar{n}' = \min(n_2, n_3),\ \lambda^2 = \frac{mc}{e\mathcal{H}}$$

$$\begin{aligned} X &= \tfrac{\lambda}{\sqrt{2}} \left[\tfrac{1}{\lambda^2}(y_0^{(1)} - y_0^{(4)}) sign(n_1 - n_4) + i q_y\right], \\ X' &= \tfrac{\lambda}{\sqrt{2}} \left[\tfrac{1}{\lambda^2}(y_0^{(2)} - y_0^{(3)}) sign(n_2 - n_3) - i q_y\right]. \end{aligned}$$

Let's introduce Green function [2]

$$G_{\alpha\alpha'}(t - t') = -i \left\langle T(a_{\alpha}(t)\, a^{+}_{\alpha'}(t')\right\rangle, \tag{2.6}$$

where $a_\alpha(t)$ is Fermi operator in the Heisenberg representation with the Hamiltonian (2.1). Considering diagram technique for such Green function at $T = 0$, one obtains the conclusion, that the appearance of these diagrams coincides with those without field, but notation of their analytical expressions requires such rules:

1. Each solid line corresponds to Green function of noninteracted electrons, described by H_0 (2.2),

$$G_n^0(k_z,\omega) = \{\omega - \varepsilon_n(k_z) - \mu + i\delta sign[\varepsilon_n(k_z) - \mu]\}^{-1} \tag{2.7}$$

   with quantum numbers n, k_z and frequency ω.

2. Each wave line corresponds to the interaction potential with 3D momentum q, frequency ω and $U(q)$.

3. For each top, where Green functions with quantum numbers n and n' and a wave line with momentum q come to, the factor corresponds to

$$\frac{\bar{n}!}{\sqrt{n_1!n!}} \exp\left[-\frac{\lambda^2 q_\perp^2}{4}\right] \left[\frac{\lambda^2 q_\perp^2}{4}\right]^{|n-n_1|/2} L_{\bar{n}}^{|n-n_1|}\left(\frac{\lambda^2 q_\perp^2}{2}\right) \tag{2.8}$$

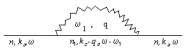
   with $\vec{q}_\perp = (q_x, q_y)$, $\bar{n} = \min(n, n_1)$.

4. Frequencies and z-components of momentum of internal lines must satisfy conservation laws in each top, and for diagrams of any order higher than the first one the conservation law of 3D-momentum occurs too.

5. Diagram of m-th order has m integrations over independent momentum (3D - momentum and z-component), as well as summation on quantum numbers of internal lines and integration over independent frequencies are carried out.

6. Before the obtained expression one should write coefficient $i^m(-1)^f$, where f is a number of closed loops.

For instance, diagram of the first order that describes exchange interaction



corresponds to the expression

$$[G_{n_1}^0(k_z,\omega)]^2 \sum_{n_1} \int \frac{d^3q}{(2\pi)^3} \int \frac{d\omega_1}{2\pi} W_{nn_1}(\vec{q}) G_{n_1}^0(k_z - q_z, \omega - \omega_1) \tag{2.9}$$

with

$$W_{nn_1}(\vec{q}) = \left[\frac{\bar{n}!}{\sqrt{n_1!n!}}\right]^2 U(\vec{q}) \exp\left[-\frac{\lambda^2 q_\perp^2}{2}\right] \left[\frac{\lambda^2 q_\perp^2}{2}\right]^{|n-n_1|} \left[L_{\bar{n}}^{|n-n_1|}\left(\frac{\lambda^2 q_\perp^2}{2}\right)\right]^2. \tag{2.10}$$

From (2.9) the function

$$V(n, n_1, q_z) = \left(\tfrac{1}{2\pi}\right)^2 \int W_{nn_1}(\vec{q}) d^2 q_\perp \tag{2.11}$$

can be organized. It can be interpreted as an interaction potential for electrons on Landau level n and n_1 with q_z momentum transfer.

It can be shown, that in the RPA frame W^{eff}_{nn} can be obtained in the form

$$W^{eff}_{nn_1} = W_{nn_1} + W_{n_1n_2}\Pi_{n_1n_2}W_{n_1n_2} + ...,$$

where

$$\Pi_{n_1n_2}(q_z) = -\frac{i}{4\pi^2}\int dk_z \int d\omega G^0_{n_1}(k_z,\omega_1)\times G^0_{n_2}(k_z+q_z,\omega+\omega_1) \quad (2.12)$$

is a polarization loop in the Landau function representation.

Calculation of the $\Re\mathrm{e}\Pi_{n_1n_2}$ at $T=0$ for electrons with the dispersion law in (2.3)

$$\varepsilon(k_z) = \frac{k_z^2}{2m}$$

gives

$$\Re\mathrm{e}\Pi_{n_1n_2} = \frac{m_z}{q_z}\times\ln\left|\frac{\left[\omega+\frac{q_z}{m}\left(d_{n_2}+\frac{q_z}{2}\right)\right]}{\left[\omega+\frac{q_z}{m}\left(d_{n_2}+\frac{q_z}{2}\right)\right]}\times\frac{\left[\omega-\frac{q_z}{m}\left(d_{n_1}+\frac{q_z}{2}\right)\right]}{\left[\omega-\frac{q_z}{m}\left(d_{n_2}-\frac{q_z}{2}\right)\right]}\right|, \quad (2.13)$$

where $d_n = \sqrt{2m_z\left[\mu-\omega_c\left(n+\frac{1}{2}\right)\right]}$, μ is the chemical potential.

$\Re\mathrm{e}\Pi(q,\Omega)$ differs from zero only at $\Im\mathrm{m}d_n = 0$. So we deal with restrictions on the integration region over momentum in the diagram technique at $T=0$ [2]. As is seen from (2.13), in static case, $\omega=0$, "diagonal" $\Re\mathrm{e}\Pi_{nn}$ has a form

$$\Re\mathrm{e}\Pi_{nn} = \frac{2m}{q_z}\ln\left|\frac{d_n+\frac{q_z}{2}}{d_n-\frac{q_z}{2}}\right|. \quad (2.14)$$

Using (2.14) and considering connection between $V(n,n',q_z)$ and $W_{nn'}(q)$ (2.11) one can show that singularity of $V(n,n',q_z)$ in the long wave approximation (i.e. at $q_z\to 0$) disappears when polarization effects are taken into account. By the way, the terms diagonal over Landau index play the main role here.

Two more conclusions, which come from the requirement $\Im\mathrm{m}d_n = 0$, are:

1. Renormalized $V(n,n',q_z)$ has an oscillating character at changing of the field or band occupancy (μ).
2. In the ultraquantum case all the polarization effects are determined only by electron state $n=0$, when an electron moves infinitely along k_z. That's why such behaviour can be considered formally as 1D case.

3. Polarization properties in the narrow band crystal

Using above results, let's consider polarization properties of 1D narrow band crystal with the dispersion law

$$\varepsilon(k) = a+\beta(1-\cos k), \quad (3.1)$$

where β is the integral of the electron mixing neighbouring atoms and it equals to the half bandwidth; here the lattice constant along c-axis is chosen to be equal to unity. In layered crystal the system of stage ordered

intercalant atoms can be described by just such a dispersion law, because these atoms are bound by weak van der Waals interaction. That's why in this case, at the electron system description, one can use tight-binding approximation, that gives (3.1).

Comparing (3.1) with (2.3), it can be seen, that $a = \omega_c(n + 1/2)$ when magnetic field is applied. Thus form for a in $\varepsilon(k)$ (3.1) describes law dispersion of the chain crystal with field, coinciding with its axis or without it.

Applying of such a nonparabolic dispersion law for the screen effect study distinguishes this work from a numerous ones, where similar problems were solved for the electrons with a square or linear (at the Fermi level) dispersion law (see for instance [5]).

A polarization loop with electron dispersion law (3.1) has been obtained in [6,7] in extreme magnetic field. After integration over frequency in (2.12) we'll have [6]

$$\Pi\left(q,\Omega\right) = \frac{1}{2\pi}\left[\int\limits_{\{B\}} R_2 dk - \int\limits_{\{A\}} R_1 dk\right], \tag{3.2}$$

where

$$R_\alpha^{-1} = \varepsilon\left(k - \tfrac{q}{2}\right) - \varepsilon\left(k + \tfrac{q}{2}\right) + \Omega + (-1)^\alpha\, i\delta, \quad (+\alpha = 1,2).$$

It has nonzero value in the case

$$\{A\} \in \left\{\begin{array}{l}\varepsilon\left(k - q/2\right) > \mu\\ \varepsilon\left(k + q/2\right) < \mu\end{array}\right\} \text{ and/or } \quad \{B\} \in \left\{\begin{array}{l}\varepsilon\left(k - q/2\right) < \mu\\ \varepsilon\left(k + q/2\right) > \mu\end{array}\right\}. \tag{3.3}$$

Real and imaginary components of $\Pi(q,\Omega)$ are

$$\Re\mathrm{e}\Pi\left(q,\Omega\right) = -\frac{1}{2\pi}\int\limits_{\{B\}-\{A\}} \left(\Omega - b\sin k\right)^{-1} dk, \tag{3.4}$$

$$\Im\mathrm{m}\Pi\left(q,\Omega\right) = \frac{1}{2}\int\limits_{\{B\}+\{A\}} \delta\,\left(\Omega - b\sin k\right) dk, \tag{3.5}$$

where $b = 2\beta\sin(q/2)$. Integrals (3.4) and (3.5) can be found analytically, but integration limits determined from (3.3) have different analytical forms depending on $Q = (a + \beta - \mu)/\beta$.

Let us present $\Re\mathrm{e}\Pi$ in the static limit. It has a form

$$\Re\mathrm{e}\Pi\left(q,0\right) \equiv \Re\mathrm{e}\Pi\left(q\right) = -\frac{1}{2\pi\beta\sin\left(q/2\right)}\ln\left|\frac{\tan\left(k_1/2\right)}{\tan\left(k_0/2\right)}\right|, \tag{3.6}$$

where k_0, k_1 are lower and upper limits of integration. They are determined by Q. As it follows from mentioned above situation

- $\Re\mathrm{e}\Pi(q) = 0$ at $|Q| > 1$, i.e. for entirely full or empty band;
- $\Re\mathrm{e}\Pi(q)$ as function of q has two singularities: at $q = 2k_F$ and $q = 2(\pi - k_F)$ (k_F is Fermi's wave vector). The first one (at $q = 2k_F$) coincides with the same for electrons with k^2 dispersion law and shows

itself as Peierls transition in 1D lattice or Kohn's anomaly in the phonon spectrum which appears in a softening of the phonon mode [8]. In the given case such an additional effect can occur at $q = 2(\pi - k_F)$. It should be noted that such an complemental point was overlooked in [7]. Behaviour of $\Im\mathrm{m}\Pi(q,\omega)$ is analysed in [9].

Let's research renormalization of interelectron interaction in the narrow band crystal. Let a bare potential of interelectron interaction has a form of the Lorentz-type curve

$$V_0(r) = \frac{D}{r^2 + D^2}, \tag{3.7}$$

where $r = |r_i - r_j|$, and D is its halfwidth. The choice of such a potential will not change the qualitative character of the conclusions about the screening. From another point of view, this potential doesn't have any singularities (as for instance Coulomb potential at $r = 0$) and thus one will have no doubts on received below conclusions, as the result of such singularities.

Fourier transformation of (3.7) is

$$V_0(q) = \sqrt{(\pi/2)}\exp(-qD). \tag{3.8}$$

The screened potential in the RPA is [10]

$$\tilde{V}(q) = \frac{V_0(q)}{1 + \Pi(q,\Omega)V_0(q)}. \tag{3.9}$$

Considering the connection of real and imaginary parts of dielectric function with $\Pi(q)$, we can write [10]

$$\varepsilon_1(q) = 1 + \Re\mathrm{e}\Pi(q)V_0(q), \tag{3.10}$$

$$\varepsilon_2(q) = \Im\mathrm{m}\Pi(q)V_0(q). \tag{3.11}$$

Using (3.9) screened potential

$$\tilde{V}(r) = \int \tilde{V}(q)\cos(qr)\,dq \tag{3.12}$$

has been found in the static case [11]. All energy values below are written in eV.

As it was mentioned above

- the value and character of $\Pi(q)$ essentially depends on the value Q, i.e. on the degree of band filling (fig.1);
- with band width increasing, at fixed μ, the area of q, where $\Re\mathrm{e}\Pi(q)$ and $\Im\mathrm{m}\Pi(q)$ differs from zero, is significantly restricted (fig.1; curve 4). Thus, in the limit $\beta \to \infty$, $\tilde{V}(r) \to V_0(r)$.
- $\varepsilon_1(q)$ and $\varepsilon_2(q)$ sharp extrema (fig.2, curves 1,2) correspond to singularities in $\Re\mathrm{e}\Pi(q)$ at $q = 2k_F$ and $q = 2(\pi - k_F)$.

Screened potential $\tilde{V}(r)$ at different band occupancy is depicted on figs.3,4 (for different $Q = (\beta - \mu)/\beta$ at fixed $\beta = 0.1$):

1. At $|Q| > 1$ ($\mu < 0$) screening is absent and $\tilde{V}(r)$ coincides with the bare potential $V_0(r)$ (3.7) (fig. 4) exhibits monotonous dependence on r.

2. At Q decreasing below unity $\tilde{V}(r)$ oscillates as it's shown in fig.4.

3. Further band filling ($Q < 0.91$ i.e. $\mu > 0.009$) is accompanied by reducing of $\tilde{V}(r)$ oscillations (fig. 4). Observing the behaviour, for instance, of the first left minimum $\tilde{V}(r)$ (value of the screened potential of two electrons interaction at the distance r, equals a lattice constant), we can see that with the Q decrease from unity (that corresponds to the decrease of β and/or the increase of the band filling) such minimum behaviour is nonmonotonous (fig. 3,4): at first it decreases sharply (at $0.9 < Q < 1$) and then increases changing nature of some extrema: minimum is changed to maximum or vice versa.

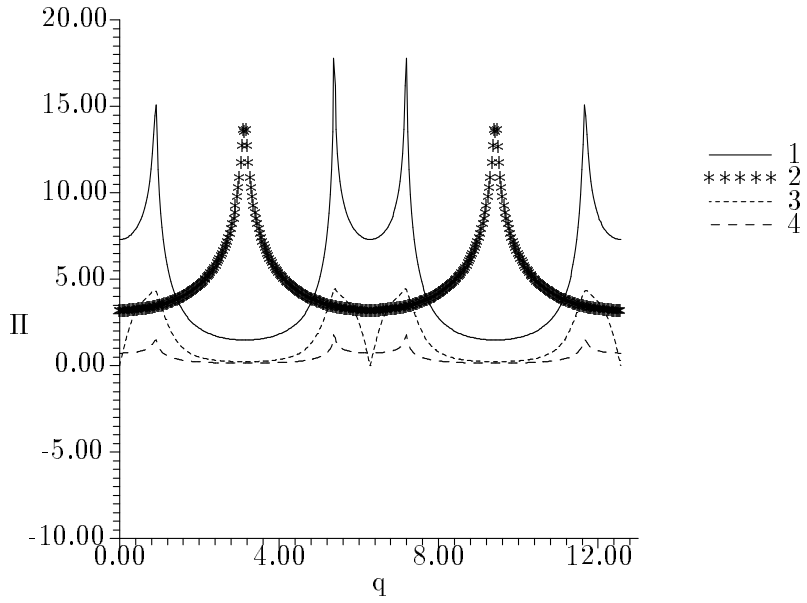


Figure 1. Dependence of $\Pi(q, \Omega)$ on q at fixed $\beta = 0.1$ (curves 1-3,5-6). 1). $\Re\mathrm{e}\Pi(q)$ at $Q = 0.9$; 2). $\Re\mathrm{e}\Pi(q)$ at $Q = 0$; 3). $\Im\mathrm{m}\Pi(q)$ at $Q = 0.9$; 4). $\Re\mathrm{e}\Pi(q)$ at $Q = 0.9$ and $\beta = 10$.

4. Conclusions

Interaction between electrons in 1D crystal with a narrow nonparabolic band leads to the oscillating sign-variable character of potential $\tilde{V}(r)$ depending on the interelectron distance. Physically it means, that depending on a distance such an interaction has different nature - attractive or repulsive. Similar $\tilde{V}(r)$ dependence on r (at large r) takes place for the ion-ion interaction at the considering of the indirect exchange "ion-electron-ion" (so-called Friedel oscillations [12]). It's significant to point out that in our

case oscillations of $\tilde{V}(r)$ are the result of the *direct* 1D electron-electron interaction.

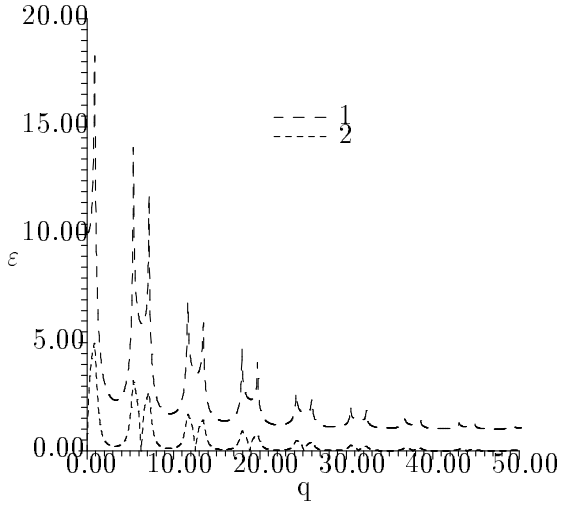


Figure 2. Dielectric function dependence on q at $\beta = 0.1$, $Q = 0.9$ $\varepsilon_1(q)$ (curve 1) and $\varepsilon_2(q)$ (curve 2).

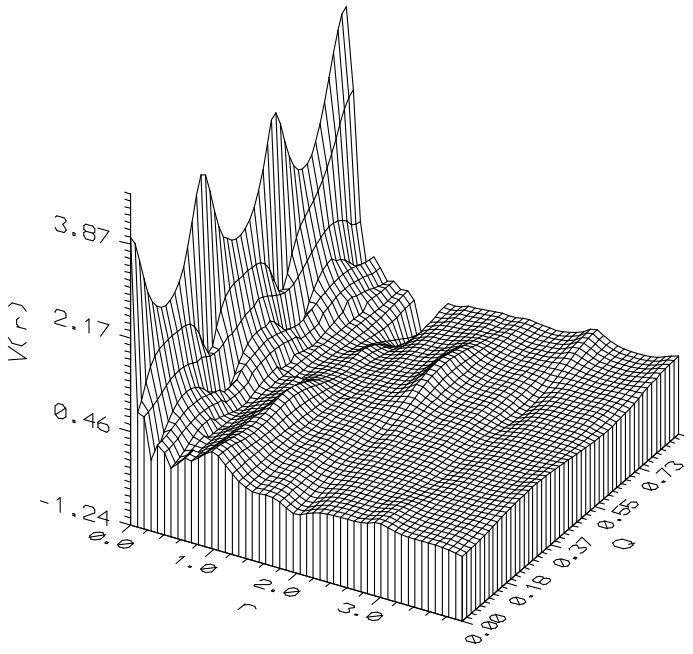


Figure 3. Dependence of a screened potential $\tilde{V}(r)$ on r at $\beta = 0.1$ and $0 < Q < 0.9$.

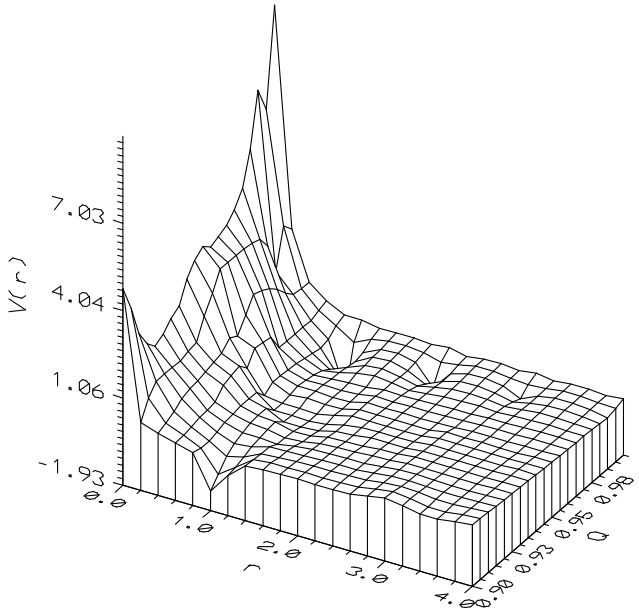


Figure 4. Dependence of a screened interelectron potential $\tilde{V}(r)$ on r at $\beta = 0.1$ and $0.9 < Q < 1$.

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ДО ЕКРАНУВАННЯ В НИЗЬКОРОЗМІРНИХ КРИСТАЛАХ

Б.А.Лукіянець, Н.К.Товстюк

На основі запропонованої діаграмної техніки для електронів в квантуючому магнітному полі проведений аналіз екранування потенціалу міжелектронної взаємодії в двох випадках. В першому в рамках наближення хаотичних фаз розглянуто фур'є-образ кулонівського потенціалу. Отримано, що він має осциляційний характер при зміні магнітного поля чи заповнення зони. В ультраквантовому випадку діагональна по квантових числах Ландау поляризаційна петля формально співпадає з аналогічною в одномірному випадку. В другому випадку в наближенні хаотичних фаз аналізується перенормування потенціалу електронної взаємодії в одномірних кристалах з вузькою зоною. Отримано, що при деяких умовах такий потенціал є осцилюючою знакозмінною функцією відстані між електронами.