LOCAL-FIELD CORRECTION FUNCTION OF THE FERMI SYSTEM WITH A SHORT-RANGE INTERACTION

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A model of fermion liquid with a short-range interaction potential which was simulated by the Yukawa repulsion potential was studied by the reference system approach. The local-field correction function of such model and its dependences on potential parameters have been studied. The difference between the local-field correction function in the case of the electron liquid and the model under consideration has been shown. The energy of the ground state and the stability region of such model have been calculated.

1. Introduction

The local-field conception holds a prior place in the modern electron liquid theory and the local-field correction function is believed to be the fundamental characteristic of any many-particle system with a local interaction potential. The local-field correction function was studied in detail for the electron liquid case [1, 2]. Up to the present, the investigation of this function for the case of a Coulomb repulsion potential cannot be considered to be completed. We do not know any investigation of the local-field correction function of many-particle system with a non-Coulomb interaction potential.

Being a functional over the interaction potential, the local-field correction function must possess the features, which are inherent to a particular physical system. But the local-field correction function of a degenerate Fermi system also must possess common features caused by Fermi surface. In this paper we want to investigate influence of the interaction potential on the local-field correction function and other model characteristics. We shall use the reference system approach for investigation a model with a non-Coulomb interaction potential between particles.

We consider the degenerate Fermi system model of \( N \) fermions with charge \( A_e \), which are located in a volume \( V \) with compensated background charge \(-\frac{A_e}{N}A_e\). We describe the interaction between particles and between particles and background charge by the Yukawa repulsion potential

\[
V(r_{ij}) = A^2 e^2 (r_{ij})^{-1} \exp[-\xi r_{ij}/a_0].
\]  

(1.1)

Here \( e \) is the charge of the electron, \( a_0 \) is the Bohr radius. Let us consider the thermodynamical limit \( N, V \to \infty, N/V = \text{const} \). The suggested potential has two parameters, which control the coupling strength and the
interaction range. $A^2$ is the interaction constant and $\xi$ defines the range of the potential. Such choice of the potential was caused, firstly, by our wish to have a look on the features of the nature of the electron liquid model with a general position, and secondly by possible use for the description of nuclear matter. The third parameter of the model is the particle mass $m$. A dimensionless coupling parameter of this model, defined as the ratio of the average potential energy of the particle to its kinetic energy, has the form

$$a = \left(\frac{3}{5} \frac{1}{\xi} \right)^{-1} \frac{1}{V} N \int dr V(r) \left[ g_2^{\text{int}}(r) - 1 \right] =$$

$$= \frac{20\pi A^2 e^2}{3\xi F} \frac{N}{V} R \int_0^R dr \exp \left[ -\xi r/a_0 \right] = \frac{10 A^2 r_s}{\eta^4 - m^* f(\xi^*)}, \quad (1.2)$$

$$f(\xi^*) = (\xi^*)^{-2} \{ 1 - [1 + \xi^*] \exp (-\xi^*) \}.$$  

Here $\xi_F = \frac{k_F^2}{2m}$ is the energy of a free particle on the Fermi surface, $m^* = m/m_0$ ($m_0$ is the mass of the electron), $g_2^{\text{int}}(r)$ is the pair distribution function of the ideal fermion system (without interaction) [3]. $R = k_F^{-1}$ is the correlation length of the degenerate ideal fermion system, $r_s = (3V/4\pi N)^{1/3} a_0^{-1}$ is the Wigner parameter, $\xi^* = \xi r_s/a_0$, where $\eta = (9\pi/4)^{1/3}$. Taking into account the asymptotic behavior of $f(\xi^*)$, one can see that the coupling parameter $\alpha$ changes from $10 A^2 r_s \eta^{-4}$ (at $\xi^* \to 0$) to $10 A^2 r_s \eta^{-4}(\xi^*)^{-2}$ (at $\xi^* \gg 1$). The electron liquid model is a limiting case of the model under consideration in the limit $A \to 1, \xi \to 0$. Its coupling parameter $r_s$ has statistical meaning and is to a certain extent formal. Varying the parameters $\lambda, \xi, m^*$, we can change the coupling parameter $\alpha$ in a wide region. For example, the weakly nonideal limit can be obtained in the different pathways

1) $r_s \to 0$: $A, \xi, m^* = \text{const}$;
2) $A \to 0$: $r_s, \xi, m^* = \text{const}$;
3) $\xi \to 0$: $A, r_s, m^* = \text{const}$. \quad (1.3)

The principal aim of our paper is to investigate the influence of the interaction potential on the local-field correction function and other model characteristics.

The local-field approximation in the electron liquid theory generalizes expressions, which occur in the random phase approximation, to systems with arbitrary value of the coupling parameter $r_s$. In general, the dynamic local-field correction function $G(x)$ can be defined by the generalization of two-particle correlation function $\mu_n^{\text{int}}(x, -x)$, which defines the pair distribution function

$$g_2(r) = 1 + \beta N(N - 1)^{-1} \sum_{\nu} \sum_{\nu \neq 0} \mu_2(x, -x) \exp (iqr), \quad (1.4)$$

where $\beta$ is the reciprocal temperature, $x = (q, \nu), q$ is the wave vector, $\nu$ is the Bose-Matsubara frequency [4], $r$ is the distance between two particles, and $N$ is the number of particles.

Substituting the Fourier-transform of the interaction potential (1.1) $V_q$ by the effective one $V_q[1 - G(x)]$, we obtain the pair correlation function in
the form

\[ \mu_2(x, -x) = \tilde{\mu}_2^0(x, -x)\{1 + \frac{V_0}{V} \tilde{\mu}_2^0(x, -x)[1 - G(x)]\}^{-1}. \]  \hfill (1.5)

Here as was already explained a p.1 \( \tilde{\mu}_2^0(x, -x) \) is the pair correlation of the ideal system function [5].

2. Local-field correction function of the model with short-range interaction potential

A set of integral equation for the local-field correction function \( G(x) \) of the electron liquid model has been obtained in [6]. The positive value of the Fourier-transform of the interaction potential has been applied in this procedure. Therefore, the equation set is valid for any potential, which satisfies the condition \( V_0 > 0 \),

\[
\begin{align*}
G(x) &= G_1(x) + G_2(x), \\
G_1(x) &= -(2\beta V_0)^{-1}[\tilde{\mu}_2^0(x, -x)]^{-2} \sum_{x_1} \left[V_0(x_1) - V_0 G_2(x_1) \right] \times \\
&\quad \times \tilde{\mu}_2^0(x, -x_1, -x_1), \\
G_2(x) &= (2\beta V_0)^{-1}[\tilde{\mu}_2^0(x, -x)]^{-2} \sum_{x_1} V_0(x_1 - x) \times \\
&\quad \times \left[V_0(x_1) - V_0 G_2(x_1) \right] \tilde{\mu}_3^0(x, x_1, -x_1 - x) \tilde{\mu}_2^0(-x, -x_1, x_1 + x).
\end{align*}
\hfill (2.1)
\]

Here \( \tilde{\mu}_2^0(\ldots) \) is the three-particle correlation function, \( \tilde{\mu}_4^0(\ldots) \) is the normal part of the four-particle one for the ideal Fermi system [5], \( x_1 = (q, \nu_1) \). They can be represented in terms of elementary functions in the case \( T = 0K \) (see [5, 7]). In (2.1) \( V_0(x) = V_0 [1 + \frac{V_0}{V} \tilde{\mu}_2^0(x, -x)]^{-1} \) is the screened interaction potential in the random phase approximation. As one can see from (2.1) the ratio \( G_2(x)G_1(x)^{-1} \) is proportional to \( \alpha \) in a weakly nonideal region (see (1.3)). Therefore, we can neglect the component \( G_2(x) \) in this region. Representing \( G_1(x) \) in the integral form, we obtain the following expression:

\[
G_1^{RPA}(x) = -4(4\pi)^{-1}[q^2 + (\xi^*)^2] I_{2,0}^0(q, \vec{p}/q) \times \\
\times \int_{q_1}^q dq_1 q_1^2 \int_0^{q_1} dq_1 \int_{-1}^{+1} dt I_{4,1}(q, q_1; \vec{p}/q, \vec{p}_1/q_1; t) \times \\
\times [q_1^2 + (\xi^*)^2 + 4A^2m^*r_s(\pi q_1)^{-1}I_{2,0}(q_1, \vec{p}_1/q_1)]^{-1}.
\]  \hfill (2.2)

The dimensionless variables \( q \equiv |q|/k_F, \ \vec{p} \equiv \nu/(2\varepsilon_F)^{-1}m^* \) and functions \( I_{2,0}(q, \vec{p}/q) = 2\varepsilon_F(3N)^{-1} \tilde{\mu}_2^0(x, -x), I_{4,1}(q, \ldots; t) = (3N)^{-1}(m^*)^{-3} \times (2\varepsilon_F)^3 \tilde{\mu}_4^0(x, -x_1, -x_1, -x_1) \) have been used. As one can see \( G_1^{RPA}(x) \) becomes the local-field correction function of the Fermi system in the limit \( r_s \to 0 \) and \( q, \xi = \text{const} \), which coincides with the local-field correction function of the ideal degenerate electron gas \( G_{id}^{RPA}(x) \) in the variables \( q, \vec{p} \) (figure 1).
This is a universal function, which does not depend on any parameters. It has the following asymptotic behavior:

\[
G^{EL}_{id}(x) = \begin{cases} 
\gamma(\bar{\nu})q^2 + \cdots & \text{for } q \ll 1, \\
1/3 + \cdots & \text{for } q \gg 1,
\end{cases}
\]  

(2.3)

where \(\gamma(\bar{\nu})\) is monotonic function of the dimensionless frequency \(\bar{\nu}\) [6, 8]. It decreases from 1/4 (at \(\bar{\nu} = 0\)) to 3/20 (at \(\bar{\nu} = \infty\)).

Figure 1. Dynamic local-field correction function of the electron liquid model \((\xi \rightarrow 0, A = 1)\) \(G^{EL}_{id}(q; \nu)\) (2.2) at \(r_s \to 0\).

Figure 2. Static local-field correction function \(G_{id}(q; 0)\) (2.2) in for different values of the parameter \(\xi^*\).

The function \(G_{id}(x)\) depends only on the parameter \(\xi^*\) in the limit \(A \to 0\), at \(r_s, \xi = \text{const}\). Let us use the representation (2.7) from [8] for \(\tilde{\rho}_{id}(x, -x, x_1, -x_1)\) to investigate the asymptotic behavior of \(G_{id}(x)\). We can obtain the following asymptotic for \(G_{id}(x)\) in the short-wavelength region:

\[
G_{id}(q, \bar{\nu}/q) = \frac{1}{2} [q^2 + (\xi^*)^2]^{-2} \times 
\left\{ \frac{1 - D(\xi^*) + 2D(\xi^*) \bar{\nu}^2}{(\bar{\nu}/q)^2 + q^2/4} \right\}
\]

(2.4)

at \(q \geq 4, \bar{\nu} \geq 2q\), where

\[
D(\xi^*) = \frac{1}{3} - \frac{3}{4} (\xi^*)^2 + \frac{1}{8} (\xi^*)^4 + (\xi^*)^3 \arctan \frac{2}{\xi^*} - 
\frac{3}{8} (\xi^*)^4 \left[ 1 + \frac{1}{12}(\xi^*)^2 \right] \ln \left[ 1 + \frac{4}{(\xi^*)^2} \right],
\]

(2.5)
and

$$G_{i,d}(q; 0) = C_0(\xi^*) + C_2(\xi^*) \frac{q^2}{2} + \cdots,$$

$$G_{i,d}(p; q) = B_0(\xi^*) + B_2(\xi^*) \frac{q^2}{2} + \cdots, \quad p \gg q,$$

$$C_0(\xi^*) = \frac{1}{4}(\xi^*)^2 \left(1 - \frac{(\xi^*)^2}{4} \ln \left[1 + \frac{4}{(\xi^*)^2}\right]\right),$$

$$B_0(\xi^*) = \frac{3}{20}(\xi^*)^2 \left(1 - (\xi^*)^2 + \frac{(\xi^*)^2}{4}[1 + (\xi^*)^2] \ln \left[1 + \frac{4}{(\xi^*)^2}\right]\right)$$

in the long-wavelength region. As one can see from (2.4), (2.7) the long-wavelength region asymptote changes from 0 to 1/2, when $\xi^*$ changes from zero to infinity and the short-wave one from 1/3 to 1/2. The function $G_{i,d}(x)$ changes very essentially near the point $|q| = 2k_F$. All features of $G_{i,d}(q; 0)$ are depicted in figure 2.

As one can see from the asymptotes (2.3) - (2.7) the behavior of the local-field correction function is defined by the effective range of the interaction between particles $R_0 = \xi^{-1} a_0$ in the long-wavelength region. The local-field correction function for any short-range potential has a finite value at $q = 0$, which rises, when the parameter $\xi^*$ rises. The asymptote $\gamma(p)q^2 + \cdots$ occurs only in the Coulomb potential limit ($R_0 = \infty$, $C_0(\xi^*) = 0$). In this way, the local-field correction function of the system with the short-range interaction potential is more important than the one of the Coulomb system.

Approximations $G_{i,d}(x)$ and $G_{i,d}^{EL}(x)$ correspond to the result of [9], in which, for the first time, the dynamic local-field correction function of the electron-liquid model $G_{i,d}^{EL}(q, \omega)$ in terms of $(q, \omega)$, where $\omega$ is the Heisenberg frequency, has been investigated. As a function of $\omega$ the expression $G_{i,d}^{EL}(q, \omega)$ has strong singularities. In the terms of $(q, \nu)$ the function $G_{i,d}(x)$ has no singularities. This is convenient for its further use.

Taking into account the existence of extreme of the functions $\tilde{\mu}_0^0(x, x_1, \ldots, x_i, x_i)$ and $\tilde{\mu}_{4,1}^0(x, \ldots, x_1, -x_i)$ near the surface $x = x_1$, we can calculate the local-field correction function in the region of middle and strong nonideality [8]. Using the mean-value theorem of the integral, we obtain the approximate solution of the set (2.1),

$$G_i(x) \approx G_i^{RPA}(x) \left[1 + G_{2,RPA}(x)\right]^{-1}, \quad i = 1, 2,$$

$G_{1,RPA}(x)$ is computed by (2.2),

$$G_{2,RPA}(x) = [q^2 + (\xi^*)^2 + \xi^*/4] \frac{r_s m^* (\pi^2 q)^{-1}}{[2I_{2,0}(q, u)]^{-2} A^2} \times$$

$$\times \int_{-\infty}^{+\infty} du \int_{-\infty}^{+\infty} dq \int_0^1 dt \, P(q_1; u_1)P(q_2; u_2)I_{3,0}(q, q_1; u, u_1; t),$$

where $u_1 = p_1/q_1$, $u = p/q$, $q_2 = [q^2 + q_1^2 + 2q_1 q t]^{1/2}$, $u_2 = q_2^{-1}[p + p_1]$, $P(q; u) = [q^2 + (\xi^*)^2 + 4A^2 r_s m^* (\pi^2 q)^{-1} I_{2,0}(q, u)]^{-1}$, $I_{3,0}(q, q_1; u, u_1; t) = (2k_F)^2 (3N)^{-1} (m^*)^{-2} \tilde{\mu}_0^0 (x, x_1, x_{i,1}, -x, -x_i)$.

Functions $\tilde{\mu}_0^0 (x, x_1, \ldots, x_i)$ and $\tilde{\mu}_{4,1}^0(x, \ldots, x_1, -x_i)$ in terms of $(q, \nu)$ do not have not singularities, therefore for the calculation of (2.2) and (2.9) standard numerical methods of integral calculation may be used.

The results of the local-field correction function calculation in the approximation (2.2), (2.8), (2.9) are depicted in figures 3, 4. When the parameter
A changes, \( G(x) \) changes weakly in the region \( 0 \leq |q| \leq 2k_F \), but a strong dependence is noticed in the region \( |q| > 2k_F \). The increase of the local-field correction function with increasing \( A \) is similar to the dependence of the electron liquid local-field correction function on the parameter \( r_s \) [7]. The dependence of \( G(x) \) on the parameter \( \xi \) at \( A, r_s, \tilde{\nu} = \text{const} \) is presented in figure 3. As one can see \( G(x) \) weakly depends on the parameter \( \xi \) in the short-wavelength region. The range \( R_0 \) has a strong influence on the local-field correction function in the region of small and medium wave vectors. The dependence of \( G(x) \) on the parameter \( r_s \) at \( \xi = \text{const} \) is depicted in figure 4. The behavior of \( G(x) \) is very similar to the electron liquid local field correction function in the region \( q > 2k_F \). Comparing \( G^{EL}(x) \) with \( G(x) \) of our model, we notice that in the region \( q \leq 2k_F \), \( G^{EL}(x) \) and \( G(x) \) are very different, \( G(x) \) has the following asymptotic behavior:

\[
G(x) \rightarrow \begin{cases} 
\alpha(\xi^*, r_s, \tilde{\nu})[q^2 + (\xi^*)^2] + \cdots & \text{for } q \ll 1, \\
G_{\infty}(A, r_s, \xi^*) + \cdots & \text{for } q \gg 1.
\end{cases} \tag{2.10}
\]

![Figure 3](image3.png)

Figure 3. The dependence of the dynamic local-field correction function \( G(x) \) on the parameter \( \xi \) in the approximation (2.8), (2.9) at \( A = 1, r_s = 1, u = 1 \).

![Figure 4](image4.png)

Figure 4. The dependence of the dynamic local-field correction function \( G(x) \) on the parameter \( r_s \) in the approximation (2.8), (2.9) \( r_s \) has the values 0.0; 0.1; 0.5; 1.0; 2.0; 3.0; 4.0; 5.0; 7.0; 10.0) at \( A = 1.0, \xi = 0.25, u = 1.0 \).

3. **Ground state energy of the model**

As is known, the local-field correction function defines the integral and local characteristics of the system with a local two-particle interaction. In accordance with (1.5), the ground state energy expression has the form

\[
E = E_0 + \lim_{\beta \to \infty} \sum_{q \neq 0} \sum_{n} \int_{0}^{1} \frac{d\lambda}{\lambda} V_0^\lambda \hat{\mu}_2^n(x, -x) \times
\]

\[
\times \left\{ 1 + \frac{V_0^\lambda}{\lambda} \hat{\mu}_0^n(x, -x)[1 - G_\lambda(x)] \right\}^{-1},
\]
where \( Y^3_0 \) and \( G_\lambda(x) \) depend on the coupling parameter \( \lambda A^2 \), \( E_0 \) is the ground state energy of the ideal system. Extracting the ideal correlation contribution, we can represent the total energy in the traditional dimensionless form:

\[
E = N \left[ R_y \varepsilon(r_s, A, \xi) + \varepsilon_{HF}(r_s, A, \xi) + \varepsilon_c(r_s, A, \xi) \right],
\]

where \( \varepsilon_0(r_s) = 3/5\eta^2 r_s^{-2}(m^*)^{-1} \) is the ideal system energy at \( T = 0 \) K in \( R_y \) per particle,

\[
\varepsilon_{HF}(r_s, A, \xi) = -2\lambda A^2 \eta^2 \frac{m^*}{r_s} \int_0^\infty dq \int_0^\infty du \int_0^r \frac{r_s}{r^2} I_{2,0}(q, u) \times \\
\left( 1 - G(q, u) \right) \left[ q^2 + (\xi^*)^2 \right]^{-\frac{1}{2}} \left( 1 + \frac{4}{(\xi^*)^2} \right) - 1 \right] 
\]

is the Hartree-Fock energy contribution,

\[
\varepsilon_c(r_s, A, \xi) = -2\lambda A^2 \eta^2 \frac{m^*}{r_s} \int_0^\infty dq \int_0^\infty du \int_0^r \frac{r_s}{r^2} I_{2,0}(q, u) \times \\
\left( 1 - G(q, u) \right) \left[ q^2 + (\xi^*)^2 \right]^{-\frac{1}{2}} \left( 1 + \frac{4}{(\xi^*)^2} \right) - 1 \right] 
\]

is the correlation energy. The function \( G(q, u) \) depends on the parameter \( r_s \equiv \lambda r_s \) in (3.4) (but \( \xi^* \equiv \xi r_s / \eta \)). The Hartree-Fock energy contribution has the following asymptote:

\[
\varepsilon_{HF}(r_s, A, \xi) \to - \frac{2\lambda A^2 \eta}{\pi r_s} \left\{ \frac{1}{2} \right\} \frac{1}{\xi} \left( \frac{1}{\xi^*} \right)^2 \text{ for } \xi \to 0, \\
\varepsilon_{HF}(r_s, A, \xi) \to - \frac{2\lambda A^2 \eta}{\pi r_s} \left\{ \frac{1}{2} \right\} \frac{1}{\xi} \left( \frac{1}{\xi^*} \right)^2 \text{ for } \xi \to \infty.
\]

The correlation energy \( \varepsilon_c \) has been computed by numerical method in a wide region of its parameters. The dependence of the total energy on the parameters \( r_s \) and \( \xi \) is depicted figure 5. The total energy increases with the rise of the parameter \( \xi \) at fixed value of \( r_s \). The stability region also decreases, when the total energy is negative. The curve

\[
\varepsilon(r_s, 1, \xi) = 0
\]

is depicted in figure 6 as a solid line (curve 1). The shaded part of the picture corresponds to \( \varepsilon(r_s, 1, \xi) > 0 \) and the unshaded part (below curve 1) corresponds to \( \varepsilon(r_s, 1, \xi) < 0 \). The solid line defines the particle equilibrium density in the system with minimum of the total energy (at a given magnitude of the parameter \( \xi \)) (curve 2),

\[
\frac{d}{dr_s} \varepsilon(r_s, 1, \xi) = 0.
\]
4. Conclusion

The local-field approximation is one of the most significant achievements in the electron liquid theory during the last decades and the local-field correction function is one of many universal characteristics of the model. The generalized Fermi-system model with the interaction described by the Yukawa repulsion potential has been proposed. On the basis of this model the dependence of the local-field correction function on the interaction range of the potential $R$ has been investigated. As one can see from fig. 2-4, the local field correction function in such a model has a behavior different from the one for the electron liquid model. Especially the region $0 < q < 2k_F$ is important, where the Fourier-transform of the potential $V_q$ is large. On the basis of the computation we may assert that the local field correction function in the model with a short-range interaction potential is always larger than the model with the Coulomb potential in the region of small and medium values of the wave vector $q$. This fact shows the relative importance of the short-range part of the interaction potential for the system with a finite value of the interaction range.

As is known, the electron liquid model is stable, has negative total energy in the region $r_s > 2.0$, and has the equilibrium density at $n^e_0 = 4.1825 \ldots$ which corresponds to the minimum of the total energy (~ 0.15533 Ry per electron). As one can see from fig. 5 the total energy of the generalized model in the ground state is smaller than that for the electron-liquid model for any value of the parameter $\xi$ at the same value of the parameter $r_s$. Every value of $r_s$ in the generalized model has been proved to correspond to a critical range of interaction $R_c(r_s) = a_0 q^{-1}(r_s)$. If the potential range is less than $R_c$, the correlation effects which have the range $R_F = k_F^{-1}$ cannot provide the stability of the model and a negative value of the total energy. Qualitative conclusions concerning the influence of the range of the interaction potential between particles on the character of the local-field correction function and the stability are valid not only for a model with the
Yukawa potential but for any Fermi system with an arbitrary short-range potential.

The consideration of the represented model, firstly, has heuristic importance, and secondly, the model with a short-range interaction potential can be used as a reference system for the description of neutral fermion systems at $\xi \neq 0$. In this case the term $V(\mathbf{q} = 0)$ must be added to the expression of the total energy (3.2), and its coupling parameter will have the form

$$
\alpha' = \left( \frac{3}{5} \varepsilon_F \right)^{-1} \frac{N}{V} \int d\mathbf{r}' V(\mathbf{r}) g^d_2(\mathbf{r}') = \frac{10A^2}{\eta^4} r_s m^* f(\xi^*),
$$

$$
f'(\xi^*) = \left\{ 2(\xi^*)^{-2} - (1 + \xi^*) \exp \left( -\xi^* \right) \right\}.
$$

References


ПОПРАВКА НА ЛОКАЛЬНЕ ПОЛЕ МОДЕЛІ
ФЕРМІ-СИСТЕМ З КОРОТКОСЯЖНОЮ ВЗАЄМНОСТЮ

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В рамках базисного підходу досліджено динамічну поправку на локальне поле для узагальненої моделі фермі-рідини з короткосяжною взаємодією відштовхування, яка моделюється потенціалом Юкави. Вивчено особливості цієї функції в залежності від параметра неідентичності та радіуса дії потенціалу, а також її відмінності від поправки на локальне поле моделі електронної рідини. На цій основі розраховано енергію основного стану узагальненої моделі та визначено область термодинамічної стабільності як функцію зазначених параметрів.