

# CALCULATION OF THE COLLECTIVE EXCITATIONS SPECTRUM FOR THE ELECTRON LIQUID MODEL IN THE LOCAL-FIELD APPROXIMATION

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Within the reference system approach a method of calculation of plasmons excitations spectrum for the electron liquid model is proposed. It was made by transition from Matsubara's frequency representation to Heisenberg's one and to the mixed representation for the many-particle dynamical correlation functions of the reference system (ideal degenerated electron system) and for the dynamical local field correction. For the ground state of model the plasmon dispersion curves are investigated in the wide region of the coupling parameter  $r_s$ .

## Introduction

The local-field correction function for the electron liquid model was investigated for the first time in the papers [1-3]. It was done in the terms of reference system approach in the variables  $(\mathbf{q}, \nu)$ , where  $\mathbf{q}$  is the wave-vector and  $\nu = 2\pi n\beta^{-1}$  is the Bose-Matsubara frequency [4]. The local-field correction  $G(\mathbf{q}, \nu)$  in these variables has no any singularities at all which makes it very convenient for the calculations of different thermodynamic and structural characteristics [1, 2]. However, the mentioned approach makes also possible the investigation of dynamical characteristics. One of them is the spectrum of collective excitations - plasmons  $\omega = \omega(\mathbf{q})$  which, as usual, is obtained as the root of equation

$$\varepsilon(\mathbf{q}, \hbar\omega) = 0, \quad (0.1)$$

where  $\varepsilon(\mathbf{q}, \hbar\omega)$  is the dielectric function in ordinary Heisenberg representation (see [5, 6]).

## 1. The reference system correlation functions in $(\mathbf{q}, \omega)$ variables

It is well known [4] that for the transition from thermodynamical perturbation theory to dynamical it is sufficient to make the substitution of Matsuba-

ra's frequencies  $\nu$  by  $i\hbar\omega - \delta$  in the expressions for the corresponding characteristics. As a result of such substitution we obtain

$$\begin{aligned}\varepsilon(x) &\Longrightarrow \varepsilon(\mathbf{q}, \hbar\omega); \\ \varepsilon(\mathbf{q}, \hbar\omega) &= 1 + V_q V^{-1} \tilde{\mu}_2^0(\mathbf{q}, \hbar\omega) \cdot [1 - V_q V^{-1} \tilde{\mu}_2^0(\mathbf{q}, \hbar\omega) G(\mathbf{q}, \hbar\omega)]^{-1}; \\ \tilde{\mu}_2^0(x, -x) &\Longrightarrow \tilde{\mu}_2^0(\mathbf{q}, \hbar\omega), \quad G(x) \Longrightarrow G(\mathbf{q}, \hbar\omega).\end{aligned}\quad (1.1)$$

Here  $\tilde{\mu}_2^0(x, -x)$  is the pair correlation function of the reference system (noninteracting electron gas),  $x \equiv (\mathbf{q}, \nu)$ ,  $G(x)$  is the local-field correction function of electron liquid,  $V_q \equiv 4\pi e^2 q^{-2}$ ,  $V$  - volume. In this case equation (0.1) takes the form:

$$1 + V_q V^{-1} \tilde{\mu}_2^0(\mathbf{q}, \hbar\omega) \cdot [1 - G(\mathbf{q}, \hbar\omega)] = 0. \quad (1.2)$$

The calculation of  $\tilde{\mu}_2^0(\mathbf{q}, \hbar\omega)$  can be made without any difficulties:

$$\begin{aligned}\tilde{\mu}_2^0(x, -x) &= - \sum_{\mathbf{k}, s} n_{\mathbf{k}, s}^0 \sum_{\sigma=\pm 1} [\sigma i\nu + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}]^{-1}, \\ \tilde{\mu}_2^0(\mathbf{q}, \hbar\omega) &= - \sum_{\mathbf{k}, s} n_{\mathbf{k}, s}^0 \sum_{\sigma=\pm 1} [\sigma(\hbar\omega + i\delta) + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}]^{-1},\end{aligned}\quad (1.3)$$

at  $\delta \rightarrow 0$ . Now the function  $\tilde{\mu}_2^0(\mathbf{q}, \hbar\omega)$  has the real and imaginary components which determine the real and imaginary components of dielectric function in the random phase approximation (RPA). It is a common observation that the imaginary component of this function tends to zero at high frequencies. On account of this we shall neglect the imaginary components both of  $\tilde{\mu}_2^0(\mathbf{q}, \hbar\omega)$  and the correlation functions of higher order in the problem of the plasmon spectrum calculation. In the case of absolute zero of the temperature for the real component of  $\tilde{\mu}_2^0(\mathbf{q}, \hbar\omega)$  we obtain

$$\begin{aligned}\tilde{\mu}_2^0(\mathbf{q}, \hbar\omega) &= 3N(2\varepsilon_F)^{-1} f(\mathbf{q}, \tilde{\omega}), \\ 2f(\mathbf{q}, \tilde{\omega}) &= 1 + (2q)^{-1} \sum_{\sigma=\pm 1} \left[1 - \left(q + \frac{\sigma}{q}\tilde{\omega}\right)^2 / 4\right] \times \\ &\times \ln \left| \left[1 + \left(q + \frac{\sigma}{q}\tilde{\omega}\right)^2 / 2\right] / \left[1 - \left(q + \frac{\sigma}{q}\tilde{\omega}\right)^2 / 2\right] \right|.\end{aligned}\quad (1.4)$$

Here the dimensionless variables are used:  $q \equiv |\mathbf{q}|k_F^{-1}$ ,  $\tilde{\omega} = \hbar\omega/\varepsilon_F = \omega/\omega_F$ ,  $k_F$  and  $\varepsilon_F$  are Fermi impulse and energy correspondingly, and  $N$  is the number of electrons. The function (1.4) has the following long-wave asymptotics

$$\begin{aligned}\tilde{\mu}_2^0(\mathbf{q}, \hbar\omega) &= -\frac{2N}{\varepsilon_F} \cdot \frac{q^2}{\tilde{\omega}_q^2 - q^4} \cdot \left[1 + \frac{12}{5} \cdot \frac{q^2}{\tilde{\omega}_q^2 - q^4} + \right. \\ &\left. + \frac{16q^4}{(\tilde{\omega}_q^2 - q^4)^2} (3/7 + q^2/5 + \dots)\right],\end{aligned}\quad (1.5)$$

which become useful for the investigation of spectrum at small  $q$  region. The calculation of high order correlation functions can be made as before. So the third order correlation function in the variables  $(\mathbf{q}, \nu)$  takes the following form

$$\tilde{\mu}_3^0(x_1, x_2, x_3) = \delta_{x_1+x_2+x_3, 0} \{\gamma_3(x_1, -x_2) + \gamma_3(x_2, -x_3) + \gamma_3(x_3, -x_1)\}. \quad (1.6)$$

After the transition to the mixed frequency representation for the real component of function  $\gamma_3(x_1, x_2)$  at  $\nu_1 = i\hbar\omega - \delta$  we obtain

$$\begin{aligned} \gamma_3(\mathbf{q}_1, \mathbf{q}_2 | \hbar\omega, \nu_2) = & -\frac{3N}{(2\varepsilon_F)^2} [q_1, q_2(1-t^2)]^{-1} \times \quad (1.7) \\ & \times \left\{ \sum_{\sigma=\pm 1} \int_0^1 d\alpha [A_\sigma^{(1)} B_\sigma^{(1)} - A_\sigma^{(2)} B_\sigma^{(2)}] [(A_\sigma^{(1)})^2 + (A_\sigma^{(2)})^2]^{-1} + \right. \\ & + \frac{1}{4} \sum_{\sigma=\pm 1} \left[ q_2 - t \left( q_1 - \sigma \frac{\tilde{\omega}}{q_1} \right) \right] \ln \left| \frac{1 + \left( q_1 + \sigma \frac{\tilde{\omega}}{q_1} \right) / 2}{1 - \left( q_1 + \sigma \frac{\tilde{\omega}}{q_1} \right) / 2} \right| + \\ & + \frac{1}{8} \sum_{\sigma=\pm 1} \left[ q_1 + \sigma \frac{\tilde{\omega}}{q_1} - tq_2 \right] \ln \left| \frac{u_2^2 + (1 + q_2/2)^2}{u_2^2 + (1 - q_2/2)^2} \right| - \\ & \left. - tu_2 \left[ \arctan \frac{1 + q_2/2}{u_2} + \arctan \frac{1 - q_2/2}{u_2} \right] \right\}. \end{aligned}$$

Here the following notation are used

$$\begin{aligned} A_\sigma^{(1)} &= \rho^2 - \frac{1}{4} \left[ (1 - \alpha)q_2 + \alpha \left( q_1 + \sigma \frac{\tilde{\omega}}{q_1} \right)^2 \right] + u_2^2(1 - \alpha)^2, \\ A_\sigma^{(2)} &= u_2(1 - \alpha) \left[ (1 - \alpha)q_2 + \alpha \left( q_1 + \sigma \frac{\tilde{\omega}}{q_1} \right) \right], \quad (1.8) \\ B_\sigma^{(1)} &= t^2 - 1 + \frac{1}{4} \left( q_1 + \sigma \frac{\tilde{\omega}}{q_1} \right)^2 + \frac{1}{4} q_2^2 - \frac{1}{2} q_2 t \left( q_1 + \sigma \frac{\tilde{\omega}}{q_1} \right) - u_2^2, \\ B_\sigma^{(2)} &= u_2 \left[ q_2 - t \left( q_1 + \sigma \frac{\tilde{\omega}}{q_1} \right) \right], \quad u_2 = \nu_2 (2q_2 \cdot \varepsilon_F)^{-1}, \\ \rho^2 &= 1 - \alpha(1 - t) + 2\alpha^2(1 - t), \quad t = \cosh(\mathbf{q}_1, \mathbf{q}_2). \end{aligned}$$

## 2. The local-field correction function in $(\mathbf{q}, \omega)$ variables

The most direct way to obtain the local-field correction  $G(\mathbf{q}, \nu)$  consists in performing the substitution  $\nu \rightarrow i\hbar\omega(2\varepsilon_F)^{-1} - \delta$  in the integral representation or in equations for the function  $G(\mathbf{q}, \nu)$  [1-3]. The second way of investigation is approximate but too simple. For the well known asymptotics of function  $G(\mathbf{q}, u)$  an approximate analytical representation for not large values of  $q$  may be written

$$G(\mathbf{q}, u) = \sum_{n=1}^{m_0} q^{2n} \cdot \gamma_m(u^2 | r_s). \quad (2.1)$$

Functions  $\gamma_m(u^2 | r_s)$  are taken in the form of Pade-approximation:

$$\gamma_m(u^2 | r_s) = \sum_{k=0}^m a_{mk}(r_s) u^{2k} \left[ \sum_{n=0}^m b_{mn}(r_s) u^{2n} \right]^{-1}, \quad (2.2)$$

and coefficients  $a_{mk}(r_s), b_{mn}(r_s)$  are obtained on the base of numerical calculation of  $G(\mathbf{q}, u)$ . Carrying out the substitution  $u^2 \rightarrow [\hbar\omega(2\varepsilon_F \cdot q)^{-1}]^2$  we

obtain an approximate representation for the local-field correction function in  $(\mathbf{q}, \omega)$  variables. It is useful for the analytical investigation of the plasmon spectrum asymptotics in the small wave-vectors region.

To simplify the calculations of  $G(\mathbf{q}, \omega)$  it is very useful the frequency over which the summation must be taken to be left the Matsubara's one. For example for the weakly nonideal system ( $r_s \rightarrow 0$ ) we used an integral representation for  $G_{id}(\mathbf{q}, \nu)$  of paper [1]. Carrying out here the mentioned frequency substitution we obtain the following representation

$$G_{id}(\mathbf{q}, \hbar\omega) = \frac{q^2}{4} f^{-2}(\mathbf{q}, \tilde{\omega}) \int_{-1}^{+1} \int_{-1}^{+1} dz_1 dz_2 \sum_{\sigma_1, \sigma_2 = \pm 1} \sigma_1 \sigma_2 \times$$

$$\times \Phi_{\mathbf{q}, \tilde{\omega}}(z_1 + \sigma_1 q/2; z_2 + \sigma_2 q/2; 1 - z_1^2; 1 - z_2^2), \quad (2.3)$$

$$\Phi_{\mathbf{q}, \tilde{\omega}}(a; b; w; v) = \frac{q^2}{8} (a - b) J(s^2; w; v) (b^2 q^2 - \tilde{\omega}^2/4)^{-1} \times$$

$$\times [q^2 a^2 b + (2a + b)\tilde{\omega}^2/4] (a^2 q^2 - \tilde{\omega}^2/4)^{-2}.$$

In the region of intermediate nonideality the local field correction function is approximately determined by formulae (2.1) in which [1] the substitution  $s^2 = (a - b)^2 + 4\pi\alpha_s \zeta(r_s)$  must be made. Here  $\zeta(r_s)$  is the dimensionless function of the nonideality parameter  $r_s$  and takes the value close to 0.5;  $\alpha_s = e^2 k_F (2\pi\epsilon_F)^{-1} \simeq 0.0628 r_s$ .

### 3. Dispersion coefficient of plasmons

We shall confine the analytical investigation of the long-wave plasmon spectrum limit to the weakly nonideal systems approximation, using  $G_1(\mathbf{q}, \hbar\omega)$  and  $G_1^{RPA}(\mathbf{q}, \hbar\omega)$  as a local field correction. At the mentioned limit the solution of equation (1.2), as usual, we represent in the following form

$$\omega_q = \omega_p + 2\alpha\omega_F q^2, \quad (3.1)$$

where  $\omega_p = [4\pi N e^2 / mV]^{1/2}$  is the so called plasmons frequency,  $\omega_F = \epsilon_F / \hbar$ , and  $\alpha$  is the plasmons dispersion coefficient. Using formulae (1.5) and (2.1) one may obtain the following relation:

$$\frac{\alpha}{\alpha_{RPA}} = 1 - \frac{5}{12} \left( \frac{\omega_p}{\omega_F} \right)^2 \gamma_2 \left( -\frac{\omega_p^2}{4\omega_F^2 q^2} \mid r_s \right). \quad (3.2)$$

Here  $\alpha_{RPA} = \frac{3}{5}\omega_F/\omega_p$  is plasmons dispersion coefficient calculated in RPA.

Dependence of the ratio  $\alpha/\alpha_{RPA}$  on coupling parameter  $r_s$  is the important characteristic being considered by many authors. There are many experimental papers where this characteristic has been studied (see [7] where  $\alpha/\alpha_{RPA}$  for the metals *Be, Mg, Ba, Li, Na, K* was considered). As far as  $(\omega_p/2\omega_F)^2 = 4r_s(3\pi\eta)^{-1}$  and  $\eta = (9\pi/4)^{1/3}$  in the static approximation of local field correction we obtain

$$\gamma_2 \left( -\frac{\omega_p^2}{4\omega_F^2 q^2} \mid r_s \right) \Rightarrow \gamma_2(0|0) = \frac{1}{4}. \quad (3.3)$$

This formally corresponds to the weakly nonideal system ( $r_s \rightarrow 0$ ) and the relationship

$$\frac{\alpha}{\alpha_{RPA}} = 1 - \frac{5}{9\pi\eta} r_s \quad (3.4)$$

has been obtained in [8] for the first time. Taking a formal limit  $\gamma_2(\infty|0) = 3/20$  which corresponds to great frequencies and weakly nonideal system we have a result

$$\frac{\alpha}{\alpha_{RPA}} = 1 - \frac{1}{3\pi\eta} r_s, \quad (3.5)$$

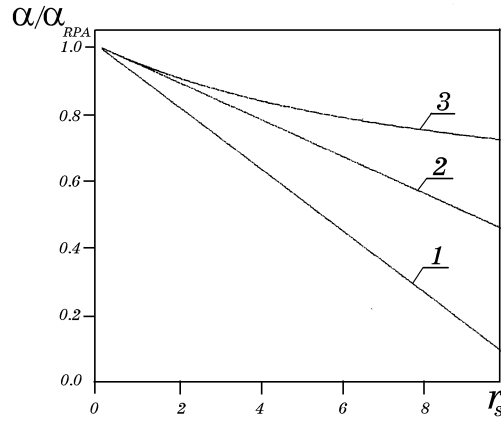


Figure 1.

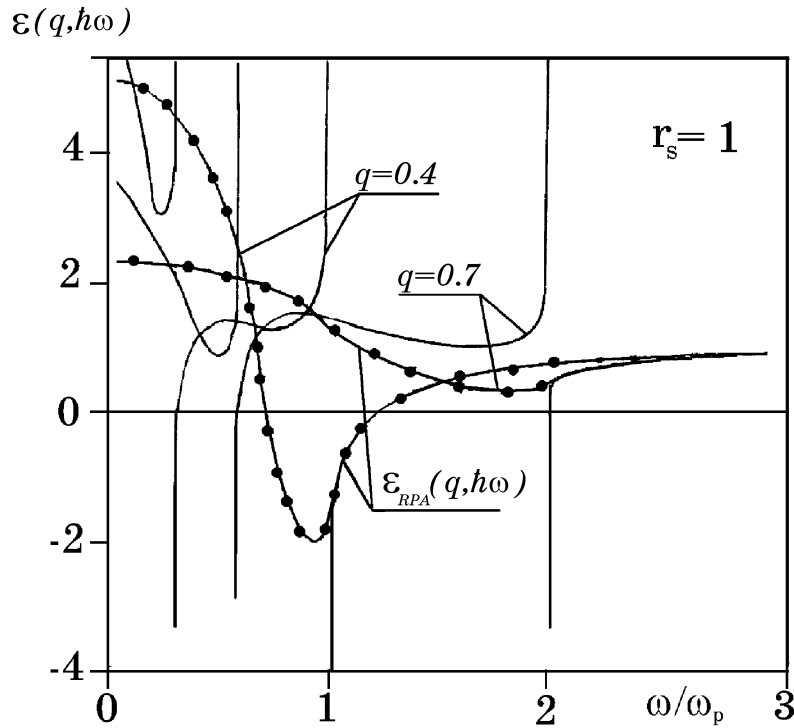


Figure 2.

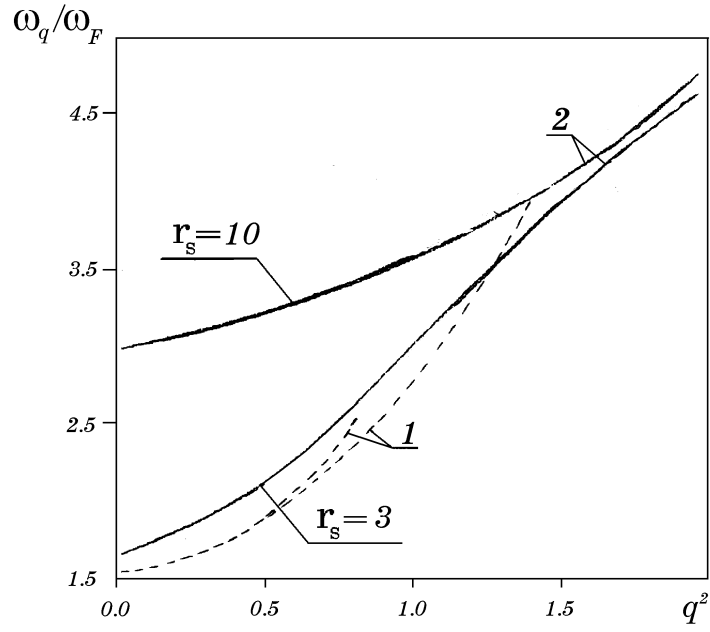


Figure 3.

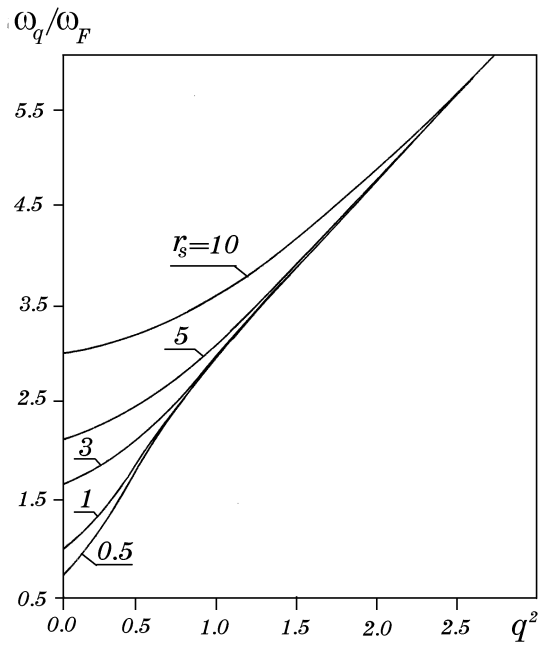


Figure 4.

which was obtained for the first time in the paper [9]. The relation-

ships (3.4) and (3.5) represent the limiting cases of (3.2) and show the linear dependence  $\alpha/\alpha_{RPA}$  on  $r_s$ , presented in the figure 1 (curve 1 and 2 correspondingly). Actually at the finite values of  $r_s$  we have nonlinear dependence approximately defined by the function

$$\gamma_2(\infty|r_s) = \frac{3}{20} \left\{ 1 - Q^2 + \frac{Q^2}{4} (1 + Q^2) \ln[1 + 4/Q^2] \right\}. \quad (3.6)$$

which corresponds to the longwave limit (curve 3);  $Q^2 = 4r_s\zeta(r_s)(\pi\eta)^{-1}$ . In this approximation we obtain the following asymptotics

$$\frac{\alpha}{\alpha_{RPA}} = \begin{cases} 1 - \frac{r_s}{4\pi\eta} \left[ 1 - \frac{r_s\zeta(r_s)}{\pi\eta} \ln \frac{\pi\eta}{r_s\zeta(r_s)} + \dots \right], & r_s \ll 1; \\ 1 - \frac{5}{18\zeta(r_s)} + \dots & r_s \gg 1. \end{cases} \quad (3.7)$$

#### 4. Calculation of plasmon spectrum

In contrast to  $G_{id}(\mathbf{q}, \nu)$ , function  $G_{id}(\mathbf{q}, \hbar\omega)$  is not a smooth function of frequency because it has first order poles. The numerical calculation of this function by its integral representation or especially as its analytical approximation makes up a pronounced mathematical difficulties.

The dielectric function  $\varepsilon(\mathbf{q}, \hbar\omega)$  calculated in different approximations (RPA and  $G_1(\mathbf{q}, \hbar\omega)$ ) as a function of variable  $\omega/\omega_p$  at the given values of wavevector  $q = 0.4, q = 0.7$  for the case  $r_s = 1$  is presented in figure 2. As it is visible the equation  $\varepsilon(\mathbf{q}, \hbar\omega) = 0$  has two real roots at not great values of  $q$ . Curve  $\varepsilon(\mathbf{q}, \hbar\omega)$  calculated in  $G_{id}(\mathbf{q}, \hbar\omega)$  approximation has a complicated form and the function  $\varepsilon(\mathbf{q}, \hbar\omega)$  has a pole near to its greatest zero. The high – frequency (plasmon) branch of the spectrum calculated in RPA exists only at nongreat values of  $q$ . At the same time in  $G_{id}(\mathbf{q}, \hbar\omega)$  or  $G_{id}^{RPA}(\mathbf{q}, \hbar\omega)$  approximation it exists when  $\mathbf{q}$  takes great values too. For the first time this result was established in paper [1], where the exchange correction to  $\varepsilon(\mathbf{q}, \hbar\omega)$  in variables  $(\mathbf{q}, \hbar\omega)$  immediately was investigated numerically.

In figure 3 the solution of equation (1.2) at  $r_s = 3, r_s = 10$  in different approximations: RPA (curve 1) and  $G_{id}(\mathbf{q}, \hbar\omega)$  (curve 2), is shown. As one can see, in the long-wave region these different approximations give almost the same results, and in the great wave vectors region the solution of (1.2) in the RPA escapes at all. A family of solutions of equation (1.2) in the region  $0, 5 \leq r_s \leq 10$  in  $G_1^{RPA}(\mathbf{q}, \hbar\omega)$  approximation is shown in figure 4.

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## ОБЧИСЛЕННЯ СПЕКТРУ КОЛЕКТИВНИХ ЗБУДЖЕНЬ МОДЕЛІ ЕЛЕКТРОННОЇ РІДИНИ В НАБЛИЖЕННІ ЛОКАЛЬНОГО ПОЛЯ

В.Б.Солов'ян

В рамках базисного підходу запропоновано спосіб розрахунку спектру плазмових збуджень в моделі електронної рідини шляхом переходу від мацубарівського частотного зображення до зображення Гейзенберга та змішаного зображення для багаточастинкових динамічних кореляційних функцій базисної системи (ідеальної виродженої системи електронів) та динамічної поправки на локальне поле. Досліджено дисперсійні криві плазмонів в широкій області параметра неідеальності  $r_s$  для основного стану моделі.