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CORRELATION EFFECTS IN A DEGENERATE ELECTRON GAS

V. ŠIPS and M. VRTAR

Institute »Ruđer Bošković«, Zagreb

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Abstract: A modified version of the Bohm-Pines approach is obtained by transforming longitudinal long-wavelength phonons into plasmons. Taking into account the exchange processes, the electron-plasmon Hamiltonian is derived in which the electron correlation is included. The exchange and correlation contribution to the plasma frequency depends upon the influence of the crystal periodicity on the effective short-range electron-electron interaction. Full agreement with the Bohm-Pines theory is obtained if periodicity effects are completely disregarded.

1. Introduction

Bohm and Pines[1] developed the theory of an interacting electron gas in metals, which offers a simple justification for the one-electron approximation. Replacing ions by a uniform background of positive charge, they considered the influence of the electron-electron Coulomb interaction on metallic properties. The main feature of their approach, called the theory of a collective description of electrons, is a set of collective variables introduced to re-describe the long-range interaction between electrons into a plasma field. Although the BP theory gives an excellent physical insight into the effective electron-electron interaction, it suffers from certain difficulties. These difficulties are caused by the introduction of new terms into the Hamiltonian, whereby the number of variables is increased. To maintain the number of degrees of freedom unchanged, it is necessary to impose an equal number of subsidiary conditions on the wave function, which makes the whole approach considerably complicated. In practice, the final results are obtained by ignoring the subsidiary conditions. This treatment is based on the work by Bohm, Huang and Pines[2], who found that their effect on the ground-state energy and the specific heat is small.

Difficulties arising from the subsidiary conditions can be simply avoided in problems where we are not interested in the behaviour of longitudinal long-wavelength phonons. Then, instead of neglecting the ionic oscillations and introducing the subsidiary plasma variables, we can transform the long-wavelength longitudinal phonon field into the plasma one. Performing the calculation within the Random Phase Approximation (RPA), we found that this approach slightly affects the effective short-range electron-electron interaction term, but leaves the plasma dispersion relation unchanged[3].

Starting from the formulation developed by Bardeen and Pines[4], Hone[5] examined the influence of non-RPA corrections on electron-phonon scattering and showed that correlation effects are automatically introduced by diagonal exchange terms. The same refers to the expression for the plasmon energy[6], where the electron correlation somewhat modifies the strength of the exchange influence. While all those studies are based on the BP theory and thus involve an auxiliary plasma field, in the present paper we treat correlation effects in a modified BP approach which is free from the subsidiary conditions. Owing to the fact that correlation effects depend on the effective screened electron-electron interaction, our method will not lead to the same results as derived within the original BP theory. Nevertheless, it confirmes the main features of their results. Full agreement is obtained if different contributions to the effective electron-electron interaction coming from the ionic periodicity mutually compensate.

2. *Transformation to plasma modes*

An approximation calculation of the electron-phonon interaction can be obtained by assuming that phonons are either longitudinal or transversal and that the latter ones do not interact with electrons. This is essentially the long-wavelength approximation. Then the longitudinal electron-phonon Hamiltonian for a monoatomic metal can be written in the form[7]

$$H = \sum_{\substack{\rightarrow \\ s\kappa}} E_\kappa N_{s\kappa} + \frac{1}{2}\sum_k V_k \rho_k^+ \rho_k + \frac{1}{2}\sum_k (p_k^+ p_k + \Omega_k^2 q_k^+ q_k) + \sum_k \nu_k^l q_k \rho_k^+ . \quad (1)$$

E_κ is the energy of an independent electron moving in the periodical potential, V_k is the square of the electron-electron matrix element, ρ_k is the electron density fluctuation

$$\rho_k = \sum_{s\kappa} c_{s\kappa}^+ c_{s\kappa+\kappa} , \quad (2)$$

$N_{s\kappa}$ is the electron occupation number in the state of spin s and wave number κ, q_k and p_k are the phonon coordinate and the conjugate momenta, respectively, Ω_k is the bare longitudinal phonon frequency, and v_k^i is the unscreened electron-phonon matrix element.

In the first step we transform the Hamiltonian with the help of the generating function

$$S' = \sum_{k<k_c} \frac{v_k^{i*}}{\Omega_k^2} p_k \rho_k , \tag{3}$$

where k_c is the maximum wave vector for which electrons exhibit the collective behaviour. In the RPA we neglect plasmon scattering and hence we arrive at the result

$$H' = \sum_{s\kappa} E_\kappa N_{s\kappa} + \frac{1}{2} \sum_{k<k_c} \{ p_k^+ p_k \left(1 + \frac{|v_k^i|^2 k^2 N}{\Omega_k^4 m}\right) + \Omega_k^2 q_k^+ q_k \} +$$

$$+ \frac{1}{2} \sum_{k<k_c} \left(V_k - \frac{|v_k^i|^2}{\Omega_k^2} \right) \rho_k^+ \rho_k + \frac{1}{2} \sum_{k<k_c} V_k \rho_k^+ \rho_k +$$

$$+ \frac{i}{\hbar} \sum_{s\kappa k} \frac{v_k^{i*}}{\Omega_k^2} p_k c_{s\kappa}^+ c_{s\kappa+k} \left(E_\kappa - E_{\kappa+k} \right) + \tilde{H} , \tag{4}$$

m being the electron mass, N the number of electrons in unit volume (which is assumed to be equal to the number of ions), and $\tilde{H}$ represents that part of the electron-phonon Hamiltonian which is not affected by our transformation

$$\tilde{H} = \sum_{k>k_c} v_k^i q_k \rho_k^+ + \frac{1}{2} \sum_{k>k_c} (p_k^+ p_k + \Omega_k^2 q_k^+ q_k). \tag{5}$$

In writing the coefficient of $p_k^+ p_k$ in (4), we have applied the sum rule[8]

$$V_k \sum_{s\kappa} N_{s\kappa} \left(E_{\kappa - k} - E_\kappa \right) = \hbar^2 \omega_p^2 , \tag{6}$$

with

$$\omega_p^2 = 4 \pi N e^2/m. \tag{7}$$

A new canonical transformation is very simple. It just replaces q_k, p_k by P_k^+, Q_k^+ in the following way

$$q_k = \frac{1}{\Omega_k} P_k^+, \qquad p_k = \Omega_k Q_k^+. \tag{8}$$

Then the transformed Hamiltonian can be written as

$$H' = H_0 + H_{\text{int}} + \Delta H_F + \tilde{H}, \tag{9}$$

where

$$H_0 = \sum_{s\kappa} E_\kappa N_{s\kappa} + \frac{1}{2} \sum_{k<k_c} W_k \rho_k^+ \rho_k + \frac{1}{2} \sum_{k<k_c} V_k \rho_k^+ \rho_k + \frac{1}{2} \sum_{k<k_c} (P_k^+ P_k + \omega_k^2 Q_k^+ Q_k), \tag{10}$$

$$H_{int} = \frac{i}{\hbar} \sum_{k<k_c} \frac{\nu_k^i}{\Omega_k} Q_k \sum_{s\kappa} c_{s\kappa}^+ c_{s\kappa-k} (E_{\kappa-k} - E_\kappa). \tag{11}$$

$$\Delta H_F = \frac{1}{2} \sum_{k<h_c} (\Omega_k^2 + \frac{|\nu_k^i|^2 k^2 N}{m\Omega_k^2} - \omega_k^2) Q_k^+ Q_k . \tag{12}$$

Here

$$W_k = V_k - \frac{|\nu_k^i|^2}{\Omega_k^2}, \tag{13}$$

and ω_k is the plasma frequency, which will be determined later on.

It is important to note that the electron-electron interaction in (10), in comparison with the Coulomb term is drastically reduced. The third term in H_0 is the same as in the BP theory, while the second one gives an additional contribution. To understand its structure and importance, we remind that for small momentum transfers[7]

$$V_k = \frac{4\pi e^2}{k^2} + \alpha_1 + \dots , \tag{14a}$$

$$|\nu_k^i|^2 = \frac{4\pi e^2}{k^2} (\Omega_p^2 + \alpha_2 k^2 + \dots), \tag{14b}$$

$$\Omega_k^2 = \Omega_p^2 + \alpha_3 k^2 + \dots , \tag{14c}$$

with $\Omega_p^2 = 4\pi N e^2/M$, where M denotes the ionic mass. Thus for $k \to 0$

$$W_k = \text{Const} + O(k^2). \tag{15}$$

In other words, in the long-wavelength limit W_k behaves like $4\pi e^2/(k_s^2 + k^2)$, which is the Fourier transform of the Yukawa potential. This shows that the second term in H_0 essentially also represents the screened electron-electron interaction.

The remaining electron-plasmon interaction can be eliminated by the use of the generator

$$S'' = i \sum_{s\kappa \; k<k_C} c^+_{s\kappa} \, c_{s\kappa \; k} \, (f_{k\kappa} Q_k - i g_{k\kappa} P^+_k) \; . \tag{16}$$

Taking into account that the electron-plasmon coupling is small, we write the new system Hamiltonian in the form

$$H_N = H' + \frac{i}{\hbar}[H_0, S''] + \frac{i}{2}\left(\frac{i}{\hbar}\right)^2 [[H_0, S''], S''] + \frac{i}{\hbar}[H_{\text{int}}, S''] + \dots \tag{17}$$

From the requirement that both S'' and H_N should be hermitian we obtain the conditions

$$\sum_{s\kappa} f_{k\kappa} (N_{s\kappa} - N_{s\kappa-k}) = 0 \, , \tag{18}$$

and

$$\sum_{\kappa'} g_{k\kappa'} \Delta N_{\kappa'} \left\{ \Theta \left(\left| \vec{\kappa} - \vec{\kappa'} \right| - k_C \right) V_{\kappa - \kappa'} + \Theta \left(k_C - \left| \vec{\kappa} - \vec{\kappa'} \right| \right) W_{\kappa - \kappa'} \right\} = 0 \, , \tag{19}$$

where

$$\Delta N_\kappa = N_{s\kappa} - N_{s\kappa-k} \tag{20}$$

and Θ is the usual step function.

The parameters $f_{k\kappa}$ and $g_{k\kappa}$ will be chosen in such a way that

$$H_{\text{int}} + \frac{i}{\hbar}[H_0, S''] = 0. \tag{21}$$

This leads to

$$(E_\kappa - E_{\kappa+k})(f_{k\kappa} + i\frac{\nu_k^i}{\Omega_k}) + \hbar\omega_k^2 g_k - \sum_{\kappa'} \Delta N_{\kappa'}(f_{k\kappa} - f_{k\kappa'}) \cdot$$

$$\cdot \{\Theta(|\vec{\kappa} - \vec{\kappa}'| - k_c)\, V_{\kappa-\kappa'} + \Theta(k_c - |\vec{\kappa} - \kappa'|)\, W_{\kappa-\kappa'}\} = 0\,, \qquad (22)$$

and

$$g_{k\kappa}\{(E_\kappa - E_{\kappa-k}) - \sum_{\kappa'} \Delta N_{\kappa'}\Big[\Theta(|\vec{\kappa} - \vec{\kappa}'| - k_c)\, V_{\kappa-\kappa'} +$$

$$+ \Theta(k_c - |\vec{\kappa} - \vec{\kappa}'|)\, W_{\kappa-\kappa'}\Big]\} + \hbar f_{k\kappa} - W_k \sum_{s\kappa'} g_{k\kappa'} \Delta N_{\kappa'} = 0\,. \qquad (23)$$

With the help of (21) our Hamiltonian becomes

$$H_N = H_0 - \frac{i}{2\hbar} \sum_{k<k_c} \frac{\nu_k^{i*}}{\Omega_k} \sum_{s\kappa} g_{k\kappa}\, c_{s\kappa}^+ c_{s\kappa-k} \sum_{s'\kappa'} (E_{\kappa'+k} - E_{\kappa'})\, c_{s'\kappa'}^+ c_{s'\kappa'+k} + \tilde{H}\,, \qquad (24)$$

where the plasmon frequency is defined through the dispersion relation

$$\omega_k^2 = \Omega_k^2 + \frac{|\nu_k^i|^2 k^2 N}{\Omega_k^2 m} + \frac{1}{\hbar^2} \frac{\nu_k^{i*}}{\Omega_k} \sum_{s\kappa} f_{k\kappa}(N_{s\kappa} - N_{s\kappa-k})(E_\kappa - E_{\kappa-k})\,. \qquad (25)$$

The first term on the right-hand side arises from the ionic motion, and because of the large disparity between the electron and ion mass, it is negligible. The main contribution to ω_k^2 is contained in the second term which is of the order ω_p^2, while the last one determines the k-dependence.

Neglecting terms higher than k^2, we shall confine ourselves to the first order iteration for $f_{k\kappa}$ and $g_{k\kappa}$, using the RPA values as basic solutions. Then we can write

$$\omega_k^2 = \omega_{\mathrm{RPA}}^2 + \omega_{ex}^2, \qquad (26)$$

with

$$\omega_{\mathrm{RPA}}^2 = \omega_p^2 + \Omega_p^2 + k^2 \langle v^2 \rangle, \qquad (27)$$

and

$$\omega_{ex}^2 = \frac{V_k}{2\hbar^4 \omega_p^2} \sum_{s\kappa\kappa'} \Delta N_\kappa \, \Delta N_{\kappa'} (\Delta E_\kappa - \Delta E_{\kappa'})^2 \left\{ V_{\kappa-\kappa'} \, \Theta \left(\left| \vec{\kappa} - \vec{\kappa}' \right| - k_c \right) + \right.$$

$$\left. + \, W_{\kappa-\kappa'} \, \Theta \left(k_c - \left| \vec{\kappa} - \vec{\kappa}' \right| \right) \right\} , \tag{28}$$

where only the leading term caused by the phonon recoil has been kept.

The new feature in comparison with the results obtained in the same approximation in the framework of the BP theory is the appearance of the last term in (28). This term represents the direct contribution to the plasmon energy associated with the ionic periodicity. Together with the preceding term it gives the influence of exchange on the plasma vibration. Both these terms are caused by the screened electron-electron interaction, and hence include the correlation contribution to the plasma frequency.

The simplest approximation that in fact corresponds to our neglect of the electron-phonon interaction for non-longitudinal modes, is based on the jelly model. By ignoring the ionic periodicity the expressions for V_k, $|v_k^i|^2$ and ω_k^2 reduce to the corresponding first terms in the series expansions (14), and hence the last term in (28) vanishes. Further, by inserting the expression for the free electron-energy

$$E_\kappa = \frac{\hbar^2 \kappa^2}{2m} \tag{29}$$

into (28), it is easy to show that under these circumstances (26) goes over into

$$\omega_k^2 = \omega_p^2 + \Omega_p^2 + \frac{3\hbar^2 k^2 k_F^2}{5m^2} \left\{ 1 - \frac{m^2 \omega_p^2}{4\hbar^2 k_F^4} \left(1 + \frac{\beta^2}{4} - \frac{\beta^4}{8} \right) \right\}. \tag{30}$$

Here k_F is the wave number of an electron on the Fermi sphere, and β is the ratio k_c/k_F. Apart from the second term, which gives the ionic contribution to the plasma frequency and is of the order m/M comparated to ω_p^2, the result (30) is in agreement with that derived on the basis of the BP approach[6].

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KORELACIONI EFEKTI U DEGENERIRANOM ELEKTRONSKOM PLINU

V. ŠIPS i M. VRTAR

Institut »Ruđer Bošković«, Zagreb

Sadržaj

Efekt elektronske korelacije na plazmonsku energiju ispitan je proširenjem metode Bohma i Pinesa. Prednost pred originalnim Bohm-Pinesovim postupkom sastoji se u tome što je cijeli račun proveden bez proširenja stupnjeva slobode i odgovarajućih pomoćnih uvjeta. Pokazano je da članovi izmjene ne daju općenito isti doprinos plazmonskom kvantu kao u BP teoriji, Potpuno slaganje dobiveno je u okviru žele-modela.