

Green Function Method for Electron Gas. II

— Dispersion Relation of Plasmons —

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The shift of plasmon energy due to the electron exchange is calculated. Our result is the same as that obtained by Nozières and Pines. The analysis of the experimental values of Watanabe referring to Bohm-Pines' values is made and the agreement between our theory and the experiment seems to be good at high densities.

§ 1. Introduction

Several authors¹⁾ attempted to improve Bohm-Pines' dispersion relation of plasmons by including the effect of electron exchange and reached the conclusions that the exchange effect gives a certain correction to the term of order k^2 (k is the wave number of a plasmon). The corrections, however, vary considerably with the authors and the characters of the approximations in their theories are not quite obvious. Recently DuBois²⁾ has calculated the shift of plasmon energy due to the electron exchange, using the Feynman-Dyson techniques of field theory. In the present paper we obtain the dispersion relation by the method described in I.³⁾ The correction to the term of order k^2 is the same as that obtained by Nozières and Pines,⁴⁾ who derived the shift of the plasmon frequency by Bohm-Pines' theory.

§ 2. Dispersion relation

The two-particle Green function^{3)*}

$$G(x_1, x_2; x_3, x_4) = i(\Psi_0, T\{\phi(x_1)\phi(x_2)\phi^*(x_3)\phi^*(x_4)\}\Psi_0) \quad (2.1)$$

satisfies the Bethe-Salpeter equation;

$$\begin{aligned} G(x_1, x_2; x_3, x_4) &= iG(x_1, x_3)G(x_2, x_4) - iG(x_1, x_4)G(x_2, x_3) \\ &+ i \int \dots \int G(x_1, x_5)G(x_6, x_3)G(x_5, x_6; x_7, x_8)G(x_7, x_2; x_8, x_4) dx_5 dx_6 dx_7 dx_8. \end{aligned} \quad (2.2)$$

Let $t_1, t_3 > t_2, t_4$. Then, we have

$$G(x_1, x_2; x_3, x_4) = -i \sum_S \chi_S(x_1, x_3) \bar{\chi}_S(x_2, x_4), \quad (2.3)$$

* Throughout this paper the atomic unit, $m = \hbar = 1$, is used and the notations in I are followed.

where

$$\chi_s(x_1, x_3) = (\Psi_0, T\{\phi(x_1)\phi^*(x_3)\}\Psi_s). \tag{2.4}$$

Applying Gell-Mann and Low's procedure to (2.2), we have the following equation for the bound state amplitude $\chi_s(x_1, x_3)$ of an electron and a hole,

$$\chi_s(x_1, x_3) = i \int G(x_1, x_5)G(x_6, x_3)\Gamma(x_5, x_6; x_7, x_8)\chi_s(x_7, x_8)dx_5dx_6dx_7dx_8. \tag{2.5}$$

The interaction part Γ is given by the diagrams shown in Fig. 1 in lowest order. Then we get

$$\begin{aligned} \chi_s(x_1, x_3) = & -2i \int G(x_1, x_5)G(x_6, x_3)v(x_5-x_6)\chi(x_6, x_6)dx_5dx_6 \\ & + i \int G(x_1, x_5)G(x_6, x_3)v(x_5-x_6)\chi_s(x_5, x_6)dx_5dx_6, \end{aligned} \tag{2.6}$$

where $v(x-x') = v(\mathbf{r}-\mathbf{r}')\delta(t-t')$.

The first and the second terms on the right-hand side in (2.6) correspond to the diagrams shown in Fig. 1 (a) and Fig. 1 (b) respectively. The factor 2 of the first term is due to the



Fig. 1. First order interaction part

fact that in exciting a new pair an electron of either spin is available. The Fourier transform of (2.6) is given by*

$$\begin{aligned} \chi_{k\omega}(p) = & iG\left(p + \frac{k}{2}\right)G\left(p - \frac{k}{2}\right) \left\{ -2v(\mathbf{k}) \int \chi_{k\omega}(p) \frac{dp}{(2\pi)^4} \right. \\ & \left. + \int v(\mathbf{q}) \chi_{k\omega}(p+q) \frac{dq}{(2\pi)^4} \right\}, \end{aligned} \tag{2.7}$$

which was first derived by Galickij and Migdal.⁵⁾ If we neglect the second term in parentheses in (2.7), substitute the non-interacting one-particle Green function $G_0(p)$ for $G(p)$ and integrate the both sides over p , we get the Bohm-Pines dispersion relation⁶⁾

$$\begin{aligned} 1 = & -2iv(\mathbf{k}) \int G_0\left(p + \frac{k}{2}\right)G_0\left(p - \frac{k}{2}\right) \frac{dp}{(2\pi)^4} \\ = & -2v(\mathbf{k}) \int \frac{n_0(\mathbf{p} + \mathbf{k}/2) - n_0(\mathbf{p} - \mathbf{k}/2)}{\omega - \epsilon_0(\mathbf{p} + \mathbf{k}/2) + \epsilon_0(\mathbf{p} - \mathbf{k}/2)} \frac{d\mathbf{p}}{(2\pi)^3} \\ = & 4\pi e^2 \int \frac{2n_0(\mathbf{p})}{(\omega - \mathbf{k} \cdot \mathbf{p})^2 - (k^4/4)} \frac{d\mathbf{p}}{(2\pi)^3}. \end{aligned} \tag{2.8}$$

* Hereafter p, q and k denote the four-dimensional energy-momentum vectors, while the bold-faced \mathbf{p}, \mathbf{q} and \mathbf{k} represent the ordinary momenta, for instance, $p = (p\epsilon), k = (k\omega), dp = d\mathbf{p}d\epsilon$, etc. Confusion of the four-dimensional vector with the magnitude of the momentum will not occur, because the four-dimensional vector always appears in the argument of G or χ .

In order to improve the dispersion relation we must take into account (i) the exchange energy and (ii) the ladder type diagram. The Green function $G(\mathbf{p}, \varepsilon)$ may be written as

$$G(\mathbf{p}, \varepsilon) = G_0(\mathbf{p}, \varepsilon) + G_0(\mathbf{p}, \varepsilon) \Sigma(\mathbf{p}, \varepsilon) G(\mathbf{p}, \varepsilon), \quad (2.9)$$

or

$$G(\mathbf{p}, \varepsilon) = 1 / \{ G_0^{-1}(\mathbf{p}, \varepsilon) - \Sigma(\mathbf{p}, \varepsilon) \} = 1 / \{ \varepsilon_0(\mathbf{p}) - \varepsilon - \Sigma(\mathbf{p}, \varepsilon) \}, \quad (2.10)$$

where $\Sigma(\mathbf{p}, \varepsilon)$ is the irreducible self-energy part. The first order self-energy which is represented by the diagram shown in Fig. 2 is given by

$$\Sigma^{(1)}(\mathbf{p}) = \int v(\mathbf{p}-\mathbf{p}') n_0(\mathbf{p}') \frac{d\mathbf{p}'}{(2\pi)^3}. \quad (2.11)$$

If we substitute $\varepsilon_0(\mathbf{p}) - \Sigma^{(1)}(\mathbf{p})$ for $\varepsilon_0(\mathbf{p})$ in (2.8), we find that a term of $\ln k$ appears in the dispersion relation. This logarithmic divergence is cancelled by the second term in parentheses in (2.7), which represents the effect of the ladder type diagram. The ladder type diagrams give, in general, contributions of higher order in r_s than the pair diagrams and may be regarded as a small perturbation. Then we may solve (2.7) by successive approximation. Taking the first approximation, we get



Fig. 2. $\Sigma^{(1)}$

$$\begin{aligned} \chi_{k\omega}(\mathbf{p}) = & -2iv(\mathbf{k}) G\left(\mathbf{p} + \frac{\mathbf{k}}{2}\right) G\left(\mathbf{p} - \frac{\mathbf{k}}{2}\right) \left\{ 1 + i \int v(\mathbf{q}) G\left(\mathbf{p} + \mathbf{q} + \frac{\mathbf{k}}{2}\right) \right. \\ & \left. \times G\left(\mathbf{p} + \mathbf{q} - \frac{\mathbf{k}}{2}\right) \frac{d\mathbf{q}}{(2\pi)^4} \right\} \int \chi_{k\omega}(\mathbf{p}') \frac{d\mathbf{p}'}{(2\pi)^4}. \end{aligned} \quad (2.12)$$

Within our approximation (to the order of $r_s \ln r_s$ or r_s) it is permitted to substitute $G_0(\mathbf{p}, \varepsilon)$ for $G(\mathbf{p}, \varepsilon)$ in the second term in parentheses of (2.12). Then we have the dispersion relation

$$\begin{aligned} 1 = & -2v(\mathbf{k}) \left\{ i \int G\left(\mathbf{p} + \frac{\mathbf{k}}{2}\right) G\left(\mathbf{p} - \frac{\mathbf{k}}{2}\right) \frac{d\mathbf{p}}{(2\pi)^4} + i^2 \iint G_0\left(\mathbf{p} + \frac{\mathbf{k}}{2}\right) G_0\left(\mathbf{p} - \frac{\mathbf{k}}{2}\right) \right. \\ & \left. \times v(\mathbf{q}) G_0\left(\mathbf{p} + \mathbf{q} + \frac{\mathbf{k}}{2}\right) G_0\left(\mathbf{p} + \mathbf{q} - \frac{\mathbf{k}}{2}\right) \frac{d\mathbf{p}}{(2\pi)^4} \frac{d\mathbf{q}}{(2\pi)^4} \right\} \\ = & -2v(\mathbf{k}) \left\{ \int \frac{n_0(\mathbf{p} + \mathbf{k}/2) - n_0(\mathbf{p} - \mathbf{k}/2)}{\omega - \mathbf{k} \cdot \mathbf{p} + \Sigma^{(1)}(\mathbf{p} + \mathbf{k}/2) - \Sigma^{(1)}(\mathbf{p} - \mathbf{k}/2)} \frac{d\mathbf{p}}{(2\pi)^3} \right. \\ & + \iint \frac{n_0(\mathbf{p} + \mathbf{k}/2) - n_0(\mathbf{p} - \mathbf{k}/2)}{\omega - \mathbf{k} \cdot \mathbf{p}} \\ & \left. \times v(\mathbf{q}) \frac{n_0(\mathbf{p} + \mathbf{q} + \mathbf{k}/2) - n_0(\mathbf{p} + \mathbf{q} - \mathbf{k}/2)}{\omega - \mathbf{k} \cdot (\mathbf{p} + \mathbf{q})} \frac{d\mathbf{p}}{(2\pi)^3} \frac{d\mathbf{q}}{(2\pi)^3} \right\} \end{aligned} \quad (2.13)$$

instead of (2.8).

Expanding the terms in parentheses in (2.13) in powers of e^2 and k^2 and retaining terms up to orders e^2 and k^4 , we get

$$1 = -2v(\mathbf{k}) \left[\int \frac{n_0(\mathbf{p} + \mathbf{k}/2) - n_0(\mathbf{p} - \mathbf{k}/2)}{\omega - \mathbf{k} \cdot \mathbf{p}} \frac{d\mathbf{p}}{(2\pi)^3} \right. \\ \left. + \frac{2}{\omega^4} \iint (n_0(\mathbf{p}) - n_0(\mathbf{p} - \mathbf{k})) n_0(\mathbf{p} + \mathbf{q}) \right. \\ \left. \times v(\mathbf{q}) \left\{ 3 \left(\mathbf{k} \cdot \mathbf{p} - \frac{k}{2} \right) (\mathbf{k} \cdot \mathbf{q}) + (\mathbf{k} \cdot \mathbf{q})^2 \right\} \frac{d\mathbf{p}}{(2\pi)^3} \frac{d\mathbf{q}}{(2\pi)^3} \right]. \quad (2.14)$$

If we compare the above equation with (2.8), we see that the second term in the bracket is just the correction term to the dispersion relation of BP. Using the following relation,

$$n_0(\mathbf{p}) - n_0(\mathbf{p} - \mathbf{k}) = -\frac{(\mathbf{k} \cdot \mathbf{p})}{p} \delta(p - p_0) + \frac{k^2}{2p} \delta(p - p_0) \\ - \frac{(\mathbf{k} \cdot \mathbf{p})^2}{2p^3} (\delta(p - p_0) - p\delta'(p - p_0)) + \dots,$$

and performing the integrations over \mathbf{p} and \mathbf{q} , we find that the correction term in (2.14) yields $-3/20 \cdot \omega_p^4 / \omega^4 \cdot k^2 / p_0^2$ up to order k^2 . The dispersion relation now reads

$$\omega^2 = \omega_p^2 + \frac{3}{5} p_0^2 k^2 \left(1 - \frac{1}{4} \frac{\omega_p^2}{p_0^4} \right) + O(k^4), \quad (2.15)$$

which is to be compared with that of BP;

$$\omega^2 = \omega_p^2 + \frac{3}{5} p_0^2 k^2 + O(k^4). \quad (2.16)$$

Thus the correction factor due to the electron exchange is*

$$1 - \frac{1}{4} \frac{\omega_p^2}{p_0^4} = 1 - \frac{\alpha}{3\pi} r_s = 1 - 0.0553 r_s, \quad (2.17)$$

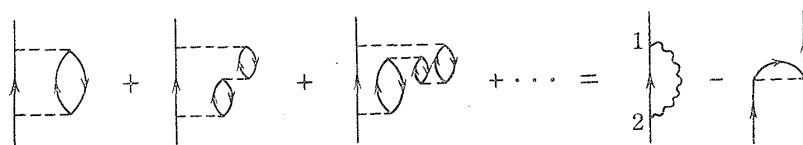
which agrees with that of NP.⁴⁾

§ 3. Further remarks

As mentioned in § 2, when the ladder type diagram is ignored the exchange energy gives a $\ln k$ term to the plasmon frequency. To avoid this difficulty we may as well include the electron correlation, which means here the action of the polarization cloud back on the electron. We consider the contributions to the self energy from the diagrams shown in Fig. 3. Then we have

$$\Sigma^{(2)}(\mathbf{p}, \varepsilon) = -i \int \frac{d\mathbf{k} d\omega}{(2\pi)^4} G_0(\mathbf{p} + \mathbf{k}, \varepsilon + \omega) v(\mathbf{k}) \left(1 - \frac{1}{\varepsilon(\mathbf{k}, \omega)} \right), \quad (3.1)$$

* The correction factor obtained by DuBois is $1 - \frac{\alpha}{12\pi} r_s$. He has taken into account the same diagrams as ours. The discrepancy might be due to his trivial mistake.

Fig. 3. $\Sigma^{(2)}$

where

$$\begin{aligned} \epsilon(\mathbf{k}, \omega) &= 1 + 2iv(\mathbf{k}) \int \frac{d\mathbf{p}}{(2\pi)^4} G_0\left(\mathbf{p} + \frac{\mathbf{k}}{2}\right) G_0\left(\mathbf{p} - \frac{\mathbf{k}}{2}\right) \\ &= 1 + 2v(\mathbf{k}) \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{n_0(\mathbf{p} + \mathbf{k}/2) - n_0(\mathbf{p} - \mathbf{k}/2)}{\omega - \mathbf{p} \cdot \mathbf{k} + i\delta(n_0(\mathbf{p} + \mathbf{k}/2) - n_0(\mathbf{p} - \mathbf{k}/2))} \end{aligned} \quad (3.2)$$

is the complex dielectric constant. Since we are concerned with the self energy up to order r_s , we may replace $\epsilon(\mathbf{k}, \omega)$ in (3.1) by static dielectric constant $\epsilon(\mathbf{k}, 0)$;⁷⁾

$$\epsilon(\mathbf{k}, 0) = 1 + \frac{2\alpha r_s}{\pi} \frac{p_0^2}{k^2} \left\{ 1 + \frac{4p_0^2 - k^2}{4p_0 k} \ln \frac{2p_0 + k}{2p_0 - k} \right\}. \quad (3.3)$$

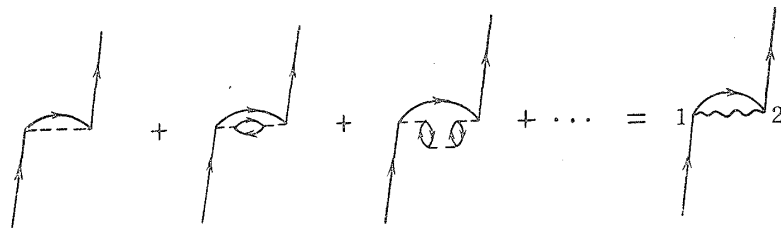
Then the sum of $\Sigma^{(1)}$ and $\Sigma^{(2)}$ yields

$$\Sigma(\mathbf{p}) = \Sigma^{(1)} + \Sigma^{(2)} = \frac{1}{2} \int \frac{d\mathbf{k}}{(2\pi)^3} v(\mathbf{k}) \left(1 - \frac{1}{\epsilon(\mathbf{k}, 0)} \right) + \int \frac{d\mathbf{k}}{(2\pi)^3} n_0(\mathbf{p} + \mathbf{k}) \frac{v(\mathbf{k})}{\epsilon(\mathbf{k}, 0)}, \quad (3.4)$$

where use has been made of the relation

$$i \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} G_0(\mathbf{p}, \varepsilon) = n_0(\mathbf{p}) - \frac{1}{2}.$$

The first term in (3.4) is simply an additive constant which has no effect on the plasmon frequency and the second one may be interpreted as the exchange energy of the screened Coulomb potential $v(\mathbf{k})/\epsilon(\mathbf{k}, 0)$. This interpretation is most easily understood by the language of diagrams; the neglect of retardation corresponds to that the times t_1 and t_2 of the vertices 1 and 2 in Fig. 3 are set equal as shown in Fig. 4. This diagram just corresponds to the first one in Fig. 3 in NP, where they evaluated the shift of the plasmon frequency caused by H_s in the BP theory.

Fig. 4. $\Sigma^{(1)} + \Sigma^{(2)}$

Our screened potential is essentially (at least, up to order r_s) equivalent to H_{sr} . If we substitute $\Sigma(\mathbf{p})$ for $\Sigma^{(1)}(\mathbf{p})$ in (2.13), we find that the logarithmic divergence disappears, as anticipated at the start.

At the same time, we must consider the effect of the ladder type diagrams, the second term in parentheses in (2.13). Here using "bare" Coulomb potential in the ladder is, also, the origin of the logarithmic divergence, which is, however, eliminated by introduction of the screening of the potential. This means, within our approximation, $v(\mathbf{q})$ must be replaced by $v(\mathbf{q})/\epsilon(\mathbf{q}, 0)$. The ladder type diagram corresponds to the second one in Fig. 3 in NP. After these modifications are both taken into account, we again get the correction factor (2.17).

It can be shown that the contribution from the plasmon state to the correlation energy is not of the simple form $\frac{1}{2}\{[\hbar\omega - (\hbar\omega)_{e^2=0}]dk/(2\pi)^3$ in our case. This might be due to the fact that the separation of the bound state from the scattering state is not clear near the cut-off momentum owing to the damping of plasmons. In the theory of BP the damping of plasmons arises mainly through the short range collisions of electrons (NP). Therefore the damping is associated with the non-RPA corrections to the plasmon frequency. DuBois has calculated the damping and discussed the determination of k_c .

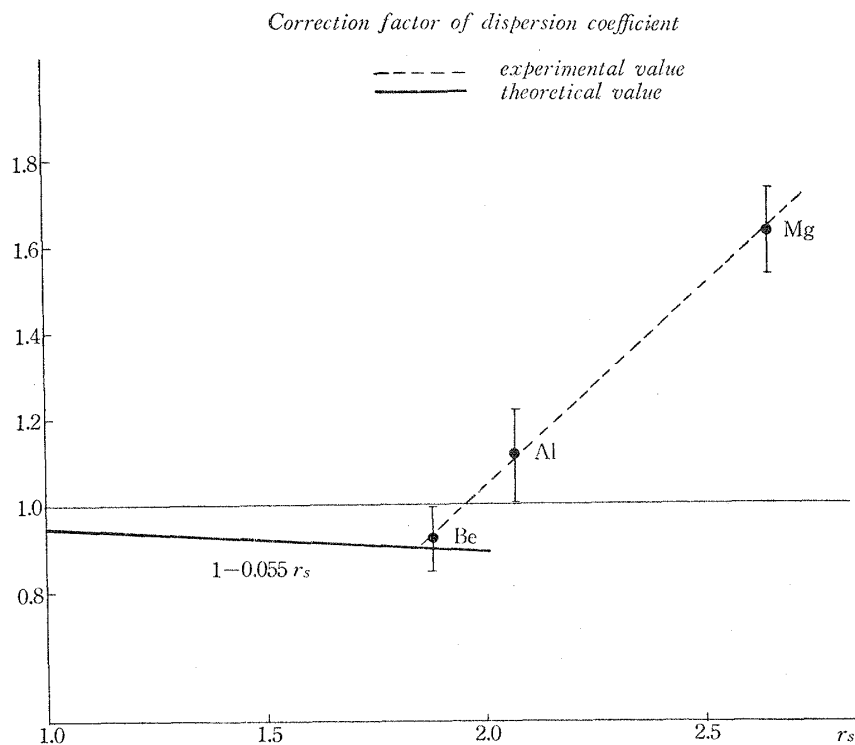


Fig. 5

Finally we add some comments on the comparison with experiment (Fig. 5). First we plot the ratios of Watanabe's experimental values⁸⁾ of the dispersion co-

efficients to BP's theoretical values as a function of r_s . Because of very singular structure of the Brillouin zone, Ge is put out of consideration. On the other hand, for Be, Al and Mg the effective mass is nearly equal to the true mass and we may regard the effect of the positive ion lattice as comparably small. In fact, the above-mentioned ratios stand in a straight line within experimental error and we entertain a hope that this curve can be approximately described by the function of r_s alone. Then we plot the theoretical correction curve (2.17). At high densities such as in Be the agreement between theory and experiment seems to be rather good, whereas at lower densities the discrepancy becomes large and we will have to proceed to the evaluation of corrections up to higher orders.

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