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Application of the Dielectric Formulation to the Multi-Component, Many-Particle System with Coulomb Interaction

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Abstract

In terms of a generalized dielectric constant $\epsilon(q, \omega)$ defined by Nozieres and Pines, a multi-component, many-particle system with Coulomb interaction is described. By this formulation, various kinds of charged particle systems can be discussed from the unified point of view.

$\epsilon(q, \omega)$ is calculated in the random phase approximation (R.P.A.). Fermi(F), Bose(B), Bose and Bose(BB), Bose and Fermi(BF), and Fermi and Fermi(FF) systems are discussed. For F, B, BB, and BF, the $\epsilon(q, \omega)$ obtained above leads directly to the results of Gell-Mann and Brueckner, Foldy, Bassichis, and Ginoza and Kanazawa, respectively.

It is made obvious in this discussion that in the high density limit, the results obtained by treating Bose components by Bogoliubov method are naturally equivalent to those obtained in terms of the R.P.A.

1. Introduction

The many particle systems with Coulomb interactions have been studied by many workers. For the free electron gas(F), the calculation of the correlation energy within the random phase approximation (R.P.A) was performed by Gell-Mann and Brueckner¹). As for the charged Bose gas (B), Foldy²) calculated the energy by the Bogoliubov method³). Lee⁴) redid the Foldy calculation by the Brandow boson linked-cluster expansion in which the particle conservation is treated exactly. The Bogoliubov method was generalized in order to permit examination of a mixture of an arbitrary number of different species of Bose particles by Bassichis⁵). He examined a neutral mixture of two types of charged Bose particles (BB) and obtained two types of elementary excitations : plasma type and free particle like. The ground state energy and the elementary excitations of the neutral system consisting of charged Bose particles and charged Fermi particles (BF) were investigated by Ginoza and Kanazawa⁶). There are two types of collective excitations in BF : optical- and acoustic -phonon like. They treated the Bose component by the Bogoliubov method and applied the field theoretical technique.

The aim of this paper is to discuss various kinds of systems described above

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from the unified point of view. This program is realized by the introduction of the generalized dielectric constant $\epsilon(q, \omega)$ defined by Nozieres and Pines⁷⁾ to the description of a multi-component, many-particle system with Coulomb interaction.

It is simple to evaluate $\epsilon(q, \omega)$ within the R.P.A. For F, B, BB, and BF, the $\epsilon(q, \omega)$ in the R.P.A. leads directly to the results of Gell-Mann and Brueckner, Foldy, Bassichis, and Ginoza and Kanazawa, respectively.

In section 2, the brief review of the dielectric formulation will be given. In section 3, an equation of motion for a correlation function will be solved with the R.P.A. and $\epsilon(q, \omega)$ is obtained. On the basis of $\epsilon(q, \omega)$ thus obtained, F, B, BB, BF, and FF are discussed. In the final section, the summary of the results in this paper is given.

2. General Formulation

Let us consider a neutral mixture of an arbitrary number of different species of charged particles in a large box of volume Ω with periodic boundary condition. We assume the nonrelativistic motions for all particles. We shall be using a second quantized representation. Let us $C_i(k\sigma)$ and $C_i^+(k\sigma)$ represent, respectively, the destruction and creation operators for a particle in the state specified by momentum k and spin σ in the i -th component. If any two operators of these belong to the same component, they satisfy the well-known commutation relations specified by the statistics obeyed by the constitutive particles of its component. Otherwise, they commute each other. The Hamiltonian of this system ($\Omega=1, \hbar=2\pi$) is written as

$$H = H_0 + H_1, \tag{2.1}$$

$$H_0 = \sum_i \sum_{k\sigma} \epsilon_i(k) C_i^+(k\sigma) C_i(k\sigma),$$

$$H_1 = \frac{1}{2} \sum_q v(q) \{ \rho(q) \rho(-q) - \sum_i e_i^2 n_i \},$$

where $\rho(q) = \sum_i \sum_{k\sigma} e_i C_i^+(k\sigma) C_i(k+q\sigma),$

$$\epsilon_i(k) = k^2 / 2m_i,$$

$$v(q) = 4\pi q^{-2} \text{ for } q \neq 0$$

$$= 0 \quad \text{for } q = 0,$$

and n_i is the number density of particle with mass m_i and charge e_i .

Let us review briefly the dielectric formulation given by Nozieres and Pines⁷⁾. We introduce adiabatically a sufficiently small, oscillating test charge of wave vector q and frequency ω to our system. The charge density of the test charge is assumed to be

$$[\gamma_q e^{i(qr-\omega t)} + c.c.] e^{\eta t}$$

where $\gamma_q \rightarrow 0$ and $\eta \rightarrow +0$. For the system with translational invariance, the dielectric constant $\epsilon(q, \omega)$ is defined by

$$1/\epsilon(q, \omega) = 1 + \overline{\rho(q)}/\gamma_q e^{-i\omega t}$$

where $\overline{\rho(q)}$ is the perturbed expectation value of $\rho(q)$.

Calculating the linear response to the test charge under the assumption that the system is initially in its ground state, we obtain

$$\overline{\rho(q)} = v(q) D^r(q, \omega) \gamma_q e^{-i\omega t}$$

where $D^r(q, \omega)$ is a Fourier transform of the retarded total density correlation function $D^r(q, t-t')$ defined as follows ;

$$D^r(q, t-t') = -i \theta(t-t') \langle [\rho(q, t), \rho(-q, t')] \rangle. \tag{2.2}$$

The $\rho(q, t)$ is the Heisenberg representation of $\rho(q)$ and the average is taken in the ground state of the Hamiltonian given by (2.1). Thus,

$$1/\epsilon(q, \omega) = 1 + v(q) D^r(q, \omega) \tag{2.3}$$

and therefore the calculation of the dielectric constant is reduced to that of $D^r(q, \omega)$.

In the field theoretical calculations, the propagator corresponding to (2.2) is introduced. It is the time ordered total density correlation function defined by

$$D^c(q, t-t') = -i \langle T \rho(q, t) \rho(-q, t') \rangle. \tag{2.4}$$

In the case that the ground state of (2.1) is invariant under the time inversion, the followings are derived from the definition :

$$D^c(q, t-t') = D^c(-q, t'-t) = D^c(q, t'-t).$$

By going over to the Lehmann representation, we can show that in the complex ω -plane, $D^r(q, \omega)$ and $\epsilon^{-1}(q, \omega)$ are analytic in the upper half, and that on the real ω -axis, the following relations are satisfied ;

$$\begin{aligned} \text{Re } \epsilon^{-1}(q, \omega) - 1 &= v(q) \text{Re } D^r(q, \omega) = v(q) \text{Re } D^c(q, \omega), \\ \text{Im } \epsilon^{-1}(q, \omega) &= v(q) \text{Im } D^r(q, \omega) = v(q) (\omega / |\omega|) \text{Im } D^c(q, \omega), \end{aligned} \tag{2.5}$$

$$D^c(q, \omega) = D^c(-q, -\omega) = D^c(q, -\omega).$$

It is shown by the direct calculations of the commutators that

$$\langle [(\rho(q), H), \rho(-q)] \rangle = (q^2 / 4\pi) \sum_i \omega_i^2, \tag{2.6}$$

where $\omega_i^2 = 4 \pi n_i e_i^2 / m_i$. From the Lehmann representation of (2.6) and the relations (2.5), the sum rule which must be satisfied by ϵ^{-1} is obtained;

$$\int_0^\infty d\omega \omega \operatorname{Im} \epsilon^{-1}(q, \omega) = (-\pi/2) \sum_i \omega_i^2. \quad (2.7)$$

Also, if $\epsilon(q, \omega)$ is analytic in the upper half of the complex ω -plane, $\epsilon(q, \omega)$ must satisfy the following sum rule ;

$$\int_0^\infty d\omega \omega \operatorname{Im} \epsilon(q, \omega) = (\pi/2) \sum_i \omega_i^2 \quad (2.8)$$

$\epsilon(q, \omega)$ may be analytic if $\epsilon(q, 0) \geq 0$.

The knowledge of the dielectric constant permits one to obtain directly the various properties of the system. The allowed energy spectra of the density fluctuations are yielded by the relation

$$\epsilon(q, \omega) = 0. \quad (2.9)$$

The ground state energy is calculated by the following :

$$E = E_{\text{HF}} + E_{\text{corr}}, \quad (2.10)$$

$$E_{\text{HF}} = E_0 - \sum_q v(q) \left\{ \int_0^\infty \frac{d\lambda}{\lambda} \int_0^\infty \frac{d\omega}{2\pi} \operatorname{Im} D_{\text{HF}}^r(q, \omega; \lambda) + \frac{1}{2} \sum_i n_i e_i^2 \right\},$$

$$E_{\text{corr}} = \sum_q v(q) \int_0^1 \frac{d\lambda}{\lambda} \int_0^\infty \frac{d\omega}{2\pi} \operatorname{Im} \left\{ D_{\text{HF}}^r(q, \omega; \lambda) - D^r(q, \omega; \lambda) \right\},$$

where E_0 , E_{HF} , and E_{corr} are the noninteracting ground state energy, the Hartree-Fock ground state energy, and the correlation energy of the system, respectively.

3. Discussions of the various kinds of systems within the R.P.A.

3.1 Let us define a function as follows ;

$$\begin{aligned} & \ll e_i C_i^+(k\sigma, t) C_i(k+q\sigma, t) : \rho(-q, t') \gg \\ & = -i \theta(t-t') \langle [e_i C_i^+(k\sigma, t) C_i(k+q\sigma, t), \rho(-q, t')] \rangle \end{aligned}$$

where $C_i^+(k\sigma, t)$ is the Heisenberg representation of $C_i^+(k\sigma)$. With the calculations of the commutators, we obtain the equation of motion of this function as

$$\begin{aligned} i \frac{\partial}{\partial t} \ll e_i C_i^+(k\sigma, t) C_i(k+q\sigma, t) : \rho(-q, t') \gg &= \delta(t-t') e_i^2 (n_i(k\sigma) - n_i(k+q\sigma)) \\ & + (\epsilon_i(k+q) - \epsilon_i(k)) \ll e_i C_i^+(k\sigma, t) C_i(k+q\sigma, t) : \rho(-q, t') \gg \\ & + \sum_{q'} (v(q') e_i^2 / 2) \ll \{ \rho(q', t) [C_i^+(k\sigma, t) C_i(k+q-q'\sigma, t) - C_i^+(k+q'\sigma, t) C_i(k+q\sigma, t)] \\ & + [C_i^+(k\sigma, t) C_i(k+q+q'\sigma, t) - C_i^+(k-q'\sigma, t) C_i(k+q\sigma, t)] : \rho(-q', t) \} : \rho(-q, t') \gg, \end{aligned} \quad (3.1)$$

where $n_i(k\sigma) = \langle C_i^+(k\sigma) C_i(k\sigma) \rangle$. This equation can not be solved due to the third term in the right hand side. Let us make the approximation of replacing the square brackets by the ground state averages, that is,

$$\llbracket \rho(q', t) C_i^+(k\sigma, t) C_i(k+q-q'\sigma, t) : \rho(-q, t') \rrbracket = \delta_{q, q'} n_i(k\sigma) \llbracket \rho(q, t) : \rho(-q, t') \rrbracket \text{etc.} \quad (3.2)$$

Now, we can solve this equation and obtain, with the use of (2.2) and (2.3),

$$D^r(q, \omega) = \sum_i D_i(q, \omega) / [1 - v(q) \sum_i D_i(q, \omega)],$$

$$\epsilon(q, \omega) = 1 - v(q) \sum_i D_i(q, \omega), \quad (3.3)$$

where $D_i(q, \omega) = e_i^2 \sum_{k\sigma} \frac{n_i(k\sigma) - n_i(k+q\sigma)}{\omega - \epsilon_i(k+q) + \epsilon_i(k) + i\delta}$ (3.4)

Incidentally, the Hartree-Fock approximation is the one of neglecting the third term in the right hand side of (3.1). In this case, we obtain

$$D_{\text{HF}}^r(q, \omega) = \sum_i D_i(q, \omega),$$

$$\epsilon_{\text{HF}}^{-1}(q, \omega) = 1 + v(q) \sum_i D_i(q, \omega). \quad (3.5)$$

It is obvious that (3.3) and (3.5) are analytic in the upper half of the complex ω -plane. It is easily shown that (3.3) and (3.5) satisfy (2.8) and (2.7), respectively.

3.2 The substitution of (3.3) and (3.5) into (2.10) and the integration over λ yield the following results

$$E_{\text{HF}} - E_0 = -\frac{1}{2} \sum_i' \sum_q \sum_{k\sigma} v(q) e_i^2 n_i(k\sigma) n_i(k+q\sigma),$$

$$E_{\text{corr}} = \sum_q \int_0^\infty \frac{d\omega}{2\pi} \text{Im} \{ \log [1 - v(q) \sum_i D_i(q, \omega)] + v(q) \sum_i D_i(q, \omega) \}$$

$$= E_{\text{corr}}^{(0)} + \Delta E \quad (3.6)$$

where $E_{\text{corr}}^{(0)} = \sum_i \sum_q \int_0^\infty \frac{d\omega}{2\pi} \text{Im} \{ \log [1 - v(q) D_i(q, \omega)] + v(q) D_i(q, \omega) \},$

$$\Delta E = \sum_q \int_0^\infty \frac{d\omega}{2\pi} \text{Im} \log \frac{1 - v(q) \sum_i D_i(q, \omega)}{\prod_i [1 - v(q) D_i(q, \omega)]}, \quad (3.7)$$

and the prime on the sum over i means the exclusion of the sum over the Bose components.

Let us assume that

$$n_i(k\sigma) = \theta(k_{\text{Fi}} - k) \quad \text{for the Fermi components}$$

$$= n_i \delta_{k,0} \delta_{\sigma,0} \quad \text{for the Bose components} \quad (3.8)$$

where $k_{Fi} = (3 \pi^2 n_i)^{1/3}$. In this case ,

$$E_{\text{corr}}^{(0)} = \sum_i' (0.062 \log r_i - 0.142) n_i m_i e_i^4 / 2 + \sum_i'' (-0.803 r_i^{-3/4}) n_i m_i e_i^4 / 2, \tag{3.9}$$

where the double prime on the sum over i means the exclusion of the Fermi components and $r_i = (3/4 \pi n_i)^{1/3} m_i e_i^2$ which is the particle density parameter in the i -th component. Let us assume that our theory is applied to the one component systems with the background of fixed and uniformly distributed charge of opposite sign. The following are obvious from (3.9) ; For the free electron gas, the decouplings (3.2) yield the ground state energy obtained by Gell-Mann and Brueckner¹⁾ in the high density limit by the perturbation theory, while for the charged Bose gas, the one obtained by Foldy²⁾ by the Bogoliubov theory³⁾. Lee⁴⁾ redid the Foldy calculation by the Brandow boson linked-cluster expansion treating the particle number conservation exactly. ΔE given by (3.7) is interpreted as the contribution of the interactions between components to the ground state energy. It is automatically zero for the one-component systems.

As for the elementary excitations of the one component systems, the well-known elementary excitations are obtained from (3.8) , (3.3), and (2.9) with the well-known discussions as shown in Fig. 1 and Fig. 2.

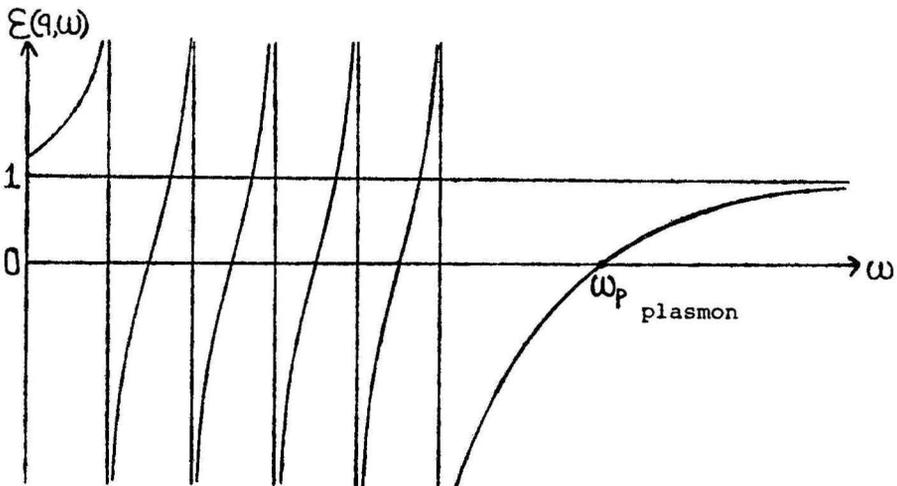


Fig. 1. $\epsilon(q, \omega)$ of the charged Fermi gas as the function of ω for the fixed q

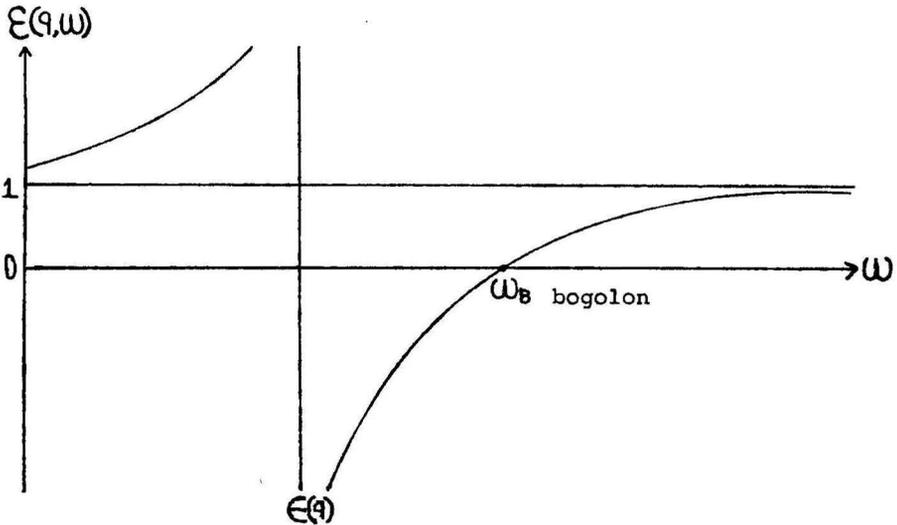


Fig. 2 $\epsilon(q, \omega)$ of the charged Bose gas

3.3 Bassichis⁵⁾ generalized the Bogoliubov method³⁾ for a Bose gas to the method to deal with a mixture of an arbitrary number of different species of Bose particles. Examining a neutral mixture of two types of charged Bose particles, he obtained two types of elementary excitations : the plasma type and the free-particle like. For the neutral, multi-component system consisting of different species of charged Bose particles, our theory yields essentially the same results as Bassichis'.

Let us consider the neutral, two-component, charged Bose system (BB, $i=1, 2$). The expression of the dielectric constant of BB is obtained from (3.8), (3.4), and (3.3). Fig. 3 shows its behaviors as a function of ω for the fixed q .

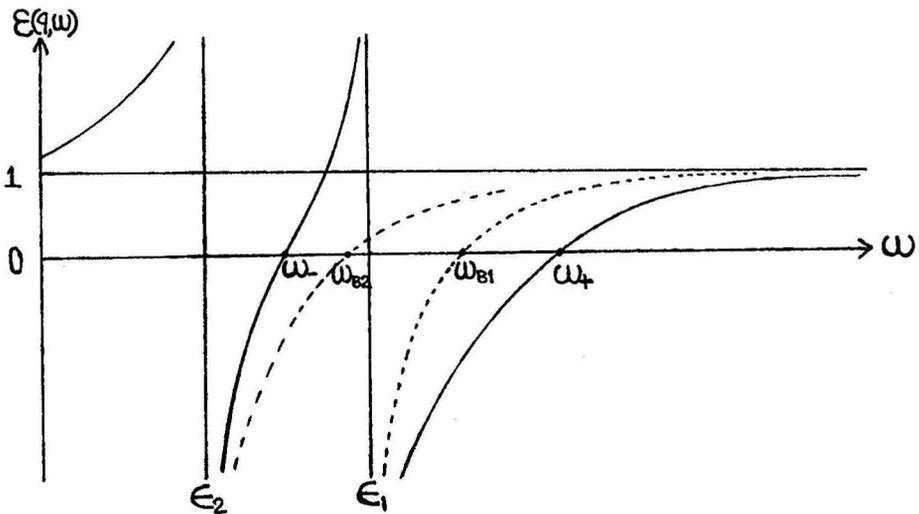


Fig. 3 $\epsilon(q, \omega)$ of BB. For the sake of comparison, the dielectric constant of each component in the absence of the interaction between components is shown by dotted curves.

The elementary excitations of BB are determined by (2.9) . As shown in Fig. 3, there are two types of elementary excitations, that is , $\omega = \omega_{\pm} - i \delta$:

$$\omega_{\pm} = \frac{1}{2} \left[(\omega_{B1}^2 + \omega_{B2}^2) \pm \{ (\omega_{B1}^2 + \omega_{B2}^2)^2 - 4(\epsilon_1^2 \epsilon_2^2 + \omega_1^2 \epsilon_2^2 + \omega_2^2 \epsilon_1^2) \}^{1/2} \right]^{1/2},$$

where $\omega_{B_i} = (\epsilon_i^2 + \omega_i^2)^{1/2}$ which gives the bogolon spectra of i -th component in the absence of the interaction between components. It is obviously seen that the shifts from ω_{B1} to ω_+ and from ω_{B2} to ω_- occur as the effect of the interaction between components. These excitations were obtained by Bassichis. The detailed discussions are found in his paper .

As for the ground state energy, we obtain from (3.6) as follows ;

$$E = E_{\text{corr}} = \sum_q \left\{ (\omega_+ - \epsilon_1 - v(q)e_1^2 n_1)/2 + (\omega_- - \epsilon_2 - v(q)e_2^2 n_2)/2 \right\}.$$

Let us consider the case that two species of Bose particles have equal mass and equal, but opposite charges, and let $m_1 = m_2 = m$, $|e_1| = |e_2| = e$, $n_1 = n_2 = n$, and $r_1 = r_2 = r_s$. In this case, the above energy can be calculated easily :

$$\begin{aligned} E &= \sum_q \frac{1}{2} \left\{ \left[\left(\frac{q^2}{2m} \right)^2 + \frac{4 \pi (2n) e^2}{m} \right]^{1/2} - \frac{q^2}{2m} - \frac{4 \pi (2n) e^2}{q^2} \right\} \\ &= (-0.803 r_s^{-3/4} \times 2^{1/4}) n m e^4, \end{aligned}$$

or, as the contribution of the interaction between components to the ground state energy, we have

$$\Delta E = 0.803 (1 - 2^{1/4}) r_s^{-3/4} n m e^4 .$$

Next, we consider BF, that is, the neutral, two-component system consisting of charged Fermi particles ($i=1$) and charged Bose particles ($i=2$). The low energy states of this system have been studied by Ginoza and Kanazawa⁶⁾ in the high density limit by the field theoretical treatment. The Bose component was treated by the Bogoliubov method. The discussion here reproduces completely the results obtained by them. The discussion in this paper is significant in that we can discuss BF as one of the various kinds of systems from the unified point of view without resort to the perturbation theory.

The contribution of the interaction between components to the ground state energy of BF is obtained from (3.8), (3.7), and (3.4). It is easily seen with the use of the relations (2.5) that the expresion (3.7) is the same as that obtained in the reference 6). This can be calculated exactly in terms of density parameter expansion at the high-density limit, resulting in

$$\Delta E / (n_2 m_2 e_2^2 / 2) = A r_2^{-1/4} + B (\log r_2)^2 + C (\log r_2) + D$$

where A and B is given in the reference 6).

Fig.4 shows the behaviors of the dielectric constant of BF as a function of ω for the fixed q .

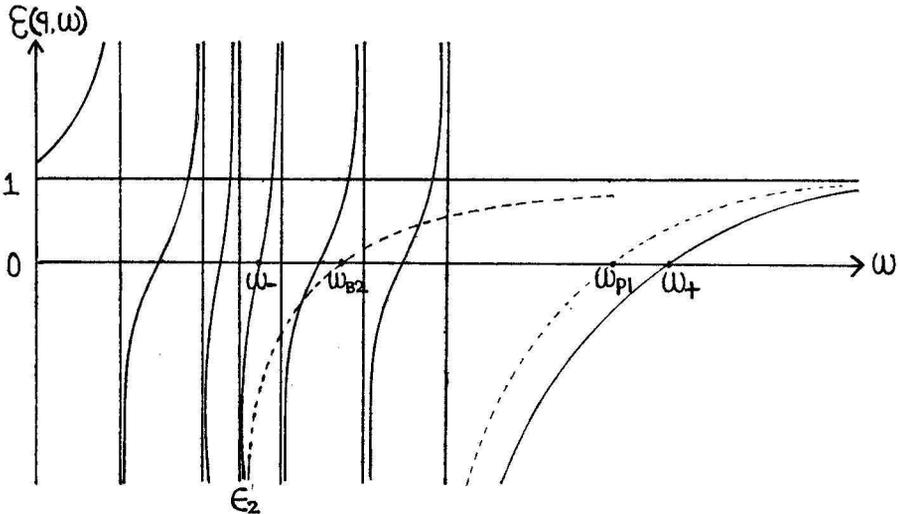


Fig. 4 $\epsilon(q, \omega)$ of BF

As shown in Fig.4, there are two types of collective excitations: optical phonon ω_+ and acoustic phonon ω_- . There are the shifts from ω_{P1} to ω_+ and from ω_{B2} to ω_- as the effect of the interaction between components. Since ω_- is in the continuum of the individual excitations, it has a finite life time. Further detailed discussions are given in the reference 6).

Finally, let us consider FF, that is, the neutral system consisting of two species of charged Fermi particles ($i=1, 2$). In Fig.5, the behaviors of the dielectric

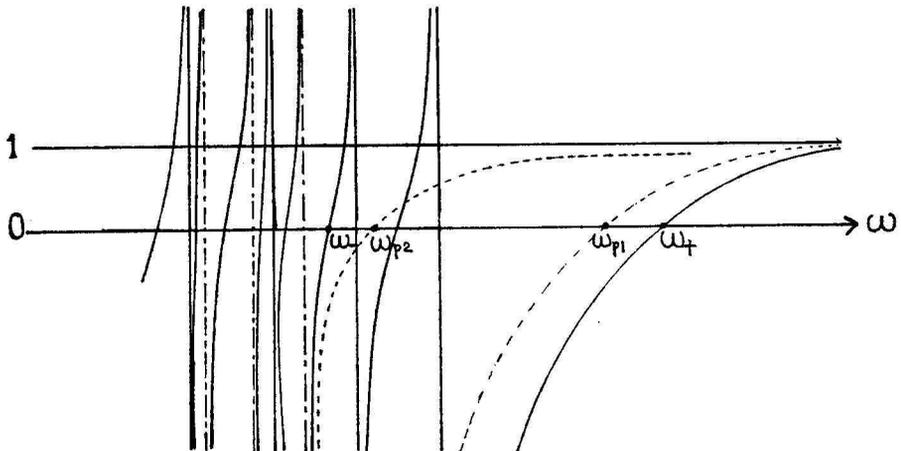


Fig. 5 $\epsilon(q, \omega)$ of the charged-Fermi and -Fermi system is drawn about the tops of continuum ($i=1$) and continuum ($i=2$) consisting of the Hartree-Fock individual excitations

constant of FF are drawn about the tops of the continuums consisting of the Hartree-Fock individual excitations ($i=1$ continuum, $i=2$ continuum), as the function of ω for the fixed q . There are two collective excitations. The dispersion relations of these are determined from (3.8), (3.3), and (2.9) and given at the low momentum as follows :

$$\omega_+ = \sqrt{\omega_1^2 + \omega_2^2} \left[1 + C_3 q^2 + \dots \right]$$

$$\omega_- = S_2 q$$

where C_3 and S_2 are the functions of mass, charge, and density. The excitation ω_- has a finite life time since it is in the continuum. Here also, the obvious shifts from ω_{P1} to ω_+ and from ω_{P2} to ω_- are seen as the effect of the interaction between components.

4. Summary

The dielectric formulation given by Nozieres and Pines has been applied to a multi-component, many-particle system with Coulomb interaction. This discussion is based on the fundamental assumptions listed below :

- (a) nonrelativistic motions for all particles
- (b) causality
- (c) time and spatial translational invariance
- (d) linearity of the response

The dielectric constant $\epsilon(q, \omega)$ of this system has been calculated with the random phase approximation (R. P. A.). It has been shown that this dielectric constant is analytic in the upper half of the complex ω -plane and satisfies the sum rule (2.8). The correlation energies and the elementary excitations of various kinds of systems with Coulomb interactions can be obtained on the basis of (3.8), (3.6), (3.3) and (2.9).

Fermi (F), Bose (B), Bose and Bose (BB), Bose and Fermi (BF), and Fermi and Fermi (FF) systems have been discussed within the R. P. A. It has been shown that for F, B, BB, and BF, the dielectric constant in the R. P. A. leads directly to the results of Gell-Mann and Brueckner, Foldy, Bassichis, and Ginoza and Kanazawa, respectively. For BB, especially in the case that two species of Bose particles have equal mass and equal, but opposite charges, the expression for the energy has been calculated :

$$E = (-0.803 r_S^{-3/4} \times 2^{1/4}) n m e^4 .$$

The collective excitations of the two-component systems at the low momentum as follows :

$$\text{For BB , } \omega_- = q^2 / 2M \text{ and } \omega_+ = \sqrt{\omega_1^2 + \omega_2^2} \left[1 + C_1 q^4 + \dots \right] .$$

$$\text{For BF , } \omega_- = S_1 q \text{ and } \omega_+ = \sqrt{\omega_1^2 + \omega_2^2} \left[1 + C_2 q^2 + \dots \right] .$$

$$\text{For FF , } \omega_- = S_2 q \text{ and } \omega_+ = \sqrt{\omega_1^2 + \omega_2^2} \left[1 + C_3 q^2 + \dots \right] .$$

where M , S_1 , S_2 , C_1 , C_2 , and C_3 are the functions of mass, charge, and density. This makes it obvious that the frequencies of these excitations at $q=0$ are independent of the statistics of the constitutive particles .

We are hoping to investigate these elementary excitations on the basis of the concept of the broken symmetry⁸⁾.

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