Note on the Nozieres-Pines Collective Approach to the Dielectric Constant

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Abstract

The extended Hamiltonian and the canonical transformation used in the Nozieres-Pines collective approach to the dielectric constant are discussed on the basis of the general theorem conjectured by Bohm, Huang, and Pines. And the corrected generating function in the transformation is given.

§ 1. Introduction

The dielectric constant serves as the unifying concept for the description of a many-particle system with Coulomb interaction.[1),2)] It can be calculated in a variety of ways, for example, the collective coordinate method,[3)] the Feynman-diagram method,[4)] etc.

For the statement of the aim of this paper and the preparations for the discussions in the following sections, let us review briefly the Nozieres-Pines collective approach to the calculation of the dielectric constant in solids. we consider a solid introduced the appropriate test-charge. The starting Hamiltonian for this system is (for convenience, $h=2\pi$)

$$H_{\text{ext}} = H + H_1 + H_2, \tag{1}$$

$$H = H_0 + \Sigma_k M_k^2 \rho_k \rho_{-k}/2,$$

$$H_1 = \Sigma_{k<k_c} [P_k P_{-k}/2 + M_k P_k \rho_{-k}],$$

$$H_2 = H_{\text{tc}} + \Sigma_{k<k_c} [M_k^2 r_k r_{-k}/2 + M_k^2 r_k \rho_{-k} + (M_k - \mu_k) r_k P_{-k}],$$

where $M_k^2 = 4\pi e^2/k^2$, H_0 is the Hamiltonian of the non-interacting Bloch electrons in the solid, H_{tc} the Hamiltonian of the test-charge fields which vibrate with the frequency Ω such as $[H_{\text{tc}}, r_k] = \Omega r_k$, P_k the collective coordinate describing the plasmon fields, and ρ_k and r_k the k-th density fluctuation operators of electrons and test-charges, respectively. The quantity μ_k is an, at present, arbitrary constant. Tnis extended Hamiltonian is equivalent to the Hamiltonian of the system in consideration, when we impose such

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subsidiary conditions on the eigenfunctions of H_{ext} as

$$P_k \Psi = 0 \quad (k < k_c). \tag{2}$$

The dielectric constant, $\varepsilon(k, \Omega)$, is defined such that the effective Coulomb interaction between the test-charges in the system described by (1) and (2) is written as

$$\Sigma_{k<k_c} \frac{M_k^2}{2\varepsilon(k, \Omega)} r_k r_{-k}. \tag{3}$$

In order to calculate the quantity (3), we must eliminate from (1) the plasmon-test charge and electron-test charge interactions by a canonical transformation. The first transformation to do this is that generated by $S' = -\Sigma_{k<k_c} M_k Q_k \rho_k$, where Q_k is the canonical conjugate of P_k. We then obtain the following Hamiltonian and subsidiary conditions,

$$H_{ext} = H_0 + H_{field} + H_{int} + H_{sr} + U + H_{tc} + \Sigma_{k<k_c} [(M_k - \mu_k) r_{-k} P_k + \mu_k M_k r_{-k} \rho_k + M_k r_k r_{-k}/2], \tag{4}$$

$$(P_k - M_k \rho_k)\Psi = 0 \qquad (k < k_c), \tag{5}$$

where H_{field} is the Hamiltonian of the plasmon fields with the classical plasma frequency, H_{int} that of the interaction between plasmon and electron, H_{sr} that of the short range interaction between electrons, and U the so-called random phase term. Next transformation is taken so as to eliminate from (4) and (5) the plasmon-test charge and electron-test charge interactions consistently. Nozieres and Pines performed this by the following generating function and obtained

$$\varepsilon(k,\Omega) = 1 + 2M_k^2 \Sigma_n \frac{\omega_{no} |(\rho_k)_{on}|^2}{\omega_{no}^2 - \Omega^2} \tag{6}$$

in the non-interacting Bloch-electron representation:

$$S = \Sigma_{k<k_c} (\alpha_k P_k + \beta_k Q_{-k} + F_k) r_{-k}, \tag{7}$$

where

(A) Static Case ($\Omega = 0$)

$$\alpha_k = 0,$$

$$\beta_k = \mu_k - M_k,$$

$$(F_k)_{mn} = \mu_k M_k i(\rho_k)_{mn} / \omega_{mn},$$

$$\mu_k = M_k / \varepsilon(k, 0).$$

(B) Dynamical Case ($\Omega \neq 0$)

$$\alpha_k = \frac{i}{\Omega} \left[\frac{M_k}{\varepsilon(k,\Omega)} - \mu_k\right],$$

$$\beta_k = M_k [1/\varepsilon(k, \Omega) - 1],$$
$$(F_k)_{mn} = i\frac{M_k}{\Omega}\left[\mu_k - \frac{M_k}{\varepsilon(k,\Omega)}\frac{\omega_{mn}}{\omega_{mn}+\Omega}\right](\rho_k)_{mn}, \tag{8}$$
$$\mu_k = \text{(freely chosen)}.$$

The transformation generated by this generating function in the dynamical case is unsuitable due to the following reasons:

(a) $\alpha_k^* \neq \alpha_{-k}$ and $(F_k)_{mn}^* \neq (F_{-k})_{nm}$ are easily shown. Therefore, the generating function is not hermitian and the transformation not unitary.

(b) As $\Omega \to 0$, the generating function diverges and the transformation is not well-defined.

(c) The existence of the difference in the treatment between the static case and the dynamical case is physically unnatural.

In this context, Nozieres and Pines chose μ_k as

$$\mu_k = M_k/\varepsilon(k, \Omega) \quad \text{for very low frequency,}$$
$$= 0 \quad \text{for high frequency.} \tag{9}$$

However, this choice can not remove the unsatisfactory points listed above.

The purposes of this paper are (i) throwing light upon the extended Hamiltonian (1) chosen by Nozieres and Pines (in § 2), (ii) clarifying the origin of the unsatisfactory points listed above, and giving the corrected transformation (in § 3).

§ 2. On the Nozieres - Pines extended Hamiltonian

In this section, let us discuss the extended Hamiltonian (1) chosen by Nozieres and Pines on the basis of a general theorem conjectured by Bohm, Huang, and Pines[5] (BHP). By this discussion, we see that μ_k is not taken quite arbitrarily.

BHP conjectured the general theorem whose mathematical statement is represented by

$$E_{\text{ext}}^0 \geqq E_0 \tag{10}$$

where E_0 is the ground state energy of a physical system (an original system) and E_{ext}^0 that of the system consisting of the original system and parametrically fixed external fields. If we work H_{ext} given by (1) in a representation in which all P_k and r_k are diagonal with eigenvalues P_k' and r_k', respectively, then we may consider H_{ext} to be the Hamiltonian for the electron system in the presence of the parametrically fixed external fields defined by $H_1 + H_2$.

The electrons are coupled to the external fields through $M_k P_k' \rho_{-k}$ and $M_k^2 r_k' \rho_{-k}$. Since these couplings are weak, we may regard $H_1 + H_2$ as the perturbation to the original system whose Hamiltonian is H. We consider the static test charge fields. Now, we can obtain the followings by the second-order perturbational calculation:

$$E_{ext}^0 - E_0 = \Sigma_{k<k_C} \left[\frac{P_k' P_{-k}' + M_k^2 r_k' r_{-k}'}{2\varepsilon(k, 0)} + \left(\frac{M_k}{\varepsilon(k, 0)} - \mu_k \right) P_k' r_{-k}' \right], \quad (11)$$

where $\varepsilon(k, 0)$ is the dielectric constant of the original system consistently given by the expression (6). This result is exact in the weak coupling limit, that is, $e^2 \to 0$.

Now according to the theorem (10), the right-hand side of (11) must always be positive. Since $\varepsilon(k, 0) > 0$, this fact is satisfied for *not any choiee but the specific values of* μ_k. For example, for the choices $\mu_k = M_k / \varepsilon(k, 0)$ or 0, the right-hand side of (11) is always positive. The discussion here may be satisfied also for the case that the test charge fields vibrate with the sufficiently low frequency so that the perturbation may be regarded as quasi-static.

If we choose μ_k for the sufficiently low frequency as $M_k / \varepsilon(k, \Omega)$, the quantities in (8) become

$$\begin{aligned} \alpha_k &= 0, \\ \beta_k &= M_k (1 / \varepsilon(k, \Omega) - 1), \\ (F_k)_{mn} &= \frac{iM_k^2}{\varepsilon(k, \Omega)} \frac{(\rho_k)_{mn}}{\omega_{mn} + \Omega}. \end{aligned} \quad (12)$$

The generating function (7) defined by these does not have the unsatisfactory points (b) and (c) described in § 1. This choice is the same as that of Nozieres-Pines given by (9), but there is the difference in the principle of the choice of μ_k. They chose μ_k so as to have an F_k as small as possible.

§ 3. The corrected collective approach to the dielectric constant

In the previous section, we suggested that μ_k is not quite arbitrary. In this section, by following the Nozieres-Pines transformation carefully, we shall clarify the origin of the unsatisfactory points described in § 1, and give the corrected transformation.

Now, we perform for (4) and (5) the transformation generated by (7) and expand them in the power series of S, or, r_k. In order to be eliminated the

linear terms in r_k in the transformed Hamiltonian, the following three relations must be satisfied among α_k, β_k and F_k:

$$\Omega[\Omega\,\varepsilon(k,\Omega)\;\alpha_k + i\,\varepsilon(k,\Omega)\;\mu_k - iM_k\,] = 0, \tag{13}$$

$$\beta_k = -M_k + \mu_k - i\Omega\,\alpha_k\,. \tag{14}$$

$$(F_k)_{mn} = iM_k\,[\,i\omega_{mn}\;\alpha_k + \mu_k\,]\;(\rho_k)_{mn}\,/\,(\omega_{mn} + \Omega), \tag{15}$$

where $\varepsilon(k,\Omega)$ is the function defined by (6). In order that our treatment is consistent, the linear terms in r_k in the transformed subsidiary condition must be also eliminated simultaneously. This self-consistency requirement results in

$$\beta_k = (i\Omega\,\alpha_k - \mu_k)\;[\,\varepsilon(k,\Omega) - 1\,]. \tag{16}$$

The quantity (3) is obtained from the transformed Hamiltonian and it is shown, with the use of the relations given above, that the function $\varepsilon(k,\Omega)$ is just the dielectric constant.

The substitution (14) into (16) gives us

$$\Omega\,\varepsilon(k,\Omega)\;\alpha_k + i\,\varepsilon(k,\Omega)\;\mu_k - iM_k = 0. \tag{16}'$$

It should be noted if (16)′ is satisfied, (13) is automatically satisfed, *but vice versa.* The main origin of the unsatisfactory points in the transformation of Nozieres and Pines may be related to this fact as understood from the following discussions.

In the first place, it was the way of Nozieres and Pines that μ_k is determined by the self-consistency requirement. In the static case, the self-consistency requirement is stated by (16)′, while (13) vanishes. They then could determine μ_k from (16)′. However, in the dynamical case, the self-consistency requirement is automatically satisfied since (13) is equivalent to (16)′. They then interpreted this fact as the self-consistency requirement was satisfied for any choice of μ_k. In fact, we see that all of α_k, β_k, F_k and μ_k can not be determined by (14), (15) and (16)′. Nevertheless, their interpretation is not correct.

Well, we saw in § 2 that μ_k is not quite arbitray. This suggests that there must exist another condition. We set the condition that the transformation must be unitary. Now, it is easy to determine α_k, β_k, F_k, and μ_k from (14), (15), (16)′, and the unitary conditions. We obtain $M_k\,/\,\varepsilon(k,\Omega)$ for μ_k and (12) for α_k, β_k, F_k in the range of the frequencies satisfying the following inequality;

$$\left| \frac{M_k^2}{\varepsilon(k,\Omega)} \frac{\Omega}{\omega_{mn}^2 - \Omega^2} (\rho_k)_{mn} \right| << 1 \quad .$$

Under this inequality, $F_k^+ = F_{-k}$.

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