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The total dielectric function of a metallic crystal

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Abstract. The total dielectric response of a solid has contributions from the polarizability of the electrons and that associated with ionic displacements. In this article, a method for evaluating the dielectric response of simple metals is developed. Using the dielectric function of the electron gas and the equation of motion of the ions, the explicit form of the total dielectric function is obtained. The features and applications of this method are discussed taking the example of Na. In the example, the corrections from the van der Waals interaction are evaluated and shown in the figures.

1. Introduction

The dielectric property of a metal is determined by the free electrons in it as well as by the lattice positions corresponding to its crystalline structure. The contribution of the ions has two components, one corresponding to their intrinsic induced polarization, and the other corresponding to the induced polarization associated with their displacements from equilibrium position. There have been some studies of the total dielectric response of a metal, which incorporates both the electronic and ionic contributions [1, 5].

The objective of this paper is to give directly the relationship between the total dielectric function of the metal and both the dielectric function of the constituent free electrons and that of the constituent ions through their vibration properties.

2. The equation of motion of charge fluctuations

In a simple metal represented by a monatomic lattice, we can assume that the equilibrium position of ions are at the lattice points $\{R_{i0}\}$, and the free electrons have the equilibrium density n_0 . The corresponding quantities for the disturbed system are $R_i = R_{i0} + u_i$ and $n_e(\mathbf{r}, t) = n_0(\mathbf{r}, t) + n(\mathbf{r}, t)$, where R_i is the instantaneous position of the i th ion and u_i is the displacement from R_{i0} , and $n(\mathbf{r}, t)$ is the induced electron density and $n_e(\mathbf{r}, t)$ is the total electron density. The Hamiltonian for the ionic system in the presence of an external test charge density $\rho_{\text{ext}}(\mathbf{r}, t)$ is then given by

$$\begin{aligned}
 H = & \sum_{i=1}^N \frac{P_i^2}{2M} + \frac{1}{2} \sum_{i \neq j}^N V(R_i - R_j) - Ze^2 \sum_{i=1}^N \int_{\Omega} n_e(\mathbf{r}, t) V^{ie}(\mathbf{r} - R_i) d^3r \\
 & + Ze \sum_{i=1}^N \int_{\Omega} \frac{\rho_{\text{ext}}(\mathbf{r}, t)}{|R_i - \mathbf{r}|} d^3r.
 \end{aligned} \tag{1}$$

P_i is the momentum of the i th ion with mass M , and (Ze) is its charge. N is a total number of ions in the system in the volume Ω . $V^{ie}(\mathbf{r} - \mathbf{R}_i)$ is the interaction potential between the ion at \mathbf{R}_i and the valence electron taking into consideration the pseudopotential of the ion. For simple metals such as Na, Al and Pb, we can choose an approximate pseudopotential in the form of a simple empty-core pseudopotential to evaluate the Hamiltonian [8]. The summation $V(\mathbf{R}_i - \mathbf{R}_j)$, which is the interaction potential of the ions at \mathbf{R}_i and \mathbf{R}_j , can be written in the form [16]

$$\sum_{i \neq j} V(\mathbf{R}_i - \mathbf{R}_j) = \text{constant} + \sum_{i \neq j} \mathbf{u}_i \mathbf{A}_{ij} \mathbf{u}_j \quad (2)$$

where

$$\mathbf{A}_{ij} = \sum_{\mathbf{k}} k k V_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R}_{i0} - \mathbf{R}_{j0})} \quad i \neq j \quad (3)$$

$$\mathbf{A}_{ii} = - \sum_{\mathbf{k}} \sum_j k k V_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R}_{i0} - \mathbf{R}_{j0})} \quad i \neq j. \quad (4)$$

Here $V_{\mathbf{k}} = V_{\mathbf{k}}^c + V_{\mathbf{k}}^{\text{nc}}$. $V_{\mathbf{k}}^c$ is the Coulombic part of the interaction given by $4\pi e^2/k^2$ and $V_{\mathbf{k}}^{\text{nc}}$ is the non-Coulombic part. The summation here is over all possible values of \mathbf{k} ; $V_{\mathbf{k}}$ is the Fourier transform of $V(\mathbf{r})$. Thus the equation of motion for the i th ion will be

$$M \frac{\partial^2 \mathbf{u}_i}{\partial t^2} = - \sum_j \mathbf{A}_{ij} \mathbf{u}_j + Ze^2 \nabla_i \sum_j \int_{\Omega} n_e(\mathbf{r}, t) V^{ie}(\mathbf{r} - \mathbf{R}_j) d^3r - Ze \nabla_i \int_{\Omega} \frac{\rho_{\text{ext}}(\mathbf{r}, t)}{|\mathbf{r} - \mathbf{R}_i|} d^3r. \quad (5)$$

3. Total dielectric function of the electron-ion system

The induced charge density from the small displacement of the ions, treating the ions as point charges, is

$$\rho_{\text{ion}}(\mathbf{r}, t) = Ze \sum_i [\delta(\mathbf{r} - \mathbf{R}_{i0} - \mathbf{u}_i) - \delta(\mathbf{r} - \mathbf{R}_{i0})]. \quad (6)$$

Since the external test charge density $\rho_{\text{ext}}(\mathbf{r}, t)$ is assumed to be small, the induced density of the electrons can be described in reciprocal space in the form,

$$-en(\mathbf{k}, \omega) = \left(\frac{1}{\epsilon_e(\mathbf{k}, \omega)} - 1 \right) [\rho_{\text{ext}}(\mathbf{k}, \omega) + \rho_{\text{ion}}(\mathbf{k}, \omega)]. \quad (7)$$

This follows from Gorobchenko's procedure [6]. Here $\epsilon_e(\mathbf{k}, \omega)$ is the electronic dielectric function.

Thus equation (5) in reciprocal space can be written in the form (after eliminating $n(\mathbf{k}, \omega)$, using equation (7)),

$$M\ddot{\mathbf{q}}_{\mathbf{k}} + N \left\{ \sum_m (\mathbf{k} + \mathbf{K}_m)(\mathbf{k} + \mathbf{K}_m)V'_{\mathbf{k}+\mathbf{K}_m} - K_m K_m V'_{K_m} \right\} \cdot \mathbf{q}_{\mathbf{k}} = -\frac{iM\omega_1^2 \rho_{\text{ext}}(\mathbf{k}, \omega) \mathbf{k}}{Ze\epsilon_e(\mathbf{k}, \omega)k^2} \quad (8)$$

where

$$V'_{\mathbf{k}} = V_{\mathbf{k}}^{\text{nc}} + V_{\mathbf{k}}^{\text{c}} + \left(\frac{1}{\epsilon_e(\mathbf{k}, \omega)} - 1 \right) V_{\mathbf{k}}^{\text{ie}} \quad \omega_1^2 = \frac{4\pi(Ze)^2 N}{MV}$$

and

$$\mathbf{q}_{\mathbf{k}} \equiv \sum_j \mathbf{u}_j e^{-i\mathbf{k} \cdot \mathbf{R}_{j0}}$$

If we consider the contribution to the induced charge only from the induced polarization associated with ionic displacements from equilibrium positions, the total induced charge density $\rho_{\text{in}}(\mathbf{r}, t)$ will be

$$\rho_{\text{in}}(\mathbf{r}, t) = -en(\mathbf{r}, t) + \rho_{\text{ion}}(\mathbf{r}, t). \quad (9)$$

Its form in reciprocal space is

$$\rho_{\text{in}}(\mathbf{k}, \omega) = -en(\mathbf{k}, \omega) + \rho_{\text{ion}}(\mathbf{k}, \omega). \quad (10)$$

The external test charge is assumed to have the form in space and time,

$$\rho_{\text{ext}}(\mathbf{r}, t) = \rho_{\text{ext}}(\mathbf{k}_0, \omega) e^{i\mathbf{k}_0 \cdot \mathbf{r} - i\omega_0 t}. \quad (11)$$

Using equations (7), (6) and (11) in (10), a brief calculation leads to

$$\rho_{\text{in}}(\mathbf{k}_0, \omega_0) = \left(\frac{1}{\epsilon_e(\mathbf{k}_0, \omega_0)} - 1 \right) \rho_{\text{ext}}(\mathbf{k}_0, \omega_0) - \frac{iZek \cdot \mathbf{q}_{\mathbf{k}}}{\epsilon_e(\mathbf{k}_0, \omega_0)}. \quad (12)$$

From equation (8), we get

$$\mathbf{q}_{\mathbf{k}} = -\frac{i\rho_{\text{ext}}(\mathbf{k}, \omega_0) \delta_{\mathbf{k}\mathbf{k}_0} \Phi^{-1} \cdot \mathbf{k}}{Ze\epsilon_e(\mathbf{k}, \omega_0)k^2} \quad (13)$$

where Φ is dynamic vibration matrix and has the form

$$\Phi(\mathbf{k}, \omega_0) = \frac{1}{\omega_1^2} \left[\frac{N}{M} \sum_m (\mathbf{k} + \mathbf{K}_m)(\mathbf{k} + \mathbf{K}_m)V'_{\mathbf{k}+\mathbf{K}_m} - K_m K_m V'_{K_m} - \omega_0^2 \mathbf{I} \right]. \quad (14)$$

Hence

$$\rho_{\text{in}}(\mathbf{k}_0, \omega_0) = \left(\frac{1}{\epsilon_e(\mathbf{k}_0, \omega_0)} - 1 \right) \rho_{\text{ext}}(\mathbf{k}_0, \omega_0) - \frac{\rho_{\text{ext}}(\mathbf{k}_0, \omega_0) \mathbf{k}_0 \cdot \Phi^{-1} \cdot \mathbf{k}_0}{\epsilon_e^2(\mathbf{k}_0, \omega_0) k_0^2}. \quad (15)$$

The definition of the total inverse longitudinal dielectric function $\epsilon_t(\mathbf{k}, \omega)$ is

$$\frac{1}{\epsilon_t(\mathbf{k}, \omega)} = 1 + \frac{\rho_{in}(\mathbf{k}, \omega)}{\rho_{ext}(\mathbf{k}, \omega)}. \tag{16}$$

Thus we finally get the explicit form of the total inverse dielectric function:

$$\frac{1}{\epsilon_t(\mathbf{k}_0, \omega_0)} = \frac{1}{\epsilon_e(\mathbf{k}_0, \omega_0)} - \frac{1}{\epsilon_e^2(\mathbf{k}_0, \omega_0)} \frac{\mathbf{k}_0 \cdot \Phi^{-1} \cdot \mathbf{k}_0}{k_0^2}. \tag{17}$$

If ω_0 is set equal to zero in formula (17), it has the same form as the formula given by Dolgov and Maksimov [5] for the static dielectric fomula. For a better understanding of the physics behind this formula, reading the work by them is recommended. They have very similar formulae.

As an example of the use of formula (17), we will discuss the dispersion relation for longitudinal charge oscillation modes in a metal at long wavelengths. The form of the electronic dielectric function at long wavelengths in the RPA is

$$\frac{1}{\epsilon_e(\mathbf{k}, \omega)} = 1 - \frac{\omega_p^2}{\omega_p^2 + \beta_e^2 k^2 - \omega^2} \tag{18}$$

β_e^2 is proportional to Fermi velocity, and hence $\beta_e^2 > 0$ [12].

In the small k region,

$$\Phi(\mathbf{k}, \omega) \approx \frac{1}{\omega_1^2} \left[\frac{N}{M} \mathbf{k} k V_k' - \omega^2 \mathbf{1} \right]$$

thus

$$\mathbf{k} \cdot \Phi^{-1} \cdot \mathbf{k} = \frac{k^2 \omega_1^2}{(N/M) V_k'^2 k^2 - \omega^2}.$$

If

$$\frac{N}{M} V_k'^2 k^2 = \frac{\omega_1^2}{\epsilon_e(\mathbf{k}, \omega)} + \beta_1^2 k^2$$

we can obtain the total dielectric function

$$\epsilon_t(\mathbf{k}, \omega) = 1 - \frac{\omega_e^2}{\omega^2 - \beta_e^2 k^2} - \frac{\omega_1^2}{\omega^2 - \beta_1^2 k^2}. \tag{19}$$

This can be obtained directly for a classical two-component plasma in the long wavelength limit [15]. β_1^2 is governed by the Coulombic and non-Coulombic interactions between two ions. We will discuss this in detail later.

If we set $\epsilon(\mathbf{k}, \omega) = 0$, the dispersion relations for small wavevector k [12] are

$$\begin{aligned} \omega_p^2 &\simeq \frac{1}{2} \left[\omega_p^2 + \beta_e^2 k^2 + \omega_1^2 + \beta_1^2 k^2 + \sqrt{(\omega_p^2 + \beta_e^2 k^2 - \omega_1^2 - \beta_1^2 k^2)^2 + 4\omega_1^2 \omega_p^2} \right] \\ &\simeq \omega_p^2 + \omega_1^2 + \frac{\omega_p^2 \beta_e^2 + \omega_1^2 \beta_1^2}{\omega_p^2 + \omega_1^2} k^2 \end{aligned} \tag{20}$$

$$\begin{aligned} \omega_\lambda^2 &\simeq \frac{1}{2} \left[\omega_p^2 + \beta_e^2 k^2 + \omega_1^2 + \beta_1^2 k^2 - \sqrt{(\omega_p^2 + \beta_e^2 k^2 - \omega_1^2 - \beta_1^2 k^2)^2 + 4\omega_1^2 \omega_p^2} \right] \\ &\simeq \frac{\omega_p^2 \beta_1^2 + \omega_1^2 \beta_e^2}{\omega_p^2 + \omega_1^2} k^2. \end{aligned} \tag{21}$$

We can find the longitudinal dispersion relations directly from equation (8). The way to achieve this is simply to find the roots of the equation. For long wavelengths, it has the form

$$\bar{q}_k + \frac{N}{M} V'_k k k \cdot q_k = 0. \quad (22)$$

We can then obtain the longitudinal dispersion relations through the equation of motion for $k \cdot q_k$,

$$k \cdot \bar{q}_k + \frac{N}{M} V'_k k^2 k \cdot q_k = 0. \quad (23)$$

Assuming the time dependence of $k \cdot q_k \propto e^{i\omega t}$, we get

$$-\omega^2 + \frac{N}{M} V'_k k^2 = 0. \quad (24)$$

Again, taking

$$\frac{N}{M} V'_k k^2 = \frac{\omega_1^2}{\epsilon_e(k, \omega)} + \beta_1^2 k^2$$

as before, and using (18), the solutions of (24) are obtained in the same form as (20) and (21).

4. Conclusion

It is widely believed that the net attraction leading to electron pair formation in a superconductor arises from the dielectric function at zero frequency, $\epsilon_t(k, 0)$, which occurs in the calculation of the energy gap in the BCS theory of superconductivity. It has been shown [3, 4, 9, 10] that at the static limit, $1/\epsilon_t(k, 0) \leq 1$. This condition is consistent with $\epsilon_t(k, 0)$ being negative for some values of k . For small wavevectors, however, $\epsilon_t(k, 0) > 0$ [10, 14] from the requirement that the compressibility of the medium must be positive [17].

We take equation (19) as a simple example to explore how and where $\epsilon_t(k, 0)$ can be negative. Since β_e^2 is positive, the only possibility for the total static dielectric function to be negative for small k is that β_1^2 is negative. In fact, β_1^2 is already known to be negative in the Coulomb lattice [16]. The non-Coulomb interaction between ions can accentuate this effect. The dominant non-Coulomb interaction is the attractive van der Waals interaction, the strength of which is determined by the polarizability of the ions [11, 13, 18].

We take a model which consists of point ions located on a lattice, which is embedded in a uniform non-responsive background electrons. The equation of motion of the j th ion has the form

$$M\ddot{u}_j = -\nabla_j \sum_i V^c(\mathbf{R}_i - \mathbf{R}_j) - \nabla_j \sum_i V^{nc}(\mathbf{R}_i - \mathbf{R}_j) \quad i \neq j. \quad (25)$$

V^{nc} is the van der Waals interaction and has the form

$$V^{nc}(r) \approx -\frac{1}{r^6} \frac{3\hbar}{\pi} \int_0^\infty \frac{d\xi \xi^4 \alpha_1(i\xi) \alpha_2(i\xi)}{(\omega_p^2 + \xi^2)^2} \quad (26)$$

where $\alpha_j(\omega)$ is the polarizability at the frequency ω of the j th ion. It can be assumed to have the form $\alpha_j(\omega) = e^2 n_j / m_e (\omega_j^2 - \omega^2)$ [13] where ω_j is the principal electronic absorption frequency. Equation (25) becomes

$$\Phi(k, \omega) \begin{pmatrix} q_{k(x)} \\ q_{k(y)} \\ q_{k(z)} \end{pmatrix} = 0 \quad (27)$$

where Φ is the dynamic vibration matrix in the uniform background model. It has the form

$$\Phi(k, \omega) = \frac{1}{\omega_1^2} \left[\frac{N}{M} \sum_m (k + K_m)(k + K_m) V_{k+K_m} - K_m K_m V_{K_m} - \omega^2 \mathbf{1} \right].$$

The elements of Φ are evaluated following the procedure of Clark [2] and have the following form for a body-centred-cubic lattice of sodium:

$$\begin{aligned} \Phi_{11} = & -\lambda^2 + S_{11} + \sum'_m \{ [F(K_m + k)](K_{mx} + k_x)^2 - F(K_m) K_{mx}^2 \} \\ & + \frac{1}{2\pi} \sum_l \left\{ G_l \left(\frac{6l_x^2}{l^2} - 2 \right) + H_l \left[\left(\frac{3}{l^2} + \frac{a^2 \eta}{2} \right) l_x^2 - 1 \right] \right\} \\ & \times [1 - \cos(\pi k_x l_x) \cos(\pi k_y l_y) \cos(\pi k_z l_z)] \\ & - A \left\{ \frac{20480}{81} [1 - \cos(\pi k_x) \cos(\pi k_y) \cos(\pi k_z)] + 82 [1 - \cos(2\pi k_x)] \right. \\ & \left. - 12 [2 - \cos(2\pi k_y) - \cos(2\pi k_z)] \right\} \quad (28) \end{aligned}$$

$$\begin{aligned} \Phi_{12} = & S_{12} + \sum'_m [F(K_m + k)](K_{mx} + k_x)(K_{my} + k_y) \\ & + \frac{1}{2\pi} \sum_l \left[G_l \frac{6l_x l_y}{l^2} + H_l \left(\frac{3}{l^2} + \frac{a^2 \eta}{2} \right) l_x l_y \right] \\ & \times [1 - \cos(\pi k_x l_x) \cos(\pi k_y l_y) \cos(\pi k_z l_z)] \\ & - \frac{2^{15}}{3^4} A \sin(\pi k_x) \sin(\pi k_y) \sin(\pi k_z). \quad (29) \end{aligned}$$

The dimensionless 'frequency' λ used here is related to the actual circular frequency ω by $\lambda^2 = \omega^2 / \omega_1^2$. The third terms in the right-hand side of (28) and (29) are from the van der Waals interaction. Here the prime denotes the omission of $m = 0$,

$$F(x) = \exp(-\pi^2 x^2 / a^2 \eta) / x^2$$

$$S_{ij} = F(k) k_i k_j$$

$$G_l = [1 - G(\frac{1}{2} \sqrt{\eta} a l)] / l^3$$

$$G(x) = (2/\sqrt{\pi}) \int_0^x \exp(-z^2) dz$$

$$H_l = (2a\sqrt{\eta}/\sqrt{\pi}) \exp(-\frac{1}{4} \eta a^2 l^2) / l^2$$

$$A = \frac{3\hbar(\omega_{Na} - 3\omega_p) \alpha_{Na}^2(0)}{32e^2 \pi a^5}$$

a is a lattice constant. η is an arbitrary parameter, the value of which is fixed to achieve rapid convergence in the series in the matrix elements in equation (28) and (29). The subscript l stands for the triad of integers l_x, l_y, l_z which are either all odd or all even. (h_x, h_y, h_z) are integers which are either all even or one even and two odd. The values of ω_{Na} and $\alpha_{\text{Na}}(0)$ are taken from [7]. The results are shown in figures 1 and 2. The corrections due to the van der Waals interaction are dependent on the ionic polarizability. Obviously, for Na, the corrections due to the van der Waals interaction are very small. For transition metals, large corrections can be expected because of higher ionic polarizability.

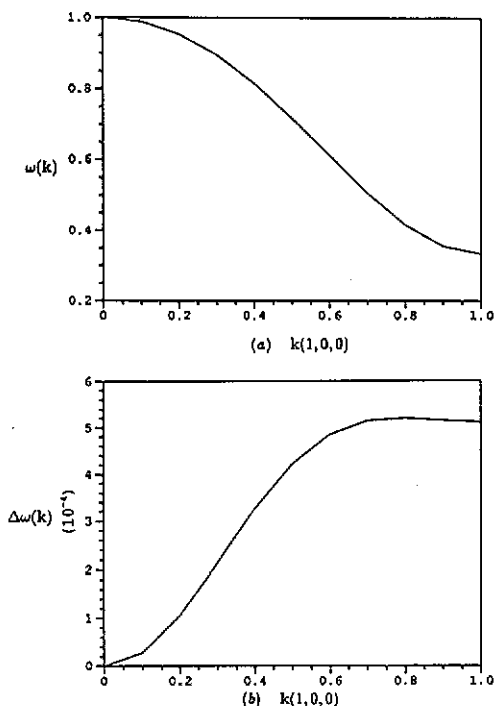


Figure 1. (a) The dispersion relation without the van der Waals interaction in a crystal of Na, along the direction $(1,0,0)$; (b) the difference between the dispersion relation with and without the van der Waals interaction in a crystal of Na, along the direction $(1,0,0)$.

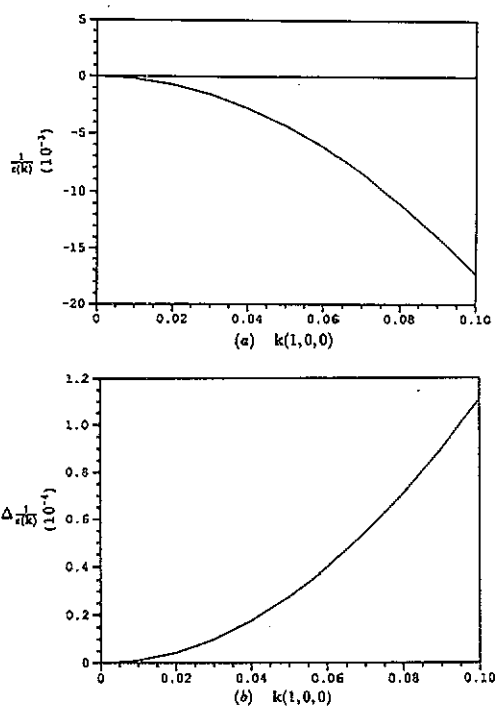


Figure 2. (a) The inverse total dielectric function without the van der Waals interaction in a crystal of Na, along the direction $(1,0,0)$ for small wavenumbers, in a unit of $(2\pi/a)$, a being the lattice constant; (b) the difference between the inverse total dielectric function with and without the van der Waals interaction in a crystal of Na, along the direction $(1,0,0)$.

Work is in progress for evaluating $\epsilon_t(k,0)$ for materials of interest in superconductivity.

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