Phenomenological derivation of the dielectric function of disordered conductors

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Abstract. For an electron gas which interacts with disordered scattering centers, the dielectric function $\varepsilon(\Omega)$ is rederived with phenomenological arguments. Elastic and inelastic scattering centers are considered. The derivation makes use of the dielectric function $\varepsilon_0(q, \omega)$ of the unperturbed electron liquid.

Introduction

The dielectric function $\varepsilon(\Omega)$ of an electron gas in interaction with static or dynamic scattering centers has already been derived quantum mechanically by several authors. Hopfield [1] found the imaginary part of $\varepsilon(\Omega)$ for static scatterers in second order perturbation theory. Helman et al. [2] used the Green's function technique to obtain $\varepsilon(\Omega)$ for static scatterers. As Dyson's equation was applied, the expression $\varepsilon(\Omega)$ is valid even for low frequencies. Pethick [3] solved the problem also with dynamic scattering by developing Kubo's formula up to second order in the scattering potential. In this form, the formula applies to high frequencies. Recently, del Castillo [4] extended the Green's function treatment to include dynamic scattering.

On the one hand the Green's function technique goes further in the perturbation treatment. On the other hand it assumes a static screening of the ions from the beginning, which is doubtful at high frequencies. Hopfield and Pethick obtain a dynamic screening. In all these results $\varepsilon(\Omega)$ can be expressed [5] in terms of the dielectric function of the unperturbed electron system. This circumstance suggests that $\varepsilon(\Omega)$ could be obtained by an argument which is phenomenological in the sense that it makes use of the dielectric function $\varepsilon_0(q, \omega)$ of the unperturbed electron system without calculating it. This work presents such a derivation. It leads to an expression which combines the advantages of the previous treatments.

The case of static scatterers

As a first step consider the electron gas without scatterers under the action of a homogeneous field $\vec{E}(t) = \vec{E} \exp(-i\Omega t)$. The resulting motion of the electrons

against the fixed positive background is transformed away using an oscillating coordinate system with origin $\vec{x}(t) = -(e/m\Omega^2)\vec{E}(t)$, where e and m are the charge and mass of the electrons.

The electrons interact with a static, disordered bare pseudo potential [6] $eV^b(\vec{r})$. In the oscillating frame of reference this has the form $eV^b(\vec{r} - \vec{x}(t))$. Since the electron gas with the field is a resting gas without field in this new frame of reference, the screening of the pseudo potential is determined by the dielectric function $\varepsilon_0(q, \omega)$. From the Fourier transform

$$V^b(\vec{q}, \omega) = \int d^3r \int dt \, \exp\left[-i(\vec{q}\vec{r} - \omega t)\right] V^b(\vec{r} - \vec{x}(t))$$

$$= \int dt \, \exp\left[-i(\vec{q}\vec{x}(t) - \omega t)\right] V_{\vec{q}}^b \tag{1}$$

the screened potential follows:

$$V(\vec{q}, \omega) = \frac{V^b(\vec{q}, \omega)}{\varepsilon_0(q, \omega)}. \tag{2}$$

From the Poisson equation the screening charge is

$$\rho(\vec{q}, \omega) = \frac{q^2}{4\pi} V^b(\vec{q}, \omega)\left[\frac{1}{\varepsilon_0(q, \omega)} - 1\right]. \tag{3}$$

The bare potential produces a field $-\vec{\nabla}V^b(\vec{r} - \vec{x}(t))$, which interacts with the screening charge leading to a force between the electrons and the scatterers. Its sign is such that it damps the motion.

$$\vec{F}(t) = -\int d^3r \, \rho(\vec{r}, t)\vec{\nabla}V^b(\vec{r} - \vec{x}(t))$$

$$= \frac{1}{4\pi} \int \frac{d^3q}{(2\pi)^3} \int \frac{d\omega}{2\pi} \int dt' i\vec{q}\, q^2 \, |V_{\vec{q}}^b|^2\left[\frac{1}{\varepsilon_0(q, \omega)} - 1\right]$$

$$\times \exp\left[i\,\vec{q}(\vec{x}(t) - \vec{x}(t'))\right] \exp\left[-i\omega(t - t')\right]. \tag{4}$$

The field $\vec{E}(t)$ and thus the factor $(\vec{x}(t) - \vec{x}(t'))$ in the exponent are arbitrarily small in a linear response theory. In the development

$$\exp\left(i\,\vec{q}(\vec{x}(t) - \vec{x}(t'))\right) = 1 + i\vec{q}(\vec{x}(t) - \vec{x}(t'))$$

the first term gives no contribution in the angular integration over $\vec{q}$ for an isotropic system. The second term gives

$$\vec{F}(t) = Nm\vec{x}(t)f(\Omega)$$

with

$$f(\Omega) = \frac{1}{3(2\pi)^3 mN} \int_0^\infty dq \, |V_{\vec{q}}^b|^2 q^6\left[\frac{1}{\varepsilon_0(q, \Omega)} - \frac{1}{\varepsilon_0(q, 0)}\right]. \tag{5}$$

The number of electrons N in the normalizing volume which is put equal to 1, has been included in the definition of $f(\Omega)$ to make this an intensive quantity. In the absence of scattering the relation between the outside field $\vec{E}$ and the polarization $\vec{P}_0$ is given by

$$4\pi\vec{P}_0 = (\varepsilon_0(\Omega) - 1)\vec{E} \tag{6}$$

where $\varepsilon_0(\Omega) = 1 - (\Omega_p/\Omega)^2$ with $\Omega_p^2 = 4\pi Ne^2/m$. In the presence of scattering an additional field $\vec{E}_{sc} = \vec{F}/Ne$ acts on the electronic charge Ne. Then the polarization becomes

$$4\pi\vec{P} = (\varepsilon_0(\Omega) - 1)(\vec{E} + \vec{E}_{sc}). \tag{7}$$

The dielectric constant in the presence of scattering is defined by

$$4\pi\vec{P} = (\varepsilon(\Omega) - 1)\vec{E}. \tag{8}$$

Since $\vec{P} = Ne\vec{x}$, the relation

$$\varepsilon(\Omega) = 1 - \frac{\Omega_p^2}{\Omega^2 - f(\Omega)} \tag{9}$$

follows. The correction term $f(\Omega)$ is related to a memory function [7]. When the bare potential is a superposition of localized pseudo potentials

$$V^b(\vec{r}) = \sum_j v^b(\vec{r} - \vec{R}_j), \tag{10}$$

where $\vec{R}_j$ is an ion position, then equation (5) becomes

$$f(\Omega) = \frac{1}{3(2\pi)^3 Nm} \int_0^\infty dq \, |v_q^b|^2 \, S^I(q) q^6 \left[\frac{1}{\varepsilon_0(q, \Omega)} - \frac{1}{\varepsilon_0(q, 0)}\right]. \tag{11}$$

Here $S^I(q) = \sum_{j,n} <\exp(i\vec{q}\vec{R}_j) \exp(-i\vec{q}\vec{R}_n)>$ is the static structure factor of the scatterers. To order $|v_q^b|^2$ this result coincides with that of Hopfield [1] and Pethick [3], whereas it differs from the quantum mechanical results of Helman [2] by order $[\varepsilon_L(q, \Omega) - \varepsilon_L(q, 0)]^2$ in the integrand, where Lindhard's function $\varepsilon_L(q, \omega)$ is used for $\varepsilon_0(q, \omega)$. This discrepancy arises from the fact that in the Green's function method static screening is used from the beginning. The logical consistency of starting with a statically screened potential is doubtful, but on the other hand a bare potential may not be a small perturbation.

Dynamic scatterers

We assume a time-dependent scattering potential

$$V^b(\vec{r}, t) = \sum_i v^b(\vec{r} - \vec{R}_i(t)) \tag{12}$$

where the $\vec{R}_i(t)$ are now ion position operators in the Heisenberg picture. Then the Fourier transform of the scattering potential in the oscillating frame becomes:

$$V^b(\vec{q}, \omega) = \int dt \, v_q^b \exp[-i(\vec{q}\vec{x}(t) - \omega t)]\rho_q^I(t) \tag{13}$$

where $\rho_{\vec{q}}^I(t) = \sum_j e^{-i\vec{q}\vec{R}_j(t)}$ is the time-dependent ion density operator. The two quantities in equation (4) $\rho(\vec{r}, t)$ and $\vec{\nabla} \cdot V^b(\vec{r}, t)$ involve in this case ion densities at different times which do not commute. The order of the factors becomes relevant; it is therefore not granted that a classical argument will lead uniquely to the correct expression. The previous reasonings have indeed to be supplemented by appropriate quantum mechanical considerations. The problem is to determine the correct statistical factors, which contain Planck's constant. This question does not occur in the high temperature limit for the ions. Then it suffices to replace the time-independent potential in (4) by (12) to obtain instead of (5)

$$f(\Omega) = \frac{1}{3(2\pi)^4 mN} \int_0^\infty dq\, q^6 |v_{\vec{q}}^b|^2 \int_{-\infty}^\infty d\omega\, S^I(q, \omega) \left[\frac{1}{\varepsilon_0(q, \Omega-\omega)} - \frac{1}{\varepsilon_0(q, -\omega)} \right]$$

(14)

where $S^I(q, \omega)$ is the dynamic structure factor of the ions. Using the relation [8]

$$\mathrm{Im} \frac{1}{\varepsilon_0(q, \omega)} = \frac{2\pi e^2}{q^2} [S^e(q, -\omega) - S^e(q, \omega)]$$

(15)

and Kramers–Kronig relations, (14) can be expressed in terms of the structure factor of the electrons $S^e(q, \omega)$:

$$f(\Omega) = -\frac{2e^2}{3(2\pi)^4 mN} \int_0^\infty dq\, q^4 |v_q^b|^2 \int_{-\infty}^\infty d\omega\, S^I(q, \nu - \omega)$$

$$\times [S^e(q, \omega) - S^e(q, -\omega)] \left(\frac{1}{\nu - \Omega - i\eta} - \frac{1}{\nu - i\eta} \right).$$

(16)

Note that (16) holds only in the ionic high temperature limit, when $S^I(q, \omega) = S^I(q, -\omega)$. The first term in the integrand is proportional to

$$\sigma(q, \nu) = \int_{-\infty}^{+\infty} d\omega\, S^I(q, \nu - \omega) S^e(q, \omega)$$

which is the structure factor for a virtual or real photon absorption with momentum and energy transfer q and ν respectively. The second term describes the corresponding emission which, generalized to all temperatures, must be written as

$$\sigma(q, -\nu) = \int_{-\infty}^{+\infty} d\omega\, S^I(q, \omega - \nu) S^e(q, -\omega)$$

in order to satisfy the detailed balance condition

$$\sigma(q, -\nu) = e^{-\beta\nu} \sigma(q, \nu).$$

(17)

The form of $f(\Omega)$ for all temperatures is therefore

$$f(\Omega) = -\frac{2e^2}{3(2\pi)^4 mN} \int_0^\infty dq\, q^4 |v_q^b|^2 \int_{-\infty}^\infty d\nu\, (1 - e^{-\beta\nu}) \sigma(q, \nu)$$

$$\times \left[\frac{1}{\nu - \Omega - i\eta} - \frac{1}{\nu - i\eta} \right].$$

Equation (18) used in (9) gives the dielectric function corrected for inelastic scattering of the electrons. It agrees to order $f(\Omega)/\Omega^2$ with Pethick's [3] result and extends it to low frequencies. It corrects the Green's function result of del Castillo [4] by including dynamic screening.

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