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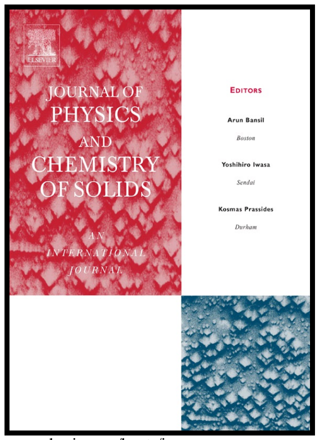

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Simple model dielectric functions for insulators

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Abstract

The Drude dielectric function is a simple way of describing the dielectric function of free electron materials, which have an uniform electron density in a classical way. The Mermin dielectric function describes a free electron gas, but is based on quantum physics. More complex metals have varying electron densities and are often described by a sum of Drude dielectric functions, the weight of each function being taken proportional to the volume with the corresponding density. Here we describe a slight variation on the Drude dielectric functions that describes insulators in a semi-classical way and a form of the Levine-Louie dielectric function including a relaxation time that does the same within the framework of quantum physics. In the optical limit the semi-classical description of an insulator and the quantum physics description coincide, in the same way as the Drude and Mermin dielectric function coincide in the optical limit for metals. There is a simple relation between the coefficients used in the classical and quantum approaches, a relation that ensures that the obtained dielectric function corresponds to the right static refractive index.

For water we give a comparison of the model dielectric function at non-zero momentum with inelastic X-ray measurements, both at relative small momenta and in the Compton limit. The Levine-Louie dielectric function including a relaxation time describes the spectra at small momentum quite well, but in the Compton limit there are significant deviations.

Keywords: dielectric function, inelastic x-ray scattering, Compton scattering, water, diamond

1. Introduction

Dielectric functions are pervasive in condensed matter physics. However, the full energy (ω) and momentum ($\boldsymbol{q}$) dependence of the dielectric function ($\epsilon(\omega, q) = \epsilon_1(\omega, q) + i\epsilon_2(\omega, q)$ with ϵ_1, ϵ_2 real) show intricate structures (see e.g. [1]) and is usually not fully known and thus widespread use is made of model dielectric functions. Knowledge of the dielectric function is also essential in medical physics to understand the penetration of charged particles in an organisms and the distribution of the associated 'damage'. The use of the dielectric function in this context has been reviewed recently [2]. Here we want to highlight some elementary properties of dielectric functions and present an alternative model dielectric function that can be of use for insulators.

2. Model dielectric functions

A frequently used model for metals is the Drude one based on the free-electron model which assumes that the target electrons have a homogeneous electron density. This Drude function (ϵ_D) is based on a classical approach and the energy loss function (ELF) $\mathrm{Im}\left[\frac{-1}{\epsilon_\mathrm{D}(\omega,q)}\right]$ is given by:

$$\mathrm{Im}\left[\frac{-1}{\epsilon_\mathrm{D}(\omega, q)}\right] = \frac{\omega\Gamma(q)\omega_i(0)^2}{(\omega^2 - \omega_i(q)^2)^2 + \omega^2\Gamma(q)^2} \tag{1}$$

and the corresponding real part:

$$\mathrm{Re}\left[\frac{1}{\epsilon_\mathrm{D}(\omega, q)}\right] = 1 + \frac{(\omega^2 - \omega_i(q)^2)\omega_i(0)^2}{(\omega^2 - \omega_i(q)^2)^2 + \omega^2\Gamma(q)^2}. \tag{2}$$

Here the plasma frequency ω_i is determined by the electron density N ($\omega_i = \sqrt{4\pi N}$, we use atomic units throughout, unless otherwise stated) and Γ is a damping constant. Both ω_i and Γ can depend on q, but for the Drude model we assume in the following that Γ does not depend on q.

For cases where the electron density is in-homogeneous one may consider the target as a sum of volumes with different electron densities. A volume fraction C_i has an electron density such that the plasmon energy is ω_i. The sum of all volume fraction should obviously add up to one: $\sum_i C_i = 1$. The dielectric function is then given by a weighted sum of their Drude functions . This approach has been quite useful for the determination of the ion stopping [3]. as well as the electron mean free path [4, 5]. The corresponding ELF is then:

$$\mathrm{Im}\left[\frac{-1}{\epsilon(\omega, q)}\right] = \sum_i C_i \frac{\omega\Gamma_i\omega_i(0)^2}{(\omega^2 - \omega_i(q)^2)^2 + \omega^2\Gamma_i^2} \tag{3}$$

and for the real part:

$$\mathrm{Re}\left[\frac{1}{\epsilon(\omega, q)}\right] = \sum_i C_i \left[1 + \frac{(\omega^2 - \omega_i(q)^2)\omega_i(0)^2}{(\omega^2 - \omega_i(q)^2)^2 + \omega^2\Gamma_i^2}\right] \tag{4}$$

Note that eq. 3 and eq. 4 only satisfy the Kramers-Kronig relations when $\sum C_i = 1$.

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