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Dynamic local field corrections for two-component plasmas at intermediate coupling

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Abstract
In non-ideal plasmas, the dielectric function has to be treated beyond the random phase approximation. Correlations as well as collisions have to be included. These corrections are known as (dynamical) local field corrections. Based on the Zubarev approach to linear response theory, a relaxation time approximation is proposed leading to an interpolation scheme between static local field corrections and the Drude model in the long-wavelength limit. The approach generalizes the Mermin approximation for the dielectric function and allows for the inclusion of a dynamical collision frequency. A numerical illustration is given for a classical two-component plasma at intermediate coupling.

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A multitude of experimental observables in the analysis of dense plasmas are directly linked to the (longitudinal) dielectric function $\epsilon(k, \omega)$. Examples range from the reflectivity and the absorption coefficient to the pair distribution function and the (dynamic) structure factor [1]. While the dielectric function for weakly coupled plasmas can be well described by the random phase approximation (RPA), it is necessary to include correlations into the dielectric function to address the physics of strongly coupled plasmas. Corrections beyond the RPA are traditionally described by the so-called local field corrections. For the interacting electron gas, local field corrections have been investigated in great detail since the pioneering work of Hubbard [2]. Also, approximative schemes for two-component plasmas have been developed [3]. For general wave vectors k and frequencies ω, the derived expressions tend to be very involved and tedious to calculate, see [4]. It is the objective of this paper to propose a scheme which interpolates between the static limit $\omega \to 0$ and the long-wavelength limit $k \to 0$. In the course of this task, we will generalize an approach due to Mermin [5] and derive an approximative expression for the response function of an electron–ion plasma in terms of local field corrections for the electron gas and an electron–ion collision frequency. To be specific, we consider a fully ionized two-component plasma of electrons and ions with temperature T and electron density n_e. The central quantities in our description are the partial density

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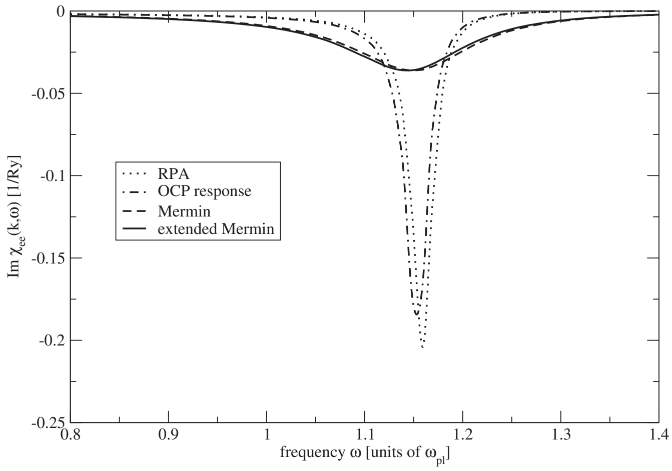

Figure 1. Imaginary part of the response function as a function of the frequency ω for wave vector $k = 0.3\ \kappa$. Parameters: $\Gamma = 0.5, \theta = 1$. Extended Mermin approach compared to other approximations.

response functions $\chi_{cc'}$, where c labels the species, $1/\epsilon(k,\omega) = 1 + \sum_{cc'} V_{cc'}(k)\chi_{cc'}(k,\omega)$. Local field corrections are introduced generalizing the random phase approximation via

$$\chi_{cc'}(k,\omega) = \chi_c^{(0)}(k,\omega)\delta_{cc'} + \chi_c^{(0)}(k,\omega)\Omega_0 V^s_{cc'}(k,\omega)\chi_{c'}^{(0)}(k,\omega),$$
$$V^s_{cc'}(k,\omega) = V_{cc'}(k)\,(1 - G_{cc'}(k,\omega))$$
$$+ \sum_d V_{cd}(k)\,(1 - G_{cd}(k,\omega))\,\chi_d^{(0)}(k,\omega)V^s_{dc'}(k,\omega),$$

where $V_{cc'}(k)$ is the Fourier transformed potential, Ω_0 is a normalization volume and $\chi_c^{(0)}$ is the response function for the non-interacting system. For $G_{cc'} = 0$, the RPA is recovered.

Mermin ansatz including local field corrections

Following Mermin [5], a relaxation time approximation that obeys particle number conservation, is given by

$$\chi^{(M)}_{\mathrm{ee}}(k,\omega) = \left(1 - \frac{\mathrm{i}\omega}{\eta}\right)\left(\frac{\chi_{\mathrm{RPA,e}}(k,\omega+\mathrm{i}\eta)\chi_{\mathrm{RPA,e}}(k,0)}{\chi_{\mathrm{RPA,e}}(k,\omega+\mathrm{i}\eta) - (\mathrm{i}\omega/\eta)\,\chi_{\mathrm{RPA,e}}(k,0)}\right), \tag{1}$$

where η is a parameter to be determined outside of the Mermin approximation. While this expression shows the desired Drude-like behaviour in the long-wavelength limit allowing to identify $\eta = \nu$ as a collision frequency, it fails to improve the static limit beyond the RPA result. Specifically, we have $\lim_{\omega\to 0}\chi(k,\omega) = \chi_{\mathrm{RPA,e}}(k,0)$ irrespective of the value of ν. We rectify this shortcoming of the Mermin approach by rederiving the approximation within the Zubarev approach to the non-equilibrium statistical operator. Starting from the Liouville–von Neumann equation for the statistical operator ρ , we approximate the general expression with the total Hamiltonian H_{tot} and $\eta \to 0$,

$$\frac{\partial\rho(t)}{\partial t} + \frac{\mathrm{i}}{\hbar}\,[H_{\mathrm{tot}}(t),\rho(t)] = -\eta(\rho(t) - \rho_{\mathrm{rel}}(t)),$$

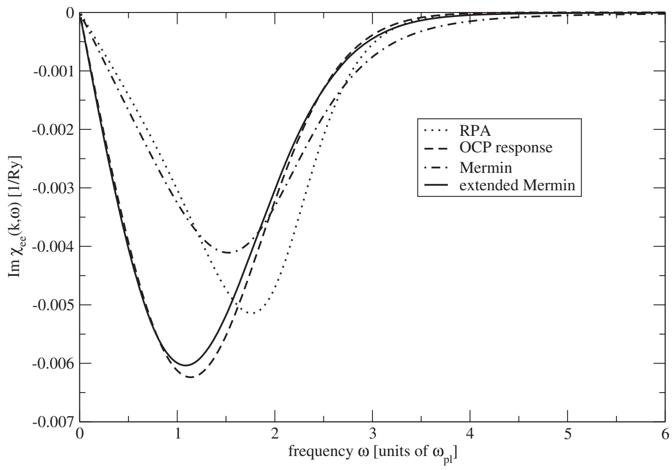

Figure 2. Imaginary part of the response function as a function of the frequency ω for wave vector $k = \kappa$. Parameters: $\Gamma = 4, \theta = 1$. Extended Mermin approach compared to other approximations.

by a relaxation time ansatz involving the external perturbation H_{ext}, the intra-species interactions, and a finite relaxation term η accounting for the electron–ion interaction

$$\frac{\partial \rho(t)}{\partial t} + \frac{\mathrm{i}}{\hbar}\left[H_{\text{kin}} + V_{ee} + V_{ii} + H_{\text{ext}}(t), \rho(t)\right] = -\eta\left(\rho(t) - \rho_{\text{rel}}(t)\right). \tag{2}$$

Using the Zubarev technique allows us to impose conserved quantities as self-consistency conditions on the relevant statistical operator ρ_{rel}. Proceeding along the lines presented in [6], the density response function $\chi_{cc'}$ is then given in linear response by correlation functions as

$$\chi_{cc'}(k,\omega) = -\beta\Omega_0 \frac{\left(n_k^c, n_k^{c'}\right)\left\langle n_k^c; \dot{n}_k^{c'}\right\rangle_{\omega+\mathrm{i}\eta}}{\left\langle n_k^c; \left(\dot{n}_k^{c'} + \mathrm{i}\omega n_k^{c'}\right)\right\rangle_{\omega+\mathrm{i}\eta}}. \tag{3}$$

$(.,.)$ is the Kubo product and $\langle .,. \rangle$ its Laplace transform. Replacing the Kubo products by response functions, the extended Mermin approximation reads

$$\chi_{ee}^{(\mathrm{xM})}(k,\omega) = \left(1 - \frac{\mathrm{i}\omega}{\eta}\right)\left(\frac{\chi_{ee}(k,\omega+\mathrm{i}\eta)\chi_{ee}(k,0)}{\chi_{ee}(k,\omega+\mathrm{i}\eta) - (\mathrm{i}\omega/\eta)\,\chi_{ee}(k,0)}\right), \tag{4}$$

where $\chi_{ee}(k,\omega)$ is the response function of interacting one-component electron gas. This expressions still results in a Drude-like form for $k \to 0$, while the static limit now reproduces the static local field correction, $\lim_{\omega\to 0} \chi_{ee}^{(\mathrm{xM})}(k,\omega) = \chi_{ee}(k,0)$.

Local field corrections for a classical two-component plasma

We present exploratory calculations which serve as a proof of principle taking $\Gamma = 0.5$ and $\Gamma = 4$ with $\theta = 1$. Here, we use the non-ideality parameter $\Gamma = e^2/(4\pi\epsilon_0 k_B T)\,(4\pi n/3)^{1/3}$ and the degeneracy parameter $\theta = (2m_e k_B T)/\hbar^2(3\pi n)^{-2/3}$ for a plasma with density n and temperature T, m_e being the electron mass. We consider an adiabatic model of interacting electrons scattering on randomly distributed but inert ions. $\chi_{ee}(k,\omega)$ is taken for a classical OCP where the static local field corrections are related to the static structure factor $S(k)$ via $G_{\text{ee}}(k) = 1 + k^2/\kappa^2(1 - 1/S(k))$, $\kappa = (e^2 n/\epsilon_0 k_B T)^{1/2}$ being the inverse Debye screening length. We approximate $G_{\text{ee}}(k,\omega) = G_{\text{ee}}(k)$. Also, the collision frequency is considered in

Born approximation with respect to a static screened potential $W_{ei}(q) = V_{ei}(q)/\epsilon_{\mathrm{RPA}}(q, 0)$, see [7],

$$\mathrm{Re}\nu(\omega) = \frac{\epsilon_0 \Omega_0^2}{6\pi^2 e^2 m_e} \int_0^\infty \mathrm{d}q\, q^6 W_{ei}^2(q) S_i(q) \frac{1}{\omega} \mathrm{Im}\epsilon_{\mathrm{RPA}}(q, \omega). \tag{5}$$

The frequency dependence of the collision frequency is neglected, $\nu(\omega) \approx \nu(0)$, to uncover the frequency dependence given by the Mermin approximation. Again, in order to keep things simple, we consider a uniform distribution of ions, i.e. $S_i = 1$. The RPA dielectric function is taken from [8]. The imaginary part for the response function in extended Mermin approximation is shown in figure 1 for $\Gamma = 0.5$, $k = 0.3\kappa$ and in figure 2 for $\Gamma = 4$, $k = \kappa$. For comparison, the original Mermin expression, the OCP response function and the RPA are presented as well. Figure 1 visualizes the broadening of the plasmonic excitation due to the account of collisions in both, the original Mermin and the extended Mermin approximation. On the other hand, for small values of ω, the extended Mermin approach approaches the static local field correction, as can be seen in figure 2. Improved calculations accounting for partial degeneracy, the frequency dependence of the collision frequency and dynamic local fields in the electronic subsystem are work in progress and subject of a forthcoming publication.

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