Interpolation between static local field corrections and the Drude model by a generalized Mermin approach

August Wierling

Universität Rostock, Institut für Physik, 18051 Rostock, Germany
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In non-ideal plasmas, the dielectric function has to be treated beyond the random phase approximation. Correlations and well as collisions have to be included. These corrections are known as (dynamical) local field corrections. With the help of 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. Exploratory calculations for a classical two-component plasma at intermediate coupling are presented.

I. INTRODUCTION

Many experimental observables in the analysis of dense plasmas are directly linked to the (longitudinal) dielectric function $\varepsilon(k, \omega)$. 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 $\omega$, the derived expressions tend to be very involved and tedious to calculate, see [4]. It is the objective of this communication to propose a scheme which interpolates between the static limit $\omega \rightarrow 0$ and the long-wave length limit $k \rightarrow 0$. 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 response functions $\chi_{cc'}$, where $c$ labels the species, $1/\varepsilon(k, \omega) = 1 + \sum_{cc'} V_{cc'}(k) \chi_{cc'}(k, \omega)$. Local field corrections are introduced generalizing the random phase approximation via

$$\chi_{cc'}(k, \omega) = \chi^{(0)}_{c}(k, \omega) \delta_{cc'} + \chi^{(0)}_{c}(k, \omega) \Omega_0 V_{cc'}(k, \omega) \chi^{(0)}_{c'}(k, \omega) ,$$

$$V_{cc'}(k, \omega) = V_{cc'}(k) (1 - G_{cc'}(k, \omega)) + \sum_{d} V_{cd}(k) (1 - G_{cd}(k, \omega)) \chi^{(0)}_{d}(k, \omega) V_{dc'}(k, \omega) ,$$

where $V_{cc'}(k)$ is the Fourier transformed potential, $\Omega_0$ is a normalization volume, and $\chi^{(0)}_{c}$ is the response function for the non-interacting system. For $G_{cc'} = 0$, the RPA is recovered.

II. MERMIN ANSATZ EXTENDED BY LOCAL FIELD CORRECTIONS

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

$$\chi^{(M)}_{cc}(k, \omega) = \left(1 - \frac{i \omega}{\eta}\right) \left(\frac{\chi_{RPA,c}(k, \omega + i \eta) \chi_{RPA,c}(k, 0)}{\chi_{RPA,c}(k, \omega + i \eta) - (i \omega/\eta) \chi_{RPA,c}(k, 0)}\right) , \quad (1)$$

*Electronic address: august.wierling@uni-rostock.de
where $\eta$ 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 $\lim_{\omega \to 0} \chi(k, \omega) = \chi_{RPA,ee}(k, 0)$ irrespective of the value of $\nu$. 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 $\rho$, we approximate the general expression with the total Hamiltonian $H_{tot}$ and $\eta \to 0$,

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

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

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

(2)

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

$$\chi_{cc'}(k, \omega) = \beta \Omega_0 \left( \frac{n_{k}^c n_{k}^{c'}}{\langle n_{k}^c \rangle \langle n_{k}^{c'} \rangle \omega + i\eta} \right) \langle \hat{n}_{k}^c; \hat{n}_{k}^{c'} \rangle \omega + i\eta .$$

(3)

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

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

(4)

where $\chi_{ee}(k, \omega)$ is the response function of the 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, $\lim_{\omega \to 0} \chi_{ee}^{(xM)}(k, \omega) = \chi_{ee}(k, 0)$.
III. DYNAMIC COLLISION FREQUENCY

A systematic approximation for the collision frequency in dense plasmas can be accomplished by a perturbative treatment of the force-force correlation function, see [7],

\[ \nu(\omega) = \frac{\beta \Omega_0}{\varepsilon_0 \omega_{pl}} \left\langle \hat{J}_0; \hat{J}_0 \right\rangle^{(2)}_{\omega+i\eta}. \]

\( J_0 \) is the current operator, \( \omega_{pl} \) is the plasma frequency. The collision frequency can be linked to a four-particle Green’s function. In particular, various effects such as dynamical screening and strong collisions relevant in non-ideal plasmas can be accounted for by partial summation of diagram sets. The net collision frequency in this so-called Gould-DeWitt approach is obtained as

\[ \nu(\omega) = \nu^{LB}(\omega) + \nu^{T}(\omega) - \nu^{Born}(\omega), \tag{5} \]

where \( \nu^{LB}(\omega) \) is the contribution due to loop diagrams, \( \nu^{T}(\omega) \) is the summation of ladder diagrams, and the Born expression has to be subtracted to avoid double counting. The interested reader is referred to Ref. [7] for details. Here, we give the final result for the first Born approximation with respect to a dynamical screened interaction, see [8],

\[ \nu^{LB}(\omega) = \frac{i\hbar}{\Omega_0 n_n e_i} \sum_q \frac{q^2}{3} V_{el}^2(q) \int \frac{\omega'}{\pi} \int \frac{\omega''}{\pi} \frac{n_B(\omega') - n_B(\omega'')}{(\omega + i\eta + \omega' + \omega'')(-\omega' - \omega'')} \times [\text{Im} \chi_{ee}(q, \omega' + i\eta) \text{Im} \chi_{ii}(-q, \omega'' + i\eta) - \text{Im} \chi_{ei}(q, \omega' + i\eta) \text{Im} \chi_{ie}(-q, \omega'' + i\eta)], \tag{6} \]

An adiabatic approximation with inert ions can be obtained from this expression by taking \( \chi_{ii}(q, \omega) = \chi_{ii}(q) \delta(\omega) \) and \( \chi_{ei}(q, \omega) = 0 \). We illustrate this discussion by presenting the collision frequency for a two-component plasma at solar core conditions \( n_e = 6.2 \times 10^{25} \text{ cm}^{-3}, \ T = 1.6 \times 10^7 \text{ K} \), see Fig. 1. As an example, we just compare the full Lenard-Balescu treatment of Eq. (6) with the adiabatic result indicated by \( m_i \rightarrow \infty \). Also, the Born result for a two-component system and for the adiabatic limit are shown. Most of the features are well known such as the difference between the two-component Born result and the adiabatic Lenard-Balescu expression at small frequencies due to a different account of screening. Similar, the jump in the adiabatic Lenard-Balescu expression at the plasma...
frequency is known to be an artifact of allowing for a undamped plasmon mode. Note, that the full calculation of 
Eq. (6) does not show such a behaviour. Instead, its overall shape is very similar to the Born approximations. The 
static limit is in accordance with a static investigation of screening in a two-component plasma of electrons and ions 
performed earlier, see [10].

![Image of a graph showing the imaginary part of the dielectric function as a function of the frequency ω for wave vector κ = k. Parameters: Γ = 4, θ = 1. Extended Mermin approach compared to other approximations.]

IV. EXPLORATORY CALCULATIONS FOR A CLASSICAL TWO-COMPONENT PLASMA

We present exploratory calculations which serve as a proof of principle taking Γ = 0.5 and Γ = 4 with θ = 1. We 
consider an adiabatic model of interacting electrons scattering on randomly distributed but inert ions. χ_{ee}(k, ω) is 
taken for a classical OCP where the static local field corrections are related to the static structure factor S(k) via 
G_{ee}(k) = 1 + k^2/κ^2 (1 − 1/S(k)), κ being the inverse Debye screening length. We approximate G_{ee}(k, ω) = G_{ee}(k).

In later applications, this has to be tuned to more realistic expressions. Also, the collision frequency is considered in 
Born approximation with respect to a static screened potential W_{ei}(q) = V_{ei}(q)/ε_{RPA}(q, 0) , see [3].

$$\text{Re} \nu(\omega) = \frac{\epsilon_0 \Omega_0^2}{6\pi^2 e^2 m_e} \int_0^\infty dq \, q^6 W_{ei}^2(q) \, S_{ii}(q) \, \frac{1}{\omega} \text{Im} \epsilon_{RPA}(q, \omega) .$$  (7)

The frequency dependence of the collision frequency is neglected, ν(ω) ≈ ν(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_{ii} = 1. The RPA dielectric function is taken from [8].

The imaginary part for the response function in extended Mermin approximation is shown in Fig. 2 for Γ = 0.5, k = 0.3 κ and in Fig. 3 for Γ = 4, k = κ. For comparison, the original Mermin expression, the OCP response function, and the RPA are presented as well. Figure 2 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 3. A similar situation is found for rather large values of k and Γ = 0.5 as in shown in Fig. 4. Here, the ideal response is given as well.

V. CONCLUSIONS

In this communication, we have proposed an interpolation scheme for the response function of a two-component 
plasma between the long-wavelength and the static limit. To this end, we combine the account of collisions via the 
Mermin ansatz with the local field description for the interacting electron gas. Thus, we obtain the broadening of
FIG. 4: Imaginary part of the dielectric function as a function of the frequency \( \omega \) for wave vector \( k = \kappa \). Parameters: \( \Gamma = 0.5, \theta = 1 \). Extended Mermin approach compared to other approximations.

the response function due to collisions in the long-wavelength limit as well as correlations beyond RPA in the static limit. Exploratory calculations have shown the expected limiting behavior and indicate a flattening of the plasmon dispersion relation as compared to the RPA.

Improved calculations accounting for partial degeneracy, the dynamics of the collision frequency, and dynamic local fields in the electronic subsystem are work in progress and subject of a forthcoming publication. In particular, standard approximations for dynamic local field correlations in the electron gas can easily be incorporated.

Acknowledgments

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[1] S. Ichimaru, Rev. Mod. Phys. 54, 1017 (1982).
[2] e.g. J. Hubbard, Proc. R. Soc London Ser. A 243, 336 (1957); K. Singwi, M.P. Tosi, R.H. Land, A. Sjölander, Phys. Rev. 176, 589 (1968); A.A. Kugler, J. Stat. Phys. 12, 35 (1975); K. Utsumi and S. Ichimaru, Phys. Rev. B 22, 5203 (1980); R.D. Dandrea, N.W. Ashcroft, A.E. Carlsson, Phys. Rev. B 34 2097 (1986); B. Farid, V. Heine, G.E. Engel, I.J. Robertson, Phys. Rev. B, 48 11602 (1993); J. Hong and M.H. Lee, Phys. Rev. Lett. 70, 1972 (1993); C.F. Richardson and N.W. Ashcroft, Phys. Rev. B 50, 7284 (1994); and references therein.
[3] e.g. S. Ichimaru, S. Mitake, S. Tanaka, X.-Z. Yan X-Z, Phys. Rev. A 32 1768 (1985); S.V. Adamyan, I.M. Tkachenko, J.L. Munoz-Cobo Gonzalez, and G. Verdu-Martin, Phys. Rev. E 48, 2067 (1993); J. Daligault and M.S. Murillo, J. Phys. A: Math. Gen. 36, 6265 (2003).
[4] G. Röpke, R. Redmer, A. Wierling, H. Reinholz, Phys. Rev. E 60, R2484 (1999).
[5] N.D. Mermin, Phys. Rev. B 1, 2362 (1973).
[6] G. Röpke, A. Selchow, A. Wierling, and H. Reinholz, Phys. Lett. A 260, 365 (1999).
[7] H. Reinholz, R. Redmer, G. Röpke, and A. Wierling, Phys. Rev. E 62, 5648 (2000).
[8] N.R. Arista and W. Brandt, Phys. Rev. A 29, 1471 (1984).
[9] A. Selchow, G. Röpke, A Wierling, H. Reinholz, T. Pschiwul and G. Zwicknagel, Phys. Rev. E 64, 056410 (2001).
[10] G. Röpke, Phys. Rev. A 38, 3001 (1988).