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Dynamics of strongly correlated ions in a partially ionized quantum plasma

P. Ludwig, M. Bonitz, and H. Kählert

Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität zu Kiel,
24098 Kiel, Germany

J.W. Dufty

Department of Physics, University of Florida, Gainesville, FL 32611, USA

Abstract. A scheme which allows to compute the dynamics of strongly correlated classical ions embedded into a partially ionized quantum plasma by first principles molecular dynamics is presented. The dynamically screened dust approach of Joyce and Lampe [Phys. Rev. Lett. **88**, 095006 (2002)] is generalized to quantum systems. The electrons are treated fully quantum-mechanically taking into account their dynamical screening of the ion-ion interaction in linear response on the basis of an extended Mermin formula. The scheme allows to include the effect of the electron dynamics, electron streaming, wake effects and electron magnetization.

1. Introduction

Strong correlation effects in ensembles of charged particles are of high importance in many fields of physics, including dense plasmas, e.g. [1, 2], the electron-hole plasma or electrons in quantum dots [3], for a recent overview see [4] and references therein. The present paper is devoted to a strongly coupled mass-asymmetric two-component plasma where only the heavy component (typically the ions) is strongly coupled whereas the light component (e.g. electrons) is weakly coupled. Such a situation is expected in various compact astrophysical systems including white dwarf stars or the crust of neutron stars where one expects ion crystallization [5]. Another relevant situation are dense laboratory plasmas produced by laser or ion beam irradiation of matter where initially again a strongly coupled ion plasma is formed – so-called “warm dense matter”, for a recent overview see the article by Gericke et al. in this volume [6]. A sketch of the density-temperature plane in this parameter range is shown in Fig. 1.

The parameters of interest for the present work are indicated by the shaded area in Fig. 1. There the ions (electrons) are classical (quantum) characterized by a degeneracy parameter $\chi_a = n_a \Lambda_a^3$ smaller (larger) than unity, with the DeBroglie wave length $\Lambda_a = h/(2\pi m_a k_B T_a)^{1/2}$. Our main interest is to describe strong ion coupling characterized by $\Gamma_i = q_i^2/(\bar{r}_i k_B T_i) > 1$, whereas the quantum coupling parameter (Brueckner parameter) of the electrons is small, $r_{se} = \bar{r}_e/a_B \ll 1$. In recent years there have been numerous attempts to develop simulations for such systems, based on path integral Monte Carlo (PIMC) [7, 8], quantum molecular dynamics (QMD) [9, 10] or the Wigner formalism (WMD) [11]. The best dynamical results so far have been obtained from QMD, however, these simulations involve a density functional treatment of the electrons which is very time-consuming. Moreover, current versions usually neglect the

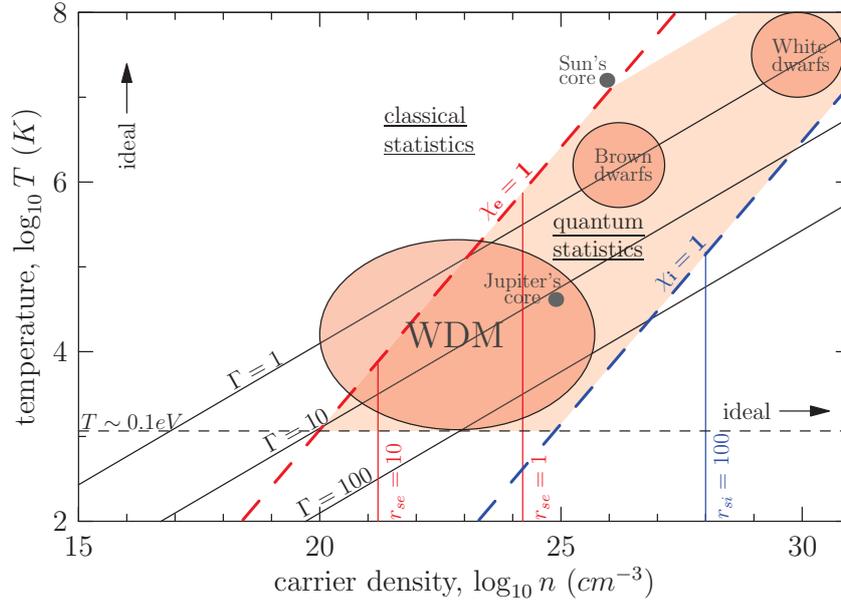


Figure 1. Phase diagram of a two-component plasma of electrons and singly charged ions in thermodynamic equilibrium with a few astrophysical examples (WDM denotes “warm dense matter”). The line $\chi_e = 1$ [$\chi_i = 1$] separates the region of classical (upper left) and quantum (lower right) behavior of the electrons [ions]. Also, the lines of constant classical (Γ) and quantum (r_s) coupling strength are shown. The present model applies to the shaded area.

dynamics of the electron subsystem. However, for dense electron-ion plasmas dynamics of the electrons, in particular dynamical screening, is expected to be important.

The approach of this paper includes these effects. It takes advantage of the weak electron coupling in the plasma phase. At the same time the ion dynamics are treated exactly, via semiclassical molecular dynamics. The model and approximations leading to effective Newtonian equations for the ions are introduced in Sec. 2. In Sec. 3 we derive the effective ion-ion pair potential which is dynamically screened by the electrons. The Mermin dielectric function is recalled in Sec. 4. A detailed derivation in the frame of quantum kinetic theory is given in the appendix. Results are summarized in Sec. 5.

2. Basic equations and approximations

The nonequilibrium dynamics of the ions in a partially ionized plasma consisting of electrons (e), ions (i), and neutrals (n) can be described by the reduced density operator for the ions, given by [12, 13]

$$i\hbar \frac{\partial \hat{F}_i(1, \dots, N_i)}{\partial t} - [\hat{H}_i(1, \dots, N_i), \hat{F}_i(1, \dots, N_i)] = \sum_{b=e,n} \sum_{k=1}^{N_i} n_b T r_{2_b} [\hat{V}_{ib}(k, 2_b), \hat{F}_{ib}(1, \dots, N_i; 2_b)], \quad (1)$$

where $b = e, n$, and $\hat{F}_{ib}(1, \dots, N_i; 2_b)$ is the joint density operator for N_i ions and one particle of type b . $\hat{H}_i(1, \dots, N_i)$ is the hamiltonian for the ions in the presence of an external field (ϕ, \mathbf{A}) and their mutual interactions

$$\hat{H}_i(1, \dots, N_i) = \sum_{k=1}^{N_i} \left[\frac{1}{2m_k} \left(\frac{\hbar}{i} \nabla_k - \frac{e_i}{c} \mathbf{A}(\mathbf{r}_k, t) \right)^2 + e\phi(\mathbf{r}_k, t) \right] + \frac{1}{2} \sum_{k \neq \ell}^{N_i} V_{ii}(|\mathbf{r}_k - \mathbf{r}_\ell|), \quad (2)$$

where \mathbf{A} and ϕ denote the vector and scalar potential of an external electromagnetic field, and \widehat{V}_{ib} is the operator of binary interactions between an ion and particle of type b . Quantum exchange effects of the ions will be irrelevant and are neglected in (1).

We now start to simplify this equation and to determine effective Newtonian equations of motion for the ions. Since the electrons are assumed strongly degenerate and weakly coupled, also the electron-ion interaction on the r.h.s. of (1) is weak and $\widehat{F}_{ie}(1, \dots, N_i; 2_e) \simeq \widehat{F}_i(1, \dots, N_i)\widehat{F}_e(2_e)$. In this approximation the electron contribution to the r.h.s. becomes $n_e Tr_{2_e} \left[\widehat{V}_{ie}(k, 2_e), \widehat{F}_{ib}(1, \dots, N_i; 2_e) \right] \simeq \left[\widehat{W}_{ie}(k), \widehat{F}_i(1, \dots, N_i) \right]$, where we defined the mean field (Hartree potential) for the ions which is created by the electrons, $\widehat{W}_{ie}(k) \equiv n_e Tr_{2_e} \widehat{V}_{ie}(k, 2_e)\widehat{F}_e(2_e)$. This gives rise to an effective single particle Hamiltonian for each ion $\widehat{H}_i(1) = \widehat{H}_i(1) + \widehat{W}_{ie}(1)$ [here $\widehat{H}_i(1)$ denotes the expression under the first sum in Eq. (2)] so that equation (1) becomes

$$i\hbar \frac{\partial \widehat{F}_i(1, \dots, N_i)}{\partial t} - \left[\widehat{H}_i(1, \dots, N_i), \widehat{F}_i(1, \dots, N_i) \right] = \sum_{k=1}^{N_i} n_n Tr_{2_n} \left[\widehat{V}_{in}(k, 2_n), \widehat{F}_{in}(1, \dots, N_i; 2_n) \right], \quad (3)$$

where $\widehat{H}_i(1, \dots, N_i)$ is given as in (2) except with the single particle hamiltonians $\widehat{H}_i(k)$ replacing $\widehat{H}_i(1)$. The l.h.s describes the effective ion dynamics driven by ion-ion and mean field ion-electron interactions, and the r.h.s. is due to the interactions with the neutrals.

Since the coupling between ions and neutrals is expected to be much weaker than between ions, an approximate treatment of the neutrals can be applied. In the following, we assume that the neutrals are close to thermodynamic equilibrium. Then the collision integral between ions and neutrals, I_{in} , can be treated using a Fokker-Planck type integral with an effective ion-neutral collision frequency ν_{in} and a diffusion coefficient D_n . The two coefficients are used as input parameters to our model. Next we take into account that the ions are classical (we briefly discuss the inclusion of quantum corrections in Sec. 5) and perform the classical limit in Eq. (3). This leads to a classical kinetic equation for the phase space distribution and possible quantum corrections [12], which is equivalent to (its characteristics are) the one set of the following Newton's equations

$$\frac{d\mathbf{p}_k}{dt} = \left(-\frac{dW_{ie}(\mathbf{r})}{d\mathbf{r}} + e_i \mathbf{E}(\mathbf{r}, t) + \frac{e_i}{c} [\mathbf{v}_k \times \mathbf{B}(\mathbf{r}, t)] \right) \Big|_{\mathbf{r}=\mathbf{r}_k} + \mathbf{F}^{i,n}(\mathbf{r}_k, \mathbf{p}_k, t), \quad k = 1, \dots, N_i, \quad (4)$$

$$\frac{d\mathbf{p}_k}{dt} = -\frac{d}{d\mathbf{r}} \left(V_i^{\text{eff}}(\mathbf{r}, t) + e_i \phi^{\text{ext}}(\mathbf{r}, t) \right) \Big|_{\mathbf{r}=\mathbf{r}_k} + \mathbf{F}^{i,n}(\mathbf{r}_k, \mathbf{p}_k, t), \quad k = 1, \dots, N_i, \quad (5)$$

The first line corresponds to the general case of an electromagnetic field (\mathbf{E}, \mathbf{B}) produced by external sources and the ions which follows from the solution of Maxwell's equations. The potential W_{ie} produced by the electrons has been separated for clarity. The second line corresponds to the case of a pure electrostatic field which is composed by an external potential ϕ^{ext} plus the total effective ion-ion interaction energy $V_i^{\text{eff}}(\mathbf{r}, t) = e_i \sum_{l=1}^{N_i} \phi_l(\mathbf{r}, t)$. Here ϕ_l is the electrostatic potential produced by ion "l" in the partially ionized plasma which will be computed in Sec. 3. Finally, $\mathbf{F}^{i,n}(\mathbf{r}_k, \mathbf{p}_k)$ describes the force acting on ion "k" from the neutral particles. Due to the weak coupling between ions and neutrals in the plasma this effect is expected to be of minor importance. Starting from the Fokker-Planck form of the collision term I_{in} the effect of the neutrals in the classical equations of motion will be a combination of a friction force plus a random force y , i.e., $\mathbf{F}^{i,n}(\mathbf{r}, \mathbf{p}, t) = -\nu_{in}\mathbf{p} + \mathbf{y}(t)$ where the amplitude of the random force will be proportional to $\sqrt{D_n}$.

In Eqs. (4), (5) we have fully retained ion-ion correlations and fluctuations and are, thus, able to treat strong correlation effects in principle exactly. The quality of the solutions thereby

depends on the quality of the potential energy V_i^{eff} which is affected (screened) by the electrons. Of particular interest for us is to include nonequilibrium situations in warm dense matter such as streaming electrons and ions, particle beams and so on. Then a full dynamic treatment of the pair interaction is crucial which we discuss now.

3. Dynamically screened ion-ion pair potential

Let us now compute the potential of a single ion moving relative to the electrons, taking into account the dielectric properties of the (unmagnetized) plasma. We start with the case of a classical charged particle, e.g. [14], and then generalize the result to quantum particles.

The Poisson equation for a polarizable medium reads ($n(\mathbf{r})$ is the number density of charged particles and n_k its Fourier component)

$$\text{div}\mathbf{D}(\mathbf{r}, t) = 4\pi e_a n_a(\mathbf{r}, t), \quad (6)$$

which, in Fourier space, becomes $i\mathbf{k} \cdot \mathbf{D}_k(t) = 4\pi e_a n_{ak}(t)$. The electrostatic potential ϕ created by the charge density on the right is $\mathbf{E}(\mathbf{r}) = -\nabla\phi(\mathbf{r})$, corresponding, in Fourier space, to $\mathbf{E}_k = -i\mathbf{k} \cdot \phi_k$. Together with the electrodynamic definition of the dielectric tensor, $D_{k,i} = \sum_j \epsilon_{k,ij} E_{k,j}$, $i, j = 1, 2, 3$, and Eq. (6) we obtain

$$\phi_k(\omega) = \frac{4\pi e_a n_{ak}(\omega)}{\sum_{ij} k_i k_j \epsilon_{k,ij}(\omega)}. \quad (7)$$

Consider now the case of a classical point charge ‘‘a’’ with initial position $\mathbf{r}(0) = \mathbf{r}_{0a}$, moving with constant velocity \mathbf{v}_a (relative to the carriers creating the dielectric function). Then

$$n_a(\mathbf{r}, t) = \delta[\mathbf{r} - \mathbf{r}_{0a} - \mathbf{v}_a t], \quad (8)$$

with the Fourier representation

$$n_{ak}(\omega) = 2\pi e^{-i\mathbf{k}\mathbf{r}_0} \delta[\omega - \mathbf{k}\mathbf{v}_a]. \quad (9)$$

Inserting this result into (7) and performing the back transform we obtain

$$\phi(\mathbf{r}, t; \mathbf{v}_a) = e_a \int \frac{d^3k}{2\pi^2} \frac{e^{i\mathbf{k}(\mathbf{r} - [\mathbf{r}_{0a} + \mathbf{v}_a t])}}{\sum_{ij} k_i k_j \epsilon_{k,ij}(\mathbf{k}\mathbf{v}_a)}. \quad (10)$$

For the special case of an isotropic medium, ϵ_{ij} has only two independent components. Concentrating on longitudinal plasma oscillations we can replace $k_i k_j \epsilon_{k,ij} \rightarrow k^2 \epsilon_k$, and the potential (10) and its Fourier transform become

$$\phi_k(\omega) = \frac{4\pi e_a n_{ak}(\omega)}{k^2 \epsilon_k(\omega)}, \quad (11a)$$

$$\phi(\mathbf{r}, t; \mathbf{v}_a) = \int \frac{d^3k}{2\pi^2} \frac{e_a e^{i\mathbf{k}(\mathbf{r} - [\mathbf{r}_{0a} + \mathbf{v}_a t])}}{k^2 \epsilon_k(\mathbf{k}\mathbf{v}_a)}. \quad (11b)$$

This result may be immediately generalized to the case of many particles. Indeed, due to linearity of Maxwell's equations, the resulting total potential is simply the sum of all potentials of the type (10), i.e. $\phi^{\text{tot}}(\mathbf{r}) = \sum_{a=1}^N \phi(\mathbf{r} - \mathbf{r}_{0a}; \mathbf{v}_a)$. From this we obtain the total potential energy entering Newton's equations (5)

$$V_i^{\text{eff}}(\mathbf{r}, t) = \sum_{a=1}^{N_i} e_a \phi(\mathbf{r} - \mathbf{r}_{0a}; \mathbf{v}_a). \quad (12)$$

We underline that this is an exact result fully including the ion-ion interaction (assuming point ions) in the presence of a partially ionized plasma the properties of which are included in the dynamic dielectric function $\epsilon_k(\omega)$. The result is applicable to equilibrium and can be extended to weakly nonequilibrium plasmas in the sense of a local approximation with a time-dependent distribution function $f(t)$ where $\epsilon_k(\omega) \rightarrow \epsilon_k(\omega, t) \approx \epsilon_k(\omega, [f(t)])$ [12]. In particular, the case of streaming electrons with a macroscopic velocity \mathbf{u}_e is trivially included by replacing on the r.h.s. of Eq. (11b) $\mathbf{v}_a \rightarrow \mathbf{v}_a - \mathbf{u}_e$. In the special case of absence of streaming, the static limit of the dielectric function is obtained, $\epsilon_k \rightarrow (k^2 + \kappa^2)/k^2$ and the pair potential of the ions becomes the isotropic Yukawa potential, $V_{ii}(r) \rightarrow e_i^2 e^{-\kappa r}/r$. In contrast, in the case of streaming charged particles, the potential is anisotropic and non-monotonic and exhibits wake effects.

The result (12) equally applies to classical and quantum electrons and its quality is fully determined by the accuracy of the dielectric function. We, therefore, now turn to the computation of the quantum electronic dielectric function. Here we will assume that linear response (weak external field) can be applied and include collision effects in relaxation time approximation within the Mermin model [16].

4. Quantum Dielectric function

The Fourier transform of the dielectric function has, in linear response, the following general form [12]

$$\epsilon_q(\hat{\omega}) = 1 - V_q \Pi_q(\hat{\omega}), \quad (13)$$

where ϵ_q is a retarded (causal) function and is complex, with $\hat{\omega} = \omega + i\nu$, where ν is the total collision frequency. Further, $\Pi_q(\hat{\omega})$ denotes the longitudinal retarded polarization function. The simplest approximation for Π is the collisionless limit – the random phase approximation (RPA) or Lindhard polarization

$$\Pi_0(q, \hat{\omega}) = 2 \int \frac{d^3Q}{(2\pi)^3} \frac{f_{-, \alpha}^{(0)} - f_{+, \alpha}^{(0)}}{\hbar\hat{\omega} - \hbar^2 \mathbf{Q} \cdot \mathbf{q}/m_\alpha}, \quad (14)$$

where $\nu \rightarrow +0$. $f_{\pm, \alpha}^{(0)}$ denotes a Fermi distribution at the argument $\mathbf{Q} \pm \mathbf{q}/2$. An improved result which takes into account electronic correlations (collisions) in a way that sum rules are fulfilled was presented for classical systems by Rostoker and Rosenbluth [17]. The generalization to quantum systems is due to Mermin [16], for a derivation see the appendix,

$$\Pi^M(q, \hat{\omega}) = \frac{\Pi_0(q, \hat{\omega})}{1 + i\hbar\tilde{\Pi}_{\nu 0}(q, \hat{\omega})}. \quad (15)$$

Further improvements of the Mermin result have been considered by various groups. Röpke et al. have derived a Mermin-type expression which, besides particle conservation contains energy conservation [19]. However, they found that the effect was small. Another modification by this group was to include a frequency dependent collision frequency into the relaxation time collision integral [20]. Finally, we mention that a selfconsistent nonequilibrium calculation within Nonequilibrium Green's functions which fully included sum rule preservation has been recently performed [21].

4.1. Dynamical screening and wake effects

The main motivation to include dynamical screening of the interaction between heavy particles in a two-component plasma is its importance for nonequilibrium situations. One such case is the existing of streaming light particles which causes wake effects which have a dramatic effect on

the arrangement of heavy particles, e.g. dust particles in a complex plasma. This was discussed in detail by Joyce and Lampe, cf. [22] and references therein. Wake effects in a quantum plasma have also been considered by one group [23] who found an important influence on stopping power of ions in a polarizable medium. However, these were only single particle effects.

5. Discussion

A new model for the simulation of dense quantum plasmas including dynamical screening of the electrons, partial ionization and strong ion correlations has been developed. It is particularly important for high density low-temperature plasmas, in situations where the ions form liquid or solid-like structures and when the electrons are in nonequilibrium. Typical situations are streaming electrons or plasma instabilities due to fast electrons or electromagnetic fields. The proposed simulation scheme is based on classical molecular dynamics simulations where the dynamical screening effects are incorporated within a linear response approach into the screening of the ion-ion pair interactions. For the screening an extension beyond the (collisionless) RPA model has been used which is due to Mermin and a strict derivation within quantum kinetic theory has been given putting the original result of Ref. [16] on solid ground and critically assessing its scope of applicability. Correlations could also be included via other approximations such as the quasilocalized charge approximation [24].

We mention that in the present version of our model the charge state of the ions is not selfconsistently computed but is used as an input. Generalizations along this line are straightforward. Also, the co-existence of several charge states maybe included via a Saha equation. The present discussion was for point-like ions. It maybe directly extended to ions with an internal structure where the pair interaction deviates from pure Coulomb repulsion, e.g. [25].

Let us briefly comment on the question how to include quantum effects in the pair interaction. This could be of importance for astrophysical applications when the ion degeneracy parameter χ_i approaches one. In this case an approximate treatment of ion degeneracy effects is sufficient which can be included in the derivation of the classical equations of motion from the quantum equation (3). As a result the ion pair potential is modified at small distances due to quantum effects which remove the divergence. This problem was first studied by Kelbg and numerous other authors. For a discussion of the Kelbg potential and improvements, see e.g. [26]. In using the expression (11b) we assumed pointlike ions and neglected any finite ion extension. This can be corrected in the final expression by replacing the Fourier transform of the Coulomb potential, i.e. the factor $1/k^2$ in Eq. (11b), by the Fourier transform of the improved Kelbg potential [26] or of any other appropriate quantum potential.

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Appendix: Kinetic derivation of the Mermin polarization

In this appendix we give a rigorous and general derivation of the Mermin polarization function (14) from quantum kinetic theory, which has not been given before. We start with the collisionless case which leads to the well-known RPA result. It is presented here to set up the notation and subsequently generalize it to include collisions. The first hierarchy equation for a multi-component system reads, in mean-field approximation, cf. Eq. (1) with $N = 1$,

$$i\hbar \frac{\partial f_{k,k',\alpha}}{\partial t} - (\epsilon_{k,\alpha} - \epsilon_{k',\alpha}) f_{k,k',\alpha} - \frac{\mathcal{V}}{N_a} \langle k | [U_{1,\alpha}^{\text{eff}}, F_{1,\alpha}] | k' \rangle = 0, \quad (16)$$

with the operator of the effective potential and the mean field potential

$$U_{1,\alpha}^{\text{eff}} = U_{1,\alpha} + W_{1,\alpha}, \quad (17)$$

$$W_{1,\alpha} = \sum_{\beta} n_{\beta} \text{Tr}_2 V_{1\alpha,2\beta} F_{2\beta}. \quad (18)$$

The normalization conditions for the density operator and the distribution function are

$$N_{\alpha} \langle k | F_{1,\alpha} | k' \rangle = \mathcal{V} f_{k,k',\alpha}, \quad (19)$$

$$N_{\alpha} = \frac{N_{\alpha}}{\mathcal{V}} \text{Tr}_1 F_{1,\alpha}(t) = 2 \sum_k f_{kk,\alpha}(t), \quad (20)$$

where \mathcal{V} is the volume and the kinetic energy of particle species “ α ” in momentum state $| \mathbf{k} \rangle$ is given by $\epsilon_{k,\alpha} = \frac{\hbar^2}{2m_{\alpha}} k^2$. Eq. (16) is the nonlinear quantum Vlasov equation (time-dependent Hartree equation).

Here we will concentrate on an unmagnetized plasma, so the external potential U is due to an electrostatic potential and $U_{1,\alpha}^{\text{eff}} = e_{\alpha}(\phi_{ext} + \phi_{ind})$, where the induced potential is the solution of Poisson's equation, $\Delta\phi_{ind} = -4\pi\rho_{ind}$ with the plasma particles acting as source. As in the classical case ϕ_{ind} functionally depends on the particle density and thus, on the distribution function, giving rise to a nonlinear kinetic equation.

We start with a plasma without external fields, $U \equiv 0$. Then the plasma will be homogeneous and all contributions to the induced potential cancel, due to charge neutrality, $\phi_{ind} \equiv 0$. We expect that the plasma will be in a (local) thermodynamic equilibrium state which, for fermions, e.g. electrons, is given by the Fermi function¹

$$f_{k,k',\alpha} = f_{k,k',\alpha}^{(0)} = f_{k,\alpha}^{(0)} \delta_{k,k'} = f_{k,\alpha}^{EQ} \delta_{k,k'} \quad (21)$$

$$f_{k,\alpha}^{EQ} = \left[e^{\beta(\epsilon_{k\alpha} - \mu_{\alpha})} + 1 \right]^{-1}, \quad (22)$$

where $\beta = 1/k_B T$ and $\mu_{\alpha}(n_{\alpha}, T)$ is the chemical potential, and the momentum delta function arises due to spatial homogeneity.

We now assume that a weak electrostatic potential ϕ_{ext} is turned on, perturbing the equilibrium state. Weakness of the potential allows us to linearize the kinetic equation and solve it with the linear response ansatz [quantities of first order in ϕ_{ext} are denoted by the superscript “(1)”]

$$U_{\alpha}^{\text{eff}}(\mathbf{r}, t) = U_{\alpha}^{\text{eff}(1)}(\mathbf{r}, t), \quad \lim_{t \rightarrow -\infty} U_{\alpha}^{\text{eff}}(\mathbf{r}, t) = 0, \quad (23)$$

$$f_{k,k',\alpha}(t) = f_{k,k',\alpha}^{(0)} + f_{k,k',\alpha}^{(1)}(t), \quad (24)$$

$$\lim_{t \rightarrow -\infty} f_{k,k',\alpha}(t) = f_{k,k',\alpha}^{(0)}.$$

Using this ansatz we can now evaluate the matrix elements of the commutator in Eq. (16). Since the potential is of first order, for the density operator the zeroth order gives the dominant contribution which is diagonal,

$$\langle k | [U_{1,\alpha}^{\text{eff}}, F_{1,\alpha}] | k' \rangle \approx \langle k | [U_{1,\alpha}^{\text{eff}(1)}, F_{1,\alpha}^{(0)}] | k' \rangle \quad (25)$$

$$= U_{k,k',\alpha}^{\text{eff}(1)} \frac{N_{\alpha}}{\mathcal{V}} \left(f_{k',\alpha}^{(0)} - f_{k,\alpha}^{(0)} \right). \quad (26)$$

¹ The only remaining contribution in Eq. (16) is the time derivative, i.e. $\frac{\partial f_{k,k',\alpha}}{\partial t} = 0$. Therefore, as in the classical case, any stationary distribution function can be used. The choice of the equilibrium distribution is based on experience. Only in the case of collisions, relaxation processes (scattering) will lead to a unique selfconsistent stationary solution.

Inserting this result into the kinetic equation (16) and taking into account that $f_{k,k'\alpha}^{(0)}$ is time-independent and diagonal, we obtain a closed equation for $f_{k,k',\alpha}^{(1)}(t)$

$$i\hbar \frac{\partial f_{k,k',\alpha}^{(1)}}{\partial t} - (\epsilon_{k,\alpha} - \epsilon_{k',\alpha}) f_{k,k',\alpha}^{(1)} - U_{k,k',\alpha}^{\text{eff}(1)} (f_{k',\alpha}^{(0)} - f_{k,\alpha}^{(0)}) = 0, \quad (27)$$

which is already a linear equation. Expanding the field into a Fourier integral of monochromatic oscillations²

$$U_{k,k',\alpha}(t) = \int d\omega \tilde{U}_{k,k',\alpha}(\omega) e^{-i(\omega+i\delta)t}, \quad (28)$$

the same expansion will also apply to $f_{k,k',\alpha}^{(1)}$ and $U_{k,k',\alpha}^{\text{eff}(1)}$.

Fourier transforming Eq. (27) and cancelling the common exponent yields the result for the perturbation of the distribution,

$$\tilde{f}_{k,k',\alpha}^{(1)}(\omega) = \frac{f_{k',\alpha}^{(0)} - f_{k,\alpha}^{(0)}}{\hbar(\omega + i\delta) - (\epsilon_{k,\alpha} - \epsilon_{k',\alpha})} \tilde{U}_{k,k',\alpha}^{\text{eff}(1)}(\omega). \quad (29)$$

This is the general result for the linear perturbation to the distribution function, and the time-dependent expression follows by a back transform. In deriving (29) we have made no assumptions on the space dependence of the external perturbation U .

In the following we consider an exciting field which is purely periodic in space without any macroscopic spatial modulation, which can be expanded in a Fourier series $U_\alpha(\mathbf{r}) = \sum_q U_{q\alpha} e^{i\mathbf{q}\mathbf{r}}$. Now introduce center of mass and relative momenta by (all quantities are vectors)

$$\begin{aligned} Q &= \frac{k + k'}{2}, & q &= k - k', & \text{or, vice versa,} \\ k &= Q + \frac{q}{2}, & k' &= Q - \frac{q}{2}. \end{aligned} \quad (30)$$

While the center of mass variable Q is related to spatial inhomogeneities, the relative momentum q is directly related to small scale spatially periodic modulations. Thus, in the present case, there will be no dependence on Q , i.e.

$$U_{k,k',\alpha} \equiv U_{Q+\frac{q}{2}, Q-\frac{q}{2}, \alpha} \longrightarrow U_q \quad (31)$$

and similarly for $\tilde{U}_{k,k',\alpha}^{\text{eff}(1)}(\omega)$. In contrast, in the unperturbed quantities ϵ_k and $f_{k,\alpha}^{(0)}$ the momentum arguments k and k' remain. Therefore, to shorten the notation, in the following we will denote $\mathbf{Q} \pm \mathbf{q}/2 \rightarrow \pm$. Via ϵ_k and $f_{k,\alpha}^{(0)}$, the dependence on Q remains also in the perturbed distribution function. Thus, we can rewrite the result (29) for a single Fourier component q of a periodic monochromatic excitation

$$\tilde{f}_{+,-,\alpha}^{(1)}(\omega) = \frac{f_{-,\alpha}^{(0)} - f_{+,\alpha}^{(0)}}{\hbar(\omega + i\delta) - (\epsilon_{+,\alpha} - \epsilon_{-,\alpha})} \tilde{U}_{q,\alpha}^{\text{eff}(1)}(\omega). \quad (32)$$

This is still not an explicit result for $\tilde{f}^{(1)}$ because the function also appears in the effective potential. To make further progress we consider the density disturbance and compute its Fourier components

$$\tilde{n}_{q,\alpha}^{(1)}(\omega) = 2 \int \frac{d^3Q}{(2\pi)^3} \tilde{f}_{Q+\frac{q}{2}, Q-\frac{q}{2}, \alpha}^{(1)}(\omega), \quad (33)$$

² δ is a small positive constant which assures causality, i.e. $\lim_{t \rightarrow -\infty} U_{k,k'} = 0$.

and the prefactor 2 accounts for the spin summation. Below, we will also need the current density which is calculated in similar way

$$\tilde{\mathbf{j}}_{q,\alpha}^{(1)}(\omega) = 2 \int \frac{d^3Q}{(2\pi)^3} \frac{\hbar\mathbf{Q}}{m_\alpha} \tilde{f}_{Q+\frac{q}{2}, Q-\frac{q}{2}, \alpha}^{(1)}(\omega). \quad (34)$$

Particle and current density are connected via the continuity equation

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} + \text{div } \mathbf{j}(\mathbf{r}, t) = 0. \quad (35)$$

Since the unperturbed expressions are time and space independent we can replace the total density and current density by the perturbed functions. The Fourier transform of this expression then reads

$$\omega \tilde{n}_{q,\alpha}^{(1)}(\omega) = \mathbf{q} \cdot \tilde{\mathbf{j}}_{q,\alpha}^{(1)}(\omega). \quad (36)$$

We can now explicitly compute the density perturbation by inserting the distribution function (32) into Eq. (33) and obtain

$$\tilde{n}_{q,\alpha}^{(1)}(\omega) = \Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega}) \tilde{U}_{q,\alpha}^{\text{eff}(1)}(\omega), \quad (37)$$

$$\Pi_{n\alpha}^{\text{RPA}}(q, \hat{\omega}) = 2 \int \frac{d^3Q}{(2\pi)^3} \left(\frac{\hbar\mathbf{Q}}{m_\alpha} \right)^n \frac{f_{-, \alpha}^{(0)} - f_{+, \alpha}^{(0)}}{\hbar\hat{\omega} - [\epsilon_{+, \alpha} - \epsilon_{-, \alpha}]}, \quad (38)$$

where we defined $\hat{\omega} = \omega + i\delta$. Here $\Pi_{n\alpha}^{\text{RPA}}$ denotes the n -th moment of the polarization function $\Pi_{0\alpha}^{\text{RPA}}$.

The simplest way to obtain the longitudinal quantum dielectric function is to use the continuity equation and relation (13) which is valid for classical *and* quantum plasmas. Computing the total electric charge density perturbation

$$\tilde{\rho}_q^{(1)}(\omega) = \sum_{\alpha} q_{\alpha} \tilde{n}_{q,\alpha}^{(1)}(\omega), \quad (39)$$

and using the relation of the effective potential to the total electrostatic potential

$$\tilde{U}_{q,\alpha}^{\text{eff}(1)}(\omega) = q_{\alpha} \tilde{\phi}_q(\omega), \quad (40)$$

we only need to insert (39) with the result (37) into (11a) and obtain

$$\epsilon^{1,\text{RPA}}(\mathbf{k}, \hat{\omega}) = 1 - \sum_{\alpha} \tilde{V}_{\alpha\alpha}(k) \Pi_{0\alpha}^{\text{RPA}}(\mathbf{k}, \hat{\omega}). \quad (41)$$

This is the longitudinal retarded dielectric function for a collisionless quantum plasma. In using the superscript ‘‘RPA’’ for the dielectric function and the polarization (14) we indicated that this is the result in the so-called *random phase approximation* (RPA) which is als frequently called Lindhard polarization. Note, however, that this result was obtained by many authors independently. The first, apparently were Klimontovich and Silin [27, 28], followed by [29, 30].

We now proceed to improve this result by including correlation effects. The quantum kinetic equation in momentum representation, with collision integral reads

$$i\hbar \frac{\partial f_{k,k',\alpha}}{\partial t} - (\epsilon_{k,\alpha} - \epsilon_{k',\alpha}) f_{k,k',\alpha} - \frac{\mathcal{V}}{N_{\alpha}} \langle k | [U_{1,\alpha}^{\text{eff}}, F_{1,\alpha}] | k' \rangle = I_{k,k',\alpha}, \quad (42)$$

Prior to external perturbation, we again assume a homogeneous state with the distribution given by a diagonal matrix $f_{k,k',\alpha} = f_{k,k',\alpha}^{(0)} = f_{k,\alpha}^{(0)}\delta_{k,k'}$, and the same applies to the collision integral, $I_{k,k',\alpha} = I_{k,k',\alpha}^{(0)} = I_{k,\alpha}^{(0)}\delta_{k,k'}$. Then the kinetic equation (42) simplifies to a diagonal equation

$$i\hbar \frac{\partial f_{k,\alpha}^{(0)}}{\partial t} = I_{k,\alpha}^{(0)} \equiv I_{k,\alpha}[f_{k,\alpha}^{(0)}], \quad (43)$$

where in the collision integral the unperturbed distribution function has to be used. Following Mermin [16] we use the relaxation time approximation for the collision integral which is constructed by the ansatz (we drop all arguments)

$$I^{RTA}[f] \equiv -\frac{1}{\tau} (f - f^{EQ}), \quad f(0) = f_0. \quad (44)$$

The solution of this equation, together with the initial condition at $t = 0$, is $f(t) = f_0 e^{-t/\tau} + f^{EQ}[1 - e^{-t/\tau}]$, showing the decay of the initial state and the approach to the asymptotic state. Here, τ is the total relaxation time due to all scattering processes which has to be computed from a separate kinetic theory or taken from experiment. We use a simple static approximation where τ is frequency independent. Despite its simplicity, this approximation allows to achieve a selfconsistent relaxation of the distribution function to the equilibrium state. While we expect that f^{EQ} will be a Fermi function, we will not need the explicit form of the equilibrium distribution below.

We now again consider a weak perturbation by a longitudinal field $U_a = q_a \phi^{ext}$,

$$\begin{aligned} U_\alpha^{\text{eff}}(\mathbf{r}, t) &= U_\alpha^{\text{eff}(1)}(\mathbf{r}, t), \quad \lim_{t \rightarrow -\infty} U_\alpha^{\text{eff}}(\mathbf{r}, t) = 0, \\ f_{k,k',\alpha}(t) &= f_{k,k',\alpha}^{(0)} + f_{k,k',\alpha}^{(1)}(t), \\ \lim_{t \rightarrow -\infty} f_{k,k',\alpha}(t) &= f_{k,k',\alpha}^{(0)}. \end{aligned} \quad (45)$$

The equation for the perturbation of the distribution reads, in first order,

$$\begin{aligned} i\hbar \frac{\partial f_{k,k',\alpha}^{(1)}}{\partial t} - (\epsilon_{k,\alpha} - \epsilon_{k',\alpha}) f_{k,k',\alpha}^{(1)} - U_{k,k',\alpha}^{\text{eff}(1)} \cdot (f_{k',\alpha}^{(0)} - f_{k,\alpha}^{(0)}) &= I_{k,k',\alpha}^{(1)}, \\ \lim_{t \rightarrow -\infty} f_{k,k',\alpha}(t) &= f_{k,\alpha}^{(0)}\delta_{k,k'}. \end{aligned} \quad (46)$$

Here, $U^{\text{eff}(1)}$ is again obtained by replacing $f_{k,k'}$ by $f_{k,k'}^{(1)}$, whereas $I^{(1)}$ is obtained by keeping in all appearances of the electron distribution functions only terms of first order in $f^{(1)}$ [21]. In case of the relaxation time approximation which is linear in f we just have to use $f_{k,k'}^{(1)}$. In order to find the explicit expression for $I^{(1)}$ we consider the long time limit of the system. The complete asymptotic solution of the original kinetic equation will be the sum of the zero and first order terms, i.e. f^{EQ} and the asymptotic solution for $f_{k,k'}^{(1)}$ which we will denote $f_{k,k'}^{(1)\infty}$. To find this solution assume a purely periodic space dependence of U . Using center of mass and relative momenta Eq. (46) becomes

$$i\hbar \frac{\partial f_{k,k',\alpha}^{(1)\infty}}{\partial t} - (\epsilon_{+,\alpha} - \epsilon_{-,\alpha}) f_{k,k',\alpha}^{(1)\infty} - U_{q,\alpha}^{\text{eff}(1)\infty} \cdot (f_{-,\alpha}^{(0)} - f_{+,\alpha}^{(0)}) = I_{k,k',\alpha}^{(1)\infty}. \quad (47)$$

Since we are looking for a stationary solution, the time-dependence should vanish. Also, we expect that collisions have relaxed to zero, i.e. $I_{k,k',\alpha}^{(1)\infty} = I_{k,k',\alpha}^{(1)}[f^{(1)\infty}] = 0$, resulting in

$$\lim_{t \rightarrow \infty} f_{k,k',\alpha}^{(1)} = f_{k,k',\alpha}^{(1)\infty} = \frac{f_{+,\alpha}^{(0)} - f_{-,\alpha}^{(0)}}{\epsilon_{+,\alpha} - \epsilon_{-,\alpha}} U_{q,\alpha}^{\text{eff}(1)\infty}. \quad (48)$$

Note that also the effective potential carries the superscript ∞ since it also depends on this solution.

Performing a Fourier transform with respect to time, according to Eq. (28) we obtain

$$\tilde{f}_{k,k',\alpha}^{(1)\infty} = \frac{f_{+,\alpha}^{(0)} - f_{-,\alpha}^{(0)}}{\epsilon_{+,\alpha} - \epsilon_{-,\alpha}} \tilde{U}_{q,\alpha}^{\text{eff}(1)\infty}, \quad \omega = 0, \quad (49)$$

where, as a result of the long-time limit, this form is restricted to zero frequency.

Now we can construct the first order correction to the collision term in Eq. (46). Since $f^{(0)}$ relaxes towards f^{EQ} , in Eq. (44) only the difference of $f^{(1)}$ and $f^{(1)\infty}$ remains. Multiplying by $i\hbar$ we obtain

$$\tilde{I}_{k,k',\alpha}^{(1)}(\omega) = -\frac{i\hbar}{\tau} \left\{ \tilde{f}_{k,k',\alpha}^{(1)}(\omega) - \frac{f_{+,\alpha}^{(0)} - f_{-,\alpha}^{(0)}}{\epsilon_{+,\alpha} - \epsilon_{-,\alpha}} \tilde{U}_{q,\alpha}^{\text{eff}(1)\infty} \right\}, \quad (50)$$

which can be inserted in Eq. (46) after Fourier transform to frequency space³ yielding the solution

$$\tilde{f}_{k,k',\alpha}^{(1)}(\omega) = \left\{ \tilde{U}_{q,\alpha}^{\text{eff}(1)} - i\hbar\nu \frac{\tilde{U}_{q,\alpha}^{\text{eff}(1)\infty}}{\epsilon_{+,\alpha} - \epsilon_{-,\alpha}} \right\} \frac{f_{-,\alpha}^{(0)} - f_{+,\alpha}^{(0)}}{\hbar\hat{\omega} - [\epsilon_{+,\alpha} - \epsilon_{-,\alpha}]}, \quad (51)$$

where we defined $\hat{\omega} = \omega + i\nu$ and used $\delta \rightarrow 0$ due to the existence of a finite collisional damping $\nu = \tau^{-1}$. This result is a straightforward extension of the collisionless random phase approximation, cf. Eq. (32). Scattering effects (terms proportional to ν) are contained in two places: first, the frequency in the denominator is replaced by a complex frequency and, second, there appears an additional contribution proportional to $U^{\text{eff}(1),\infty}$ in the numerator which renormalizes the Fourier component of the effective potential.

Eq. (51) is not an explicit solution for $\tilde{f}^{(1)}$ since this function also appears in the effective potential. To solve this problem and compute the dielectric function, we proceed as in the collisionless case. We first compute the Fourier component of the density disturbance according to Eq. (33) and also of the current density, using Eq. (34) and the definition (38),

$$\tilde{n}_{q,\alpha}(\omega) = \Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega}) \tilde{U}_{q,\alpha}^{\text{eff}(1)}(\omega) - i\hbar\nu \tilde{U}_{q,\alpha}^{\text{eff}(1)\infty} \Pi_{\nu 0\alpha}(q, \hat{\omega}), \quad (52)$$

$$\tilde{\mathbf{j}}_{q,\alpha}(\omega) = \Pi_{1\alpha}^{\text{RPA}}(q, \hat{\omega}) \tilde{U}_{q,\alpha}^{\text{eff}(1)}(\omega) - i\hbar\nu \tilde{U}_{q,\alpha}^{\text{eff}(1)\infty} \Pi_{\nu 1\alpha}(q, \hat{\omega}), \quad (53)$$

where we used the definition (41) of the RPA polarization and introduced in analogy to (38) a modified polarization function which arises from the collisions

$$\Pi_{\nu n\alpha}(q, \hat{\omega}) = 2 \int \frac{d^3Q}{(2\pi)^3} \left(\frac{\hbar\mathbf{Q}}{m_\alpha} \right)^n \frac{1}{\epsilon_{+,\alpha} - \epsilon_{-,\alpha}} \times \frac{f_{-,\alpha}^{(0)} - f_{+,\alpha}^{(0)}}{\hbar\hat{\omega} - [\epsilon_{+,\alpha} - \epsilon_{-,\alpha}]}. \quad (54)$$

Eq. (52) indicates that collisions change the particle density (second term) compared to the RPA result. As a consequence of the local density conservation law also the current density has to change, cf. Eq. (53).

³ We again assume a spatially periodic excitation.

Eqs. (52) and (53) contain the still unknown function $\tilde{U}^{\text{eff}(1)\infty}$ which we determine using the continuity equation (36). We now transform $\hbar\mathbf{q}$ times the integral $\Pi_{1\alpha}$, by adding and subtracting, under the integral, $\hbar\hat{\omega}$. Taking into account that $\epsilon_{+,\alpha} - \epsilon_{-,\alpha} = \hbar^2\mathbf{Q} \cdot \mathbf{q}/m_\alpha$, we obtain the identity

$$\hbar\mathbf{q} \cdot \Pi_{1\alpha}^{\text{RPA}}(q, \hat{\omega}) = 2 \int \frac{d^3Q}{(2\pi)^3} \left(f_{-,\alpha}^{(0)} - f_{+,\alpha}^{(0)} \right) + (\hbar\omega + i\hbar\nu)\Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega}). \quad (55)$$

Assuming that the field-free distribution depends only on the modulus of the momentum, i.e. $f_{-\mathbf{k},\alpha}^{(0)} = f_{\mathbf{k},\alpha}^{(0)}$ the integrals over f_- and f_+ cancel. The same transformation is possible for the integral $\Pi_{\nu 1\alpha}$ with the result

$$\hbar\mathbf{q} \cdot \Pi_{\nu 1\alpha}(q, \hat{\omega}) = \Pi_{0\alpha}^{\text{RPA}}(q, 0) + (\hbar\omega + i\hbar\nu)\Pi_{\nu 0\alpha}(q, \hat{\omega}). \quad (56)$$

Collecting the results (55) and (56) together we may rewrite Eq. (53),

$$\begin{aligned} \hbar\mathbf{q} \cdot \tilde{\mathbf{j}}_{q,\alpha}(\omega) &= \hbar(\omega + i\nu)\Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega})\tilde{U}_{q,\alpha}^{\text{eff}(1)} \\ &\quad - i\hbar\nu \left[\Pi_{0\alpha}^{\text{RPA}}(q, 0) + (\hbar\omega + i\hbar\nu)\Pi_{\nu 0\alpha}(q, \hat{\omega}) \right] \tilde{U}_{q,\alpha}^{\text{eff}(1)\infty} \\ &= \hbar\omega \cdot \tilde{n}_{q,\alpha}(\omega) + \\ &\quad + i\hbar\nu \left\{ \Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega})\tilde{U}_{q,\alpha}^{\text{eff}(1)} - \tilde{U}_{q,\alpha}^{\text{eff}(1)\infty} \left[\Pi_{0\alpha}^{\text{RPA}}(q, 0) + i\hbar\nu\Pi_{\nu 0\alpha}(q, \hat{\omega}) \right] \right\}. \end{aligned} \quad (57)$$

Evidently, the continuity equation (36) is fulfilled if the terms on the last line (in the curly brackets) vanish which yields the required condition on $\tilde{U}^{\text{eff}(1)\infty}$

$$\tilde{U}_{q,\alpha}^{\text{eff}(1)\infty}(\omega) = \frac{\Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega})\tilde{U}_{q,\alpha}^{\text{eff}(1)}(\omega)}{\Pi_{0\alpha}^{\text{RPA}}(q, 0) + i\hbar\nu\Pi_{\nu 0\alpha}(q, \hat{\omega})} = \frac{\tilde{n}_{q,\alpha}(\omega)}{\Pi_{0\alpha}^{\text{RPA}}(q, 0)}. \quad (58)$$

With this result we can now eliminate $\tilde{U}^{\text{eff}(1)\infty}$ from all expressions. Inserting it into (52), we can solve for the density perturbation which – as in the collisionless case, cf. Eq. (37) – is proportional to the effective potential, however, with a modified coefficient

$$\tilde{n}_{q,\alpha}(\omega) = \Pi_\alpha^M(q, \hat{\omega})\tilde{U}_{q,\alpha}^{\text{eff}(1)}(\omega), \quad (59)$$

Using the result (59) we immediately obtain the dielectric function. Computing the total charge density to $\tilde{\rho}_q(\omega) = \tilde{\Phi}_q(\omega) \sum_\alpha q_\alpha^2 \Pi_\alpha^M(q, \hat{\omega})$ and inserting the result into Eq. (11a) we obtain

$$\epsilon^{l,M}(\mathbf{k}, \omega) = 1 - \sum_\alpha \tilde{V}_{\alpha\alpha}(k) \Pi_\alpha^M(\mathbf{k}, \omega). \quad (60)$$

This is the longitudinal quantum dielectric function including collisions in relaxation time approximation. This result was first obtained by Mermin [16], therefore we use the superscript “M”. The formal structure of this expression is the same as in the collisionless and classical cases, it is a general property of linear response theory. The different physical approximations are solely contained in the longitudinal polarization function, the Mermin polarization,

$$\Pi_\alpha^M(q, \hat{\omega}) \equiv \frac{\Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega})}{1 + i\hbar\nu\tilde{\Pi}_{\nu 0\alpha}(q, \hat{\omega})} \quad (61)$$

where we introduced the definition

$$\tilde{\Pi}_{\nu 0\alpha}(q, \hat{\omega}) \equiv \frac{\Pi_{\nu 0\alpha}(q, \hat{\omega})}{\Pi_{0\alpha}^{\text{RPA}}(q, 0)} = \frac{1}{\hbar\omega} \left[\frac{\Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega})}{\Pi_{0\alpha}^{\text{RPA}}(q, 0)} - 1 \right]. \quad (62)$$

In the last equality we have eliminated the function $\Pi_{\nu 0\alpha}$ and expressed it in terms of the RPA polarization where use has been made of the identity $\hbar\omega\Pi_{\nu 0\alpha}(q, \hat{\omega}) = \Pi_{0\alpha}^{\text{RPA}}(q, \hat{\omega}) - \Pi_{0\alpha}^{\text{RPA}}(q, 0)$. Obviously, the collisionless limit of the Mermin dielectric function, i.e. $\nu \rightarrow 0$ and $\hat{\omega} \rightarrow \omega + i\delta$, is given by the random phase approximation. The classical limit of Π_{α}^M gives the result derived from the the Bhatnagar/Gross/Krook collision integral which was first obtained by Rostoker and Rosenbluth [17].

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