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A Generalised Linear Response Theory applied to the Dielectric Function of Coulomb Systems*

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Abstract

A generalised linear response theory is used to derive the dielectric function at arbitrary wave numbers k and frequencies ω for interacting quantum systems. The connection to thermodynamic Green functions allows the systematic perturbative treatment going beyond RPA and treating local field corrections as well as the inclusion of collisions on the same footing. Emphasis will be on the demonstration of the formalism. Results will be presented for the three-dimensional as well as two-dimensional case of an interacting electron gas. In the long-wavelength limit, a Drude-type expression with frequency dependent relaxation time is given bridging the theories of dielectric function and electrical conductivity.

1. Introduction

The dielectric function of a physical system contains the information on how this system reacts to an external electrical field which, in general, is time and space dependent as given by the frequency ω and the wave vector \mathbf{k} . We can describe transport or optical properties, but get also information about collective excitations (plasmons) or the dynamical structure factors. To give an example, with which we will be concerned later on, the dielectric function $\epsilon(\mathbf{k}, \omega)$ in the long-wavelength limit is related to the frequency dependent conductivity $\sigma(\omega)$, as well as to the refraction index $n(\omega)$ and the absorption coefficient $\alpha(\omega)$, according to

$$\lim_{\mathbf{k} \rightarrow 0} \epsilon(\mathbf{k}, \omega) = 1 + \frac{i}{\epsilon_0 \omega} \sigma(\omega) = \left[n(\omega) + \frac{ic}{2\omega} \alpha(\omega) \right]^2. \quad (1)$$

The dielectric function describes non-equilibrium properties. According to the fluctuation-dissipation theorem these can be expressed by equilibrium properties as long as the perturbation of the system is weak. There exist different approaches to a microscopic treatment of non-equilibrium processes. The use of equations of motion (kinetic equations) to determine distribution functions is distinguished by different diffusion and collision terms (Landau and Lifschitz 1958; Balescu 1963; Ziman 1972; Klimontovich 1982). An equivalent method is the linear response theory where expectation values of operators for physical quantities are

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determined via a non-equilibrium statistical operator. Kubo (1957) made the assumption that the system is described by the equilibrium statistical operator ρ_0 for times $t \rightarrow -\infty$. This approach can be applied to responses of quantum systems to external mechanical perturbations. Problems arise with respect to the perturbative expansion of transport coefficients such as the dc-conductivity and the treatment of thermal perturbations. These can be removed within a generalised approach to linear response theory. A non-equilibrium statistical operator was derived by the projection operator method of Mori (1965) which expresses the so-called memory function by correlation functions (Götze 1981; Neilson *et al.* 1991; Zubarev *et al.* 1997). Recently, this approach was used to develop a self-consistent theory to describe the metal-insulator transition in a disordered 2-dimensional electron gas (Thakur *et al.* 1999). A quantum statistical operator of the non-equilibrium system as proposed by Zubarev (1974) allows studying mechanical and thermal perturbations within a unified approach. This microscopic theory was further developed within the last decade, for a recent introduction and overview see Zubarev *et al.* (1996, 1997), and successfully applied, e.g., to thermoelectric properties of many-component Coulomb systems (Reinholz *et al.* 1989, 1995). Recently, this approach has also been used in the theory of the dielectric function of such systems (Röpke 1998; Röpke and Wierling 1998; Reinholz *et al.* 1999), thus making it possible to treat the dielectric function and the electrical conductivity within the same approach and making approximations self-consistently.

Extensive experience in calculating thermoelectric properties can be utilised when treating the dielectric function including collisions. A general advantage of this approach is that the response functions are expressed through equilibrium correlation functions which can be related to thermodynamic equilibrium Green functions. This allows a systematic perturbative treatment. Thus, the transport as well as thermodynamic properties can be studied within a common approach starting from the system Hamiltonian (Kraeft *et al.* 1986; Redmer 1997).

In the course of this paper we will mainly be considering Coulomb systems. Coulomb forces are somehow the origin of all properties of materials, although they might appear as collective behaviour described by short-range forces. The microscopic theory presented here would allow indeed a description of the system by any Hamiltonian, at least formally. However, we want to look at systems where the interaction of charged particles is the dominant effect, described by a Coulomb potential $V(\mathbf{r}) = 1/(4\pi\epsilon_0|\mathbf{r}|)$. Thus we will have in mind plasmas, metallic systems of condensed matter, semiconductors or (expanded) liquid metals. In recent years, Coulomb systems of lower dimensionality (e.g. two-dimensional electron gas, quantum dots) have become of increasing interest due to advances in semiconductor technology and the availability of experimentally accessible probes.

The Hamiltonian for a charged particle system of components c with charge e_c is given in terms of creation and annihilation operators in momentum representation by

$$H = \sum_{p,c} E_p^c c_{p,c}^\dagger c_{p,c} + \frac{1}{2} \sum_{pp'q;cc'} e_c e_{c'} V(q) c_{p-q,c}^\dagger c_{p'+q,c'}^\dagger c_{p',c'} c_{p,c},$$

with the kinetic energy E_p^c . The Fourier transform of the Coulomb interaction $V(q)$ is

$$V_{3D}(q) = \frac{1}{\epsilon_0 \Omega_0 q^2} \quad (2)$$

for the 3-dimensional case. The 2-dimensional case is

$$V_{2D}(q) = \frac{1}{2\epsilon_0 \Omega_0 q}. \quad (3)$$

Here Ω_0 denotes the normalisation volume or area, respectively. Other internal degrees of freedom could also be included in the index c . The spin will not be treated explicitly since we consider unpolarised systems. Spin summations are contained in the \mathbf{p} -integrations. In order to focus on the concept of our approach we treat the singly charged ions at positions \mathbf{R}_j in the adiabatic approximation. We omit the index c and the Hamiltonian reads

$$H = \sum_p E_p c_p^\dagger c_p - e^2 \sum_{pq;j} V(q) e^{-i\mathbf{q} \cdot \mathbf{R}_j} c_{p-q}^\dagger c_p + \frac{e^2}{2} \sum_{pp'q} V(q) c_{p+q}^\dagger c_{p'-q}^\dagger c_{p'} c_p. \quad (4)$$

The kinetic energy of the electrons is $E_p = \hbar^2 p^2 / 2m$. The third term represents the electron-electron interaction. The same model Hamiltonian could be applied to impurity scattering in two-dimensional electron gases (2DEG) where the impurities are considered to be within the plane of the electron gas. A generalisation for impurities which are physically a distance away from the 2DEG is straight forward and due to technical realisations in MOSFETs or other interface layers of much interest.

The paper is organised as follows. Section 2 will give a short and general introduction to the linear response theory as developed by Zubarev and co-workers. In Section 3 the dielectric function is introduced and relevant limiting cases and sum rules are considered. Microscopic expression for the longitudinal dielectric function are derived in Section 4 applying the generalised linear response theory. Section 5 presents the well-known results of RPA for the three as well as the two-dimensional case. Local field factors and the inclusion of collisions will be elaborated in Sections 6 and 7 respectively. In Section 8, a generalised Drude formula with a frequency dependent relaxation time will be derived in the long-wavelength limit, treating the dielectric function on the same level of approximation as the electrical conductivity. Further improvements in order to treat the screening consistently and avoid divergencies will be discussed in Section 9, before coming to the conclusions in Section 10.

2. Generalised Linear Response Theory

Linear response theory was derived by Kubo (1957) and later further developed in different directions by Mori (1965), Zubarev (1974), Tserkovnikov (1981) and Lee (1983), to name just a few. For a recent presentation see Zubarev *et al.* (1997). The main idea of a generalised linear response theory is the construction of the statistical operator $\rho(t) = \rho_{\text{rel}}(t) + \rho_{\text{irrev}}(t)$ by introducing a relevant statistical operator ρ_{rel} . The latter characterises the non-equilibrium state of the system by the mean values $\langle A_n(\mathbf{r}) \rangle^t$ of a set of relevant observables $\{A_n(\mathbf{r})\}$. From the maximum entropy principle the generalised Gibbs state follows

$$\rho_{\text{rel}}(t) = \exp \left[-\Phi(t) - \beta H + \beta \sum_c \mu_c N_c + \beta \sum_n \int d^3r \phi_n(\mathbf{r}, t) A_n(\mathbf{r}) \right],$$

where $\Phi(t)$ is the Massieu–Planck function. The Hamilton operator H and the particle number operators N_c of the thermodynamic equilibrium are included in ρ_{rel} for reasons of convenience which will not be apparent within this short presentation. The meaning of their Lagrange multipliers $\beta = 1/k_B T$ and the chemical potential μ_c is known from thermodynamic equilibrium already. Thermal perturbations can be included by allowing a position dependence in these terms (Wegener 1989). The thermodynamic parameters (Lagrange multipliers) $\phi_n(\mathbf{r}, t)$ are determined by the self-consistency conditions

$$\text{Tr}\{A_n(\mathbf{r}) \rho_{\text{rel}}(t)\} = \text{Tr}\{A_n(\mathbf{r}) \rho(t)\} = \langle A_n(\mathbf{r}) \rangle^t. \quad (5)$$

The relevant statistical operator is not a solution of the von Neumann equation but can serve to construct suitable initial conditions. Using the principle of the weakening of the initial correlations the irrelevant part of the statistical operator can be found with the help of the time evolution operator via Abel's theorem. The time evolution of the system is determined by the total Hamiltonian $H_{\text{tot}}(t) = H + H_{\text{ext}}(t)$ which contains the system Hamiltonian H (4), restricting ourselves to an electron system, and the interaction with an external potential

$$H_{\text{ext}}(t) = \sum_p U_{\text{ext}}(\mathbf{k}, \omega) \mathbf{e}^{-i\omega t} n_{p,-k} + \text{c.c.},$$

where $n_{p,k} = c_{p-k/2}^\dagger c_{p+k/2}$ is the Wigner transform of the single-particle density. For a weak external field U_{ext} , the system remains near thermal equilibrium. We consider the system in the so-called linear response and expand the statistical operator up to first order in U_{ext} , as well as in the non-equilibrium thermodynamic parameters ϕ_n . The self-consistency conditions (5) take the form of the response equations

$$-i\mathbf{k} \Omega_0 N_{m0} U_{\text{ext}}(\mathbf{k}, \omega) = \sum_n M_{mn} \phi_n(\mathbf{k}, \omega), \quad (6)$$

where the Fourier representations

$$\phi_n(\mathbf{r}, t) = \mathbf{e}^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} \phi_n(\mathbf{k}, \omega), \quad A_n = \int d\mathbf{r} A_n(\mathbf{r}) \mathbf{e}^{-i\mathbf{k}\cdot\mathbf{r}}$$

were introduced. The coefficients N_{m0} and M_{mn} are expressions of equilibrium correlation functions

$$N_{m0} = (A_m; \mathbf{J}_k), \quad M_{mm} = \frac{\langle A_m; \dot{A}_m + i\omega A_m \rangle_{\omega+i\eta} (A_m; \mathbf{J}_k)}{\langle A_m; \mathbf{J}_k \rangle_{\omega+i\eta}} \quad (7)$$

between pairs of the relevant observables A_n , their time derivatives $\dot{A}_n = (i/\hbar) [H, A]$, and the current density operator \mathbf{J}_k which emerges in the context of the time derivative of the particle density operators

$$\sum_p \dot{n}_{p,k} = i\Omega_0 \mathbf{k} \cdot \mathbf{J}_k, \quad \mathbf{J}_k = \frac{\hbar}{\Omega_0 m} \sum_p \mathbf{p} n_{p,k}. \quad (8)$$

The equilibrium correlation functions are defined as

$$(A; B) = \frac{1}{\beta Z} \int_0^\beta d\tau \quad \text{Tr} [e^{-\beta H + \beta \mu N} A(-i\hbar\tau) B^\dagger],$$

$$\langle A; B \rangle_z = \int_0^\infty dt \quad e^{izt} (A(t); B),$$

with $A(t) = \exp(iHt/\hbar) A \exp(-iHt/\hbar)$, and $Z = \text{Tr} e^{-\beta H + \beta \mu N}$. They can be expressed in terms of thermodynamic Green functions

$$(A; B) = -\frac{1}{\beta} \int_{-\infty}^\infty \frac{d\omega}{\pi} \frac{1}{\omega} \text{Im} \mathcal{G}_{AB^\dagger}(\omega - i0),$$

$$\langle A; B \rangle_z = -\frac{i}{\beta} \int_{-\infty}^\infty \frac{d\omega}{\pi} \frac{1}{z - \omega} \frac{1}{\omega} \text{Im} \mathcal{G}_{AB^\dagger}(\omega - i0). \quad (9)$$

The relation to the thermodynamic Green functions $\mathcal{G}_{AB}(z_\mu)$, z_μ being the (bosonic) Matsubara frequencies, allows us to perform systematic perturbation expansions. The equilibrium thermodynamic properties derived from thermodynamic Green functions can be determined self-consistently within the same approximations as for the linear response.

The set of relevant observables should be chosen in such a way that the operators of the physical quantities $\{B_l\}$ we are interested in can be represented as a linear combination of the $\{A_n\}$. In that case, we can directly use the self-consistency conditions (5) and the solution of the response equations (6) in order to calculate their mean values. Applying Cramers rule, we find

$$\langle B_l \rangle^t e^{i\omega t} = \beta \sum_n (B_l; A_n) \phi_n(\mathbf{k}, \omega)$$

$$= \frac{i \mathbf{k} \beta \Omega_0 U_{\text{ext}}(\mathbf{k}, \omega)}{|M_{mn}(\mathbf{k}, \omega)|} \begin{vmatrix} 0 & N_{ln}(\mathbf{k}, \omega) \\ N_{m0}(\mathbf{k}, \omega) & M_{mn}(\mathbf{k}, \omega) \end{vmatrix}, \quad (10)$$

with the $N_{ln}(\mathbf{k}, \omega) = (B_l; A_n)$ in analogy to N_{m0} in equation (7). The choice of the relevant observables depends greatly on the physical situation considered and several principal approaches have been discussed by Zubarev *et al.* (1997). In order to introduce thermal perturbations the energy operator is assumed to be position dependent and subsequently the Lagrange multiplier $\beta = 1/k_B T$ is position dependent and leads to a temperature gradient in linear approximation. In the context of a charged particle system we would start with moments of the n -particle density operators for each of the constituents. A detailed discussion will be given in the next section.

The linear response theory expresses the response of a system (dissipation) via an equilibrium correlation function (fluctuations) which allows the systematic perturbative treatment in analogy to equilibrium properties. The generalised

linear response theory as sketched here has been successfully applied to mechanical and non-mechanical (heat and particle exchange) perturbations and the principal equivalence to the application of kinetic equations has been shown. Expressions for thermoelectric transport coefficients have been derived and, e.g., used to describe partially ionised plasmas (Höhne *et al.* 1984; Reinholz *et al.* 1995; Redmer 1997), semiconductors (Röpke and Höhne 1984), magnetic metals (Goedsche *et al.* 1983) and expanded liquid metals (Reinholz and Redmer 1993). However, this approach has the potential to calculate non-linear properties as well if the statistical operator is considered beyond the linear expansion; for conceptual examples and references see Zubarev *et al.* (1997).

3. Dielectric Function

The perturbation of the electron system shall now be specified as originating from an external longitudinal electric field, $\mathbf{D}(\mathbf{r}, t) = -\nabla U_{\text{ext}}(\mathbf{r}, t)/e$, the dielectric displacement due to an external density distribution $n_{\text{ext}}(\mathbf{r}, t)$. The dielectric response is introduced via the classical macroscopic theory of the dielectric displacement and the electric field inside the system which differs from the external due to an induced charge density $\delta f(\mathbf{r}, t)$,

$$\begin{aligned}\mathbf{k} \cdot \mathbf{D}(\mathbf{k}, \omega) &= \frac{1}{\epsilon_0} e n^{\text{ext}}(\mathbf{k}, \omega), \\ i\mathbf{k} \cdot \mathbf{E}(\mathbf{k}, \omega) &= \frac{1}{\epsilon_0} e [n^{\text{ext}}(\mathbf{k}, \omega) + \frac{1}{\Omega_0} \sum_p \delta f(\mathbf{p}; \mathbf{k}, \omega)],\end{aligned}$$

where we took the Fourier transform in space and time. The dielectric function is then defined by

$$\epsilon(\mathbf{k}, \omega) = \frac{D(\mathbf{k}, \omega)}{E(\mathbf{k}, \omega)} = 1 - V(k) \Omega_0 \Pi(\mathbf{k}, \omega). \quad (11)$$

The polarisation function

$$\Pi(\mathbf{k}, \omega) = \frac{e^2}{\Omega_0} \sum_p \delta f(\mathbf{p}; \mathbf{k}, \omega) \frac{1}{U_{\text{eff}}(\mathbf{k}, \omega)} \quad (12)$$

is the response with respect to the effective field $U_{\text{eff}} = U_{\text{ext}}/\epsilon(\mathbf{k}, \omega)$ and determines properties like the conductivity $\sigma(\mathbf{k}, \omega)$ of the system according to

$$\sigma(\mathbf{k}, \omega) = i \frac{\omega}{k^2} \Pi(\mathbf{k}, \omega). \quad (13)$$

Other physical properties of the system are rather determined by the response to the external field and we would consider the inverse dielectric function

$$\epsilon^{-1}(\mathbf{k}, \omega) = 1 + V(k) \Omega_0 \chi(\mathbf{k}, \omega) \quad (14)$$

with the dielectric susceptibility $\chi(\mathbf{k}, \omega)$ defined with respect to the external potential. As an example, the dynamical structure factor for finite temperatures is given as

$$S(\mathbf{k}, \omega) = \frac{1}{e^{-\beta\hbar\omega} - 1} \frac{\text{Im } \epsilon^{-1}(\mathbf{k}, \omega + i0)}{\pi e^2 V(k) \Omega_0} \quad (15)$$

and is directly related to the stopping power of fast electrons scattered on the charged particle system described by the dielectric function. However, both approaches are related via

$$\Pi(\mathbf{k}, \omega) = \epsilon(\mathbf{k}, \omega) \chi(\mathbf{k}, \omega) = \frac{\chi(\mathbf{k}, \omega)}{1 + V(k) \Omega_0 \chi(\mathbf{k}, \omega)}. \quad (16)$$

There are several exact relations for the dielectric function of a homogeneous charged particle system of particle density n which can be shown analytically. We will give a short summary since we refer to them later on. For an extended account see e.g. Mahan (1981). General relations are important in so far as the consistency of any approximation can be tested. Other approaches do use the sum-rules explicitly to construct improved approximations (Gold 1997; Adamyan *et al.* 1994; Hong and Lee 1993).

As a consequence of the causality of the system response the Kramers–Kronig relation connects the real and the imaginary part of the dielectric function

$$\text{Re } \epsilon(\mathbf{k}, \omega) = 1 + \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\text{Im } \epsilon(\mathbf{k}, \omega' + i0)}{\omega - \omega'}, \quad (17)$$

which can in fact be given in a more general way for any retarded correlation function. The so-called sum rules, although integrals over frequency, give general relations for certain frequency moments of the dielectric or inverse dielectric function,

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^n \text{Im } \epsilon^{\pm 1}(k, \omega) = C_n^{\pm}(\mathbf{k}). \quad (18)$$

The first moment of the inverse dielectric function known as the f-sum rule $C_1^- = -\omega_{\text{pl}}^2$ follows from particle conservation. It gives the sum of oscillator strengths for transitions from the ground states to excited states. Here ω_{pl} is the resonance frequency of collective plasma oscillations. The conductivity sum rule $C_1^+ = \omega_{\text{pl}}^2$ integrates over the dissipative part of the longitudinal conductivity $\sigma(\mathbf{k}, \omega)$ in equation (13). Amongst the higher moments the third moment sum rule C_3^- is of particular interest. It should converge. However, in RPA as well as for the Drude formula this sum rule diverges. There are also some rigorous limiting cases which should be considered in connection with any approximation. These are the perfect screening

$$\lim_{k \rightarrow 0} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{1}{\omega} \text{Im } \epsilon^{-1}(k, \omega) = -1 \quad (19)$$

and the compressibility (K) sum rule

$$\lim_{k \rightarrow 0} \text{Re } \epsilon(k, 0) = 1 + n^2 V(k) \Omega_0 K \quad (20)$$

for the long-wavelength limit as well as the high-frequency behaviour

$$\lim_{\omega \rightarrow \infty} \operatorname{Re} \epsilon(k, \omega) = 1 - \frac{\omega_{\text{pl}}^2}{\omega^2} + O(\omega^{-4}). \quad (21)$$

4. Microscopic Expressions

In this section, we want to consider the application of the linear response theory in order to find general microscopic expressions for the dielectric function. For simplicity we will restrict ourselves to an electron system scattered on adiabatic ions or impurities of density n_i according to the Hamiltonian (4). The physical quantity we are interested in is the induced single-particle density distribution in the expression for the polarisation function (12) or the dielectric susceptibility (14) and (16)

$$\delta f(\mathbf{p}; \mathbf{k}, \omega) \mathbf{e}^{-i\omega t} = \langle \delta n_{p,k} \rangle^t = \operatorname{Tr} \{n_{p,k} \rho(t)\} - \operatorname{Tr} \{n_{p,k} \rho_0\},$$

which can also be expressed via the mean value of the current operator using the continuity equation. The conservation of the particle number $n_k = \Omega_0^{-1} \sum_p n_{p,k}$, which leads to the balance equation

$$\frac{\partial}{\partial t} \langle n_k \rangle^t + i \mathbf{k} \cdot \langle \mathbf{J}_k \rangle^t = 0, \quad (22)$$

follows from the relation $(i/\hbar)[H_{\text{tot}}, n_k] = (i/\hbar)[H, n_k] = -i \mathbf{k} \cdot \mathbf{J}_k$. We find for the dielectric susceptibility

$$\chi(\mathbf{k}, \omega) = e^2 \langle n_k \rangle^t \mathbf{e}^{i\omega t} \frac{1}{U_{\text{ext}}(\mathbf{k}, \omega)} = e^2 \frac{\mathbf{k}}{\omega} \langle \mathbf{J}_k \rangle^t \mathbf{e}^{i\omega t} \frac{1}{U_{\text{ext}}(\mathbf{k}, \omega)}.$$

In the light of what has been said about a convenient choice of relevant observables we take the quantity we want to calculate the mean value of as the relevant observable and restrict ourselves to a one moment approach. Here $\{A_n\} = \{B_l\}$ is taken as n_k or \mathbf{J}_k , respectively. If we introduce a general expression

$$\chi(\mathbf{k}, \omega) = -i\beta \Omega_0 e^2 \frac{k^2}{\omega} \frac{1}{M(\mathbf{k}, \omega)}, \quad (23)$$

for the dielectric susceptibility, we find with equations (7) and (10) for the two different choices of relevant observables

$$M(\mathbf{k}, \omega) = -i \frac{k^2}{\omega} \frac{\langle n_k; \dot{n}_k + i\omega n_k \rangle_{\omega+i\eta}}{(n_k; n_k) \langle n_k; \dot{n}_k \rangle_{\omega+i\eta}} \quad (24)$$

$$= \frac{\langle \mathbf{J}_k; \dot{\mathbf{J}}_k + i\omega \mathbf{J}_k \rangle_{\omega+i\eta}}{(\mathbf{J}_k; \mathbf{J}_k) \langle \mathbf{J}_k; \dot{\mathbf{J}}_k \rangle_{\omega+i\eta}}. \quad (25)$$

The vector character of the current operator has been suppressed here. In the following, we consider an isotropic system where the correlation functions are scalars. The direction of the external longitudinal field is taken to be in the z -direction ($\mathbf{k} = k \vec{e}_z$). For the two-dimensional case, z will lie in the two-dimensional plane. Applying partial integration in the correlation functions,

$$\langle A; \dot{B} \rangle_z = -\langle \dot{A}; B \rangle_z = (A; B) + i z \langle A; B \rangle_z, \quad (26)$$

and taking into account relation (8) between the particle density and the current density operator, it can readily be seen that in the thermodynamic limit $\eta \rightarrow 0$ the above relations (24) and (25) are identical and equal to the Kubo formula (Kubo 1957; Mahan 1981)

$$\chi(\mathbf{k}, \omega) = -i \beta \Omega_0 e^2 \frac{k^2}{\omega} \langle J_k; J_k \rangle_{\omega+i\eta}. \quad (27)$$

The Kubo formula can also be derived within the generalised linear response theory by choosing an empty set of relevant observables (Röpke 1998). It is thus apparent that the actual chosen quantum statistical approach, in particular the choice of relevant observables, does lead to identical expressions as long as no approximations have been made. However, in the course of evaluating and applying perturbation theory the formulas might be differently suited to different physical situations. For instance, it is well known, that the Kubo formula leads to singularities in the static long-wavelength limit (dc conductivity). The derived expression (23) relates the inverse of the dc conductivity to correlation functions and is, as outlined below, much better suited to avoid these singularities. It also allows the inclusion of different scattering mechanisms, in particular the electron–electron interaction, on the level of collisions.

From kinetic theories (Spitzer 1962) and application of the linear response theory to thermoelectric transport (Reinholz *et al.* 1989, 1995), it is well known that higher moments need to be taken into account and lead to a better convergence of perturbation theory in the non-degenerate limit. We want to treat the dielectric function on the same level. A generalisation of the above derived expressions for higher moments is straight forward and has been considered by Reinholz *et al.* (1989, 1999) and Röpke and Wierling (1998). An expanded set of relevant observables could take the form

$$\mathbf{A}_n = \frac{\hbar}{\Omega_0 m} \sum_p (\beta E_p)^n \mathbf{p} n_{p,k}. \quad (28)$$

The first moment \mathbf{A}_0 is the current operator \mathbf{J}_k . Taking into account the second moment is relevant in connection with thermal conductivity since it is equivalent to the ideal contribution of the energy current. We then find the general expression for the dielectric susceptibility (23) with

$$M(\mathbf{k}, \omega) = |M_{nm}(\mathbf{k}, \omega)| \left/ \begin{vmatrix} 0 & N_{0m}(\mathbf{k}, \omega) \\ N_{n0}(\mathbf{k}, \omega) & M_{nm}(\mathbf{k}, \omega) \end{vmatrix} \right.,$$

$$N_{nm}(\mathbf{k}, \omega) = (A_n; A_m), \quad M_{nm}(\mathbf{k}, \omega) = \frac{N_{nm} N_{n0}}{\langle A_n; A_0 \rangle_{\omega+i\eta}}. \quad (29)$$

A different choice of relevant observables is the particle density operator and higher moments of it. This could take into account the energy operator. However, the approaches would be connected to (29) via particle conservation (22) and energy conservation laws.

In the following sections we will discuss different approximations when calculating the dielectric function using the one-moment approach (23) with $\{A_n\} \Rightarrow J_k$:

$$M(\mathbf{k}, \omega) = \frac{1}{(J_k; J_k)^2} \left[-i\omega (J_k; J_k) + \langle \dot{J}_k; \dot{J}_k \rangle_{\omega+i\eta} - \langle \dot{J}_k; J_k \rangle_{\omega+i\eta} \frac{1}{\langle J_k; J_k \rangle_{\omega+i\eta}} \langle J_k; \dot{J}_k \rangle_{\omega+i\eta} \right] \quad (30)$$

$$= \frac{1}{\langle J_k; J_k \rangle_{\omega+i\eta}}. \quad (31)$$

This is also equivalent to (25) which can be shown by partial integrations again. We apply perturbation theory to $M(\mathbf{k}, \omega) = M^{(0)}(\mathbf{k}, \omega) + M^{(1)}(\mathbf{k}, \omega) + M^{(2)}(\mathbf{k}, \omega)$ in order to calculate the susceptibility. This is in contrast to the Kubo formula (27) where we apply perturbation theory to the current-current correlation function itself. The latter can be related to the correlation function of the Wigner densities $n_{p,k}$ via

$$\langle J_k; J_k \rangle_{\omega+i\eta} = \left(\frac{\hbar}{m\Omega_0} \right)^2 \sum_{pp'} p_z p'_z \langle n_{p,k}; n_{p',k} \rangle_{\omega+i\eta}. \quad (32)$$

Thus, if in the static long-wavelength limit the perturbation theory of (32) leads to divergent terms in all orders the result is divergent. However, these terms cancel when considering the perturbation of the inverse expression giving a finite result.

The correlation function $(J_k; J_k)$ can be calculated exactly by relating it to the commutator of position and linear momentum (cf. Röpke 1988). With the electron density n we have

$$(J_k; J_k) = \frac{n}{m\beta\Omega_0}. \quad (33)$$

The evaluation of $M(\mathbf{k}, \omega)$ by perturbation theory will be detailed below. The zeroth order leads to the random phase approximation. The RPA result will be discussed in the next section. The following section considers the first order contribution which gives the so-called local field corrections. Only taking into account second order contributions allows the inclusion of collisions and the calculation of the conductivity within the theory of the dielectric function according to equation (1). We will derive a generalised Drude formula with a well-defined approach to calculate the relaxation time.

5. RPA

In order to determine the current–current correlation function (32) or the other correlation functions appearing in the formalism outlined in the last section, we need to calculate the density–density correlation function

$$\langle n_{p,k}; n_{p',k} \rangle_{\omega+i\eta} = \langle c_{p-\frac{k}{2}}^\dagger c_{p+\frac{k}{2}}; c_{p'-\frac{k}{2}}^\dagger c_{p'+\frac{k}{2}} \rangle_{\omega+i\eta}, \quad (34)$$

which can easily be done for the zeroth order by using the Wick theorem (e.g. Mahan 1981). Since we want to consider higher perturbation theory later on, we use the connection to Green functions and Feynman diagrams. According to (9), the correlation function can be evaluated considering the two-particle Green function $\mathcal{G}_{nn}(p-k/2, p+k/2; p'-k/2, p'+k/2; \omega_\mu)$. In the presentation by diagrams, \mathcal{G}_{nn} is a four-point function with frequency ω_μ , on the left-hand side with incoming $p-k/2$ and outgoing $p+k/2$, on the right-hand side with incoming $p'-k/2$ and outgoing $p'+k/2$. The Born approximation is obtained if incoming and outgoing lines are connected, corresponding to a simple bubble $\mathcal{G}_{nn}^{(0)}$. It means that the two-particle Green function is approximated by the product of two single-particle Green functions of the ideal system:

$$\begin{aligned} \mathcal{G}_{nn}^{(0)}(p-k/2, p+k/2; p'-k/2, p'+k/2; \omega_\mu) \\ = \delta_{pp'} \sum_{z_\nu} \frac{1}{z_\nu - E_{p+\frac{k}{2}}} \frac{1}{z_\nu + \omega_\mu - E_{p-\frac{k}{2}}}. \end{aligned}$$

This leads to

$$\langle n_{p,k}; n_{p',k} \rangle^{(0)} = \delta_{pp'} \frac{\hbar}{i\beta} \frac{f_{p+\frac{k}{2}} - f_{p-\frac{k}{2}}}{E_{p+\frac{k}{2}} - E_{p-\frac{k}{2}}} \frac{1}{E_{p+\frac{k}{2}} - E_{p-\frac{k}{2}} - \hbar\omega - i\eta}. \quad (35)$$

Here and in all what follows we will omit the index $\omega+i\eta$ when writing correlation functions of the type $\langle A; B \rangle_{\omega+i\eta}$. We find the well-known RPA expression (Lindhard 1954)

$$\Pi^{(0)}(\mathbf{k}, \omega) = \frac{e^2}{\Omega_0} \sum_p \frac{f_{p+\frac{k}{2}} - f_{p-\frac{k}{2}}}{E_{p+\frac{k}{2}} - E_{p-\frac{k}{2}} - \hbar\omega - i\eta}, \quad (36)$$

which is obtained from (35) irrespective of which of the above approaches (24), (25) or (27) were chosen. Here $f_p = [\exp(\beta E_p - \beta\mu) + 1]^{-1}$ denotes the Fermi distribution function and μ the chemical potential. The limit $\eta \rightarrow 0$ has to be taken after the thermodynamic limit and can be performed using Dirac's identity. Note that due to the structure of the polarisation function the validity of the Kramers–Kronig relation (17) can be seen readily.

In the static limit, the imaginary part of (36) vanishes whereas the real part can be written as

$$\lim_{\omega \rightarrow 0} \Pi(\mathbf{k}, \omega) = \frac{e^2}{\Omega_0} \sum_p f_p \left(\frac{1}{E_p - E_{p-k}} - \frac{1}{E_{p+k} - E_p} \right).$$

We consider the limits for small and large wave vectors,

$$\begin{aligned}\lim_{k \rightarrow \infty} \epsilon(\mathbf{k}, 0) &= 1 + 4n \frac{e^2 m}{\epsilon_0 \hbar^2 k^4}, \\ \lim_{k \rightarrow 0} \epsilon(\mathbf{k}, 0) &= 1 + \left(\frac{\kappa}{k}\right)^{d-1},\end{aligned}\quad (37)$$

with the dimensionality of the system being $d = 2, 3$. In the long-wavelength limit, the screening parameter in the three-dimensional case is a Fermi integral

$$\kappa_{3D}^2 = \frac{e^2 m^{\frac{3}{2}}}{\sqrt{2} \pi^2 \epsilon_0 \hbar^3} \int_0^\infty dE_p E_p^{-1/2} f_p$$

for arbitrary degeneracy and reduces to Debye screening $\kappa_D^2 = \beta e^2 n / \epsilon_0$ in the nondegenerate limit and the Thomas–Fermi parameter $\kappa_{TF}^2 = e^2 m k_F / \pi^2 \hbar^2 \epsilon_0$ in the degenerate limit. For the two-dimensional case, the screening parameter

$$\kappa_{2D} = \frac{e^2 m}{2\pi \epsilon_0 \hbar^2}$$

is density independent and comparable with an atomic size $a_B = 2/\kappa_{2D}$, whereas the three-dimensional Debye radius κ_{3D}^{-1} can vary in its dependence on temperature and density over a wide range. Typical values for a dense non-degenerate plasma would be between $10 a_B$ and $10^4 a_B$.

In the long wavelength limit, the relation

$$\lim_{k \rightarrow 0} \langle J_k; J_k \rangle^{(0)} = \frac{i}{\omega} (J_k; J_k) \quad (38)$$

holds and with (33) we find

$$\lim_{k \rightarrow 0} \Pi^{(0)}(\mathbf{k}, \omega) = \frac{n e^2}{m} \frac{k^2}{\omega^2} = \frac{1}{V(k) \Omega_0} \frac{\omega_{pl}^2}{\omega^2}, \quad (39)$$

where the plasma frequency in the three-dimensional case is $\omega_{pl}^2 = e^2 n / \epsilon_0 m$. The two-dimensional case $\omega_{pl}^2 = e^2 n k / 2 \epsilon_0 m$ is dependent on the wave vector.

Performing the integrations for a three-dimensional system, we find the RPA dielectric function for arbitrary degeneracy as given by Arista and Brandt (1984):

$$\begin{aligned}\text{Re } \epsilon(k, \omega) &= 1 + \frac{2 k_F^2}{\pi a_B k^3} [g(u+z) - g(u-z)], \\ \text{Im } \epsilon(k, \omega) &= \frac{8\pi \epsilon_0}{\beta e^2 a_B^2 k^3} \ln \frac{1 + \exp(\beta \mu - (u-z)^2 \beta E_F)}{1 + \exp(\beta \mu - (u+z)^2 \beta E_F)},\end{aligned}$$

with

$$g(x) = \int_0^\infty dy y \ln\left(\frac{|x+y|}{|x-y|}\right) f[y^2 E_F],$$

$$u = \frac{m\omega}{\hbar k k_F}, \quad z = \frac{k}{2k_F} \quad \text{and} \quad k_F^3 = 3\pi^2 n. \quad (40)$$

The general expression (36) and limiting cases are valid for two-dimensional systems as well. The explicit treatment of the integrals for $T = 0$ was first given by Stern (1967). For arbitrary temperature, the expression for the dielectric function is (Ganguly *et al.* 1977)

$$\text{Re } \epsilon(k, \omega) = 1 + \frac{k_F}{a_B k^2} [h_1(u+z) - h_1(u-z)],$$

$$\text{Im } \epsilon(k, \omega) = \frac{k_F}{a_B k^2} [h_2(u-z) - h_2(u+z)].$$

The variables u, z are defined as in (40), but the Fermi wave vector is $k_F^2 = 2\pi n$. The functions introduced above are integrals over the Fermi functions,

$$h_1(x) = \int_0^1 dy \frac{y}{\sqrt{1-y}} f[yx^2 E_F],$$

$$h_2(x) = \int_0^\infty \frac{dy}{\sqrt{u}} f[(y+x^2)E_F].$$

The RPA approximation, which describes the collisionless plasma, satisfies the first moment sum rules (18) and limiting relations (19)–(21) given in Section 3. However, it cannot describe electrical transport (conductivity) since interactions are not taken into account.

6. Local Field Corrections

Hubbard (1957) introduced a correction factor $G(\mathbf{k})$ to the RPA in order to account for the exchange and correlation hole around an electron. It increases the dielectric screening. The concept of local-field factors for two- and three-dimensional systems (Singwi *et al.* 1968; Ichimaru *et al.* 1985; Świerkowski *et al.* 1993; Gold 1997; Kalman and Golden 1993, and references therein) in the static limit ($\omega = 0$) has been extended to finite frequencies by introducing dynamical local-field factors $G(\mathbf{k}, \omega)$ in precisely the same form as the Hubbard corrections according to

$$\Pi(\mathbf{k}, \omega) = \frac{\Pi^{(0)}(\mathbf{k}, \omega)}{1 + G(\mathbf{k}, \omega) \Omega_0 V(k) \Pi^{(0)}(\mathbf{k}, \omega)}. \quad (41)$$

Different approximation methods to determine $G(\mathbf{k}, \omega)$ have been developed such as perturbation expansions (Richardson and Ashcroft 1994) and the parametrisation of the dielectric function via sum rules (Hong and Lee 1993; Iwamoto *et al.* 1984). In particular, it has been shown that the third moment sum rule (18) is important in the construction of dynamic approximations (Kalman and Golden

1998; Iwamoto 1984). A study of the dynamical local-field factors within a time-dependent mean-field theory neglecting damping effects was reported by Kalman and Golden (1990).

Within our approach, the dynamical local-field factor $G(\mathbf{k}, \omega)$ is directly related to $M(k, \omega)$ according to

$$G(\mathbf{k}, \omega) = i \frac{\omega}{\beta \Omega_0^2 e^2 V(k) k^2} M(\mathbf{k}, \omega) - \frac{1}{V(k) \Omega_0 \Pi^{(0)}(k, \omega)} + 1. \quad (42)$$

The zeroth-order contribution $M^{(0)}(k, \omega)$ is compensated by the second term, whereas contributions from reducible diagrams compensate the 1. The first-order contributions

$$M^{(1)}(\mathbf{k}, \omega) = - \frac{\langle J_k; J_k \rangle^{(1)}}{(\langle J_k; J_k \rangle^{(0)})^2} \quad (43)$$

are due to self-energy and vertex corrections in the corresponding Feynman diagrams of the Green function G_{nn} in (34) up to first order in V ,

$$\begin{aligned} \langle n_{p,k}; n_{p',k} \rangle^{(1)} &= \frac{\hbar}{i\beta} \left(\frac{m}{\hbar^2 k} \right)^3 \frac{f_{p+\frac{k}{2}} - f_{p-\frac{k}{2}}}{p_z(p_z - m\omega/\hbar k - i\eta)} \\ &\times \left[-\delta_{pp'} \sum_{p''} V(p-p'') \frac{f_{p''+\frac{k}{2}} - f_{p''-\frac{k}{2}}}{p_z(p_z - m\omega/\hbar k - i\eta)} (2p_z - m\omega/\hbar k) \right. \\ &\left. + V(p-p') \frac{f_{p'+\frac{k}{2}} - f_{p'-\frac{k}{2}}}{p'_z(p'_z - m\omega/\hbar k - i\eta)} (p_z + p'_z - m\omega/\hbar k) \right]. \end{aligned}$$

The evaluation of (42) and (43) yields the result for the dynamical local field corrections in first order at arbitrary densities and temperatures

$$\begin{aligned} G^{(1)}(k, \omega) &= \frac{1}{2} \frac{\epsilon_0 m^2 e^2}{\hbar^4 \Omega_0} [\Pi^{(0)}(k, \omega)]^{-2} \sum_{pp'} V(|\mathbf{p} - \mathbf{p}'|) \\ &\times (f_{p+\frac{k}{2}} - f_{p-\frac{k}{2}}) \left(\frac{1}{p_z - m\omega/\hbar k - i\eta} - \frac{1}{p'_z - m\omega/\hbar k - i\eta} \right)^2 \\ &\times (f_{p'+\frac{k}{2}} - f_{p'-\frac{k}{2}}). \end{aligned} \quad (44)$$

In the three-dimensional case at zero temperature, an analytical expression for $G^{(1)}(k, \omega)$ can be found; see Richardson and Ashcroft (1994) and Engel and Vosko (1990) for the static limit $G^{(1)}(k, 0)$. The limiting cases are in accordance with the compressibility sum rule (20), $\lim_{k \rightarrow 0} G^{(1)}(k, 0) = k^2/4k_F^2$, and the relation to the pair distribution at zero distance, $\lim_{k \rightarrow \infty} G^{(1)}(k, 0) = \frac{1}{3}$, which are correct within the order of perturbation theory considered here, i.e. comparing with properties of the uncorrelated fermion gas (Hong and Mahan 1994). The static local field corrections are important for large wave vectors (small distances) and

low densities. A better approach should go beyond the first order contributions and relate the local field corrections self-consistently to the structure factor or pair distribution function, as proposed in the classical work of Singwi *et al.* (1968) and elaborated further by others. Similar relations should be derived for the dynamical local field factor.

The long-wavelength limit is of particular interest when calculating optical conductivities. Using the relations

$$\lim_{k \rightarrow 0} (f_{p+\frac{k}{2}} - f_{p-\frac{k}{2}}) = -\beta f_p(1 - f_p) \frac{\hbar^2 k}{m} p_z,$$

$$\lim_{k \rightarrow 0} \left(\frac{1}{p_z - m\omega/\hbar k - i\eta} - \frac{1}{p'_z - m\omega/\hbar k - i\eta} \right) = \left(\frac{\hbar k}{\omega} \right)^2 (p'_z - p_z),$$

as well as (39), it follows from (44) that

$$\begin{aligned} \lim_{k \rightarrow 0} G^{(1)}(k, \omega) &= \frac{k^2}{2\Omega_0} \frac{\epsilon_0 \hbar^4 \beta^2}{(emn)^2} \sum_{pp'} f_p(1 - f_p) V(|\mathbf{p} - \mathbf{p}'|) f_{p'} \\ &\quad \times (1 - f_{p'}) p_z p'_z (p_z - p'_z)^2. \end{aligned} \quad (45)$$

Thus, this expression is proportional to k^2 and no contribution from terms of first order in V will modify the behaviour in the long-wavelength limit $k \rightarrow 0$.

7. Inclusion of Collisions

In order to allow for inclusion of collisions we need to consider the perturbation theory up to the quadratic order of the interaction potential,

$$\begin{aligned} M^{(2)}(k, \omega) &= - \frac{\langle J_k; J_k \rangle^{(2)}}{(\langle J_k; J_k \rangle^{(0)})^2} + \frac{(\langle J_k; J_k \rangle^{(1)})^2}{(\langle J_k; J_k \rangle^{(0)})^3} \\ &= - \frac{\langle J_k; J_k \rangle^{(2)}}{(\langle J_k; J_k \rangle^{(0)})^2} + \langle J_k; J_k \rangle^{(0)} (M^{(1)}(k, \omega))^2. \end{aligned} \quad (46)$$

Making use of partial integration (26) and the fact that $(A; \dot{A}) = 0$ we can express the current-current correlation function as

$$\langle J_k; J_k \rangle = \frac{i}{\omega} \langle J_k; J_k \rangle + \frac{1}{\omega^2} \langle \dot{J}_k; \dot{J}_k \rangle. \quad (47)$$

The first term is known from (33). Expressing the time derivative \dot{J}_k of the current operator by applying the commutator relation with the Hamiltonian, we obtain the general expression

$$\begin{aligned} \langle \dot{J}_k; \dot{J}_k \rangle &= \left(\frac{\hbar}{m\Omega_0} \right)^2 \sum_{pp'} p_z p'_z [\langle v_{p,k}; v_{p',k} \rangle + \left(\frac{\hbar k}{m} \right)^2 p_z p'_z \langle n_{p,k}; n_{p',k} \rangle \\ &\quad + \left(i \frac{\hbar k}{m} \right) \{ p'_z \langle v_{p,k}; n_{p',k} \rangle - p_z \langle n_{p,k}; v_{p',k} \rangle \}]. \end{aligned} \quad (48)$$

The v_{pk} arise from the potential dependent part of the commutator as

$$v_{pk} = -\frac{ie^2}{\hbar} \sum_{\bar{p}qj} V(q) \mathbf{e}^{-i\mathbf{q}\cdot\mathbf{R}_j} \{\delta_{\bar{p},p} - \delta_{\bar{p},p+q}\} c_{\bar{p}-\frac{k}{2}-q}^\dagger c_{\bar{p}+\frac{k}{2}} \\ + \frac{ie^2}{2\hbar} \sum_{\bar{p}p'q} \{V(q) + V(-q)\} \{\delta_{\bar{p},p} - \delta_{\bar{p},p+q}\} c_{\bar{p}-\frac{k}{2}-q}^\dagger c_{p'+q}^\dagger c_{p'} c_{\bar{p}+\frac{k}{2}}. \quad (49)$$

The first term is the electron–ion interaction. The second term contains the electron–electron interaction including exchange, but does not give any contribution to the final results within this one-moment approach due to momentum conservation. In order to collect all terms in the second order Born approximation we apply the following relations, which can be proved by partial integration, to equation (48):

$$\begin{aligned} \langle n_{p,k}; n_{p',k} \rangle &= \left(-i \frac{m}{\hbar k} \right) \frac{(n_{p,k}; n_{p',k}) + \langle v_{p,k}; n_{p',k} \rangle}{p_z - m\omega/\hbar k} \\ &= \left(-i \frac{m}{\hbar k} \right) \frac{(n_{p,k}; n_{p',k}) - \langle n_{p,k}; v_{p',k} \rangle}{p'_z - m\omega/\hbar k}, \\ \langle n_{p,k}; v_{p',k} \rangle &= \left(-i \frac{m}{\hbar k} \right) \frac{(n_{p,k}; v_{p',k}) + \langle v_{p,k}; v_{p',k} \rangle}{p_z - m\omega/\hbar k}, \\ \langle v_{p,k}; n_{p',k} \rangle &= \left(-i \frac{m}{\hbar k} \right) \frac{(v_{p,k}; n_{p',k}) - \langle v_{p,k}; v_{p',k} \rangle}{p'_z - m\omega/\hbar k}. \end{aligned}$$

The force–force correlation function in second order is

$$\begin{aligned} \langle \dot{J}_k \dot{J}_k \rangle^{(2)} &= \left(\frac{\hbar}{m\Omega_0} \right)^2 \sum_{p_z p'_z} \left[\left(\frac{m\omega}{\hbar k} \right)^2 \frac{\langle v_{p,k}; v_{p',k} \rangle^{(0)}}{(p_z - m\omega/\hbar k - i\eta)(p'_z - m\omega/\hbar k - i\eta)} \right. \\ &\quad - \left(i \frac{\hbar k}{m} \right) p_z p'_z \frac{(n_{p,k}; n_{p',k})^{(2)}}{p_z - m\omega/\hbar k - i\eta} - (n_{p,k}; v_{p',k})^{(1)} \\ &\quad - \left(\frac{m\omega}{\hbar k} \right) \frac{(n_{p,k}; v_{p',k})^{(1)} + (v_{p,k}; n_{p',k})^{(1)}}{p_z - m\omega/\hbar k} \\ &\quad \left. + \left(\frac{m\omega}{\hbar k} \right)^2 \frac{(v_{p,k}; n_{p',k})^{(1)}}{(p_z - m\omega/\hbar k)(p'_z - m\omega/\hbar k)} \right]. \quad (50) \end{aligned}$$

The first term is explicitly in second order of the interaction, whereas the other correlation functions would have to be considered including self-energy and vertex corrections and beyond. The correlation function $\langle v_{p,k}; v_{p',k} \rangle$ in zeroth-order can be related to density–density correlation functions similar to (35) and we obtain

$$\begin{aligned}
\langle v_{p,k}; v_{p',k} \rangle^{(0)} = & -i \frac{e^4 n_i \Omega_0}{\beta \hbar} \sum_q V^2(q) S_i(q) \\
& \times \left[\frac{f_{p-\frac{k}{2}-q} - f_{p+\frac{k}{2}}}{E_{p-\frac{k}{2}-q} - E_{p+\frac{k}{2}} - \hbar\omega - i\eta} \frac{\delta_{pp'} - \delta_{p,p'+q}}{E_{p-\frac{k}{2}-q} - E_{p+\frac{k}{2}}} \right. \\
& \left. + \frac{f_{p-\frac{k}{2}} - f_{p+\frac{k}{2}+q}}{E_{p-\frac{k}{2}} - E_{p+\frac{k}{2}+q} - \hbar\omega - i\eta} \frac{\delta_{pp'} - \delta_{p,p'-q}}{E_{p-\frac{k}{2}} - E_{p+\frac{k}{2}+q}} \right] \\
& + \text{electron-electron contributions,} \tag{51}
\end{aligned}$$

where $S_i(q) = \sum_{jj'} \exp[i\mathbf{q} \cdot (\mathbf{R}_j - \mathbf{R}_{j'})]/n\Omega_0$ is the ionic structure factor. Substituting this into (50) and restricting ourselves to the first term which is explicit in V^2 , we find the general expression

$$\begin{aligned}
\langle \dot{j}_k; \dot{j}_k \rangle^{(2,V)} = & -i \frac{e^4 n_i}{\beta \Omega_0 \hbar} \left(\frac{\omega}{k} \right)^2 \sum_{pq} V^2(q) S_i(q) \\
& \times \frac{f_{p-\frac{k}{2}-\frac{k}{2}} - f_{p+\frac{k}{2}+\frac{k}{2}}}{E_{p-\frac{k}{2}-\frac{k}{2}} - E_{p+\frac{k}{2}+\frac{k}{2}} - \hbar\omega - i\eta} \\
& \times \frac{1}{E_{p-\frac{k}{2}-\frac{q}{2}} - E_{p+\frac{k}{2}+\frac{q}{2}}} \left(\frac{p_z + q/2}{p_z + q/2 - m\omega/\hbar k - i\eta} \right. \\
& \left. - \frac{p_z - q/2}{p_z - q/2 - m\omega/\hbar k - i\eta} \right)^2. \tag{52}
\end{aligned}$$

Electron-electron interaction terms are omitted here since they do not contribute in the long-wavelength limit $k \rightarrow 0$ due to momentum conservation, which will be considered in the next section.

8. Frequency Dependent Conductivity

In order to calculate optical conductivities (1) we need to consider the dielectric function (11) in the long-wavelength limit $k \rightarrow 0$. Defining a collision term $\Sigma(\omega) = \omega_{\text{pl}}^2 G(0, \omega)/\omega$, we find with the polarisation function (41), where the long-wavelength limit (39) of the RPA polarisation function was substituted,

$$\epsilon(0, \omega) = 1 - \frac{\omega_{\text{pl}}^2}{\omega[\omega + \text{Re}\Sigma(\omega)] + i\omega/\tau(\omega)}. \tag{53}$$

This is a Drude-like expression with a frequency-dependent relaxation time $\tau^{-1}(\omega) = \text{Im}\Sigma(\omega)$. The perturbation expansion of $G(0, \omega)$ in equation (42) is given by the expansion of $M(0, \omega)$. According to the discussion of (45), the first-order terms $M^{(1)}$ do not contribute in the long-wavelength limit. Subsequently, the second-order terms (46) arise from the current-current correlation function in second order only. Also in this limit, the first term on the right-hand side of expression (47) contains the complete zeroth order contribution due to (38), while

the second term only contains second and higher order contributions. Therefore we can write

$$M^{(2)}(0, \omega) = \lim_{k \rightarrow 0} \frac{\langle \dot{J}_k; \dot{J}_k \rangle^{(2)}}{(J_k; J_k)^2}.$$

Substituting the correlation functions by (33) and the long-wavelength limit of (52), the collision term is

$$\Sigma(\omega) = \frac{e^4 \hbar n_i}{d m n} \sum_{pq} V^2(q) S_i(q) \frac{q^2}{E_{p-q} - E_p} \frac{f_{p-q} - f_p}{E_{p-q} - E_p - \hbar\omega - i\eta}. \quad (54)$$

It can be shown analytically that a Kramers–Kronig relation (17) holds for the collision term which will be used when making numerical calculations. The limit $\eta \rightarrow 0$ can be carried out using the Dirac identity $\lim_{\eta \rightarrow 0} (x - i\eta)^{-1} = P(1/x) + i\pi \delta(x)$. The real part of the collision term vanishes in the static limit $\omega \rightarrow 0$. It needs to be taken into account for finite frequencies and modifies the Drude form of the dielectric function. A frequency dependent relaxation time in the second Born approximation is obtained from the imaginary part of (54) as

$$\tau^{-1}(\omega) = \frac{\pi e^4 n_i}{d m n \omega} \sum_{pq} V^2(q) S_i(q) q^2 [f(E_p + \hbar\omega) - f(E_p)] \delta(E_{p-q} - E_p - \hbar\omega).$$

These are the general expressions which have to be considered when calculating the optical conductivity using the generalised Drude formula (53). The number of integrations can be reduced analytically to

$$\begin{aligned} \tau^{-1}(\omega) &= \frac{e^4 \Omega_0^2 n_i}{\hbar^2 n \omega} \frac{1}{d(2\pi)^d} \int_0^\infty dq q^d V^2(q) S_i(q) \\ &\quad \times \int_{(\frac{m\omega}{\hbar q} + \frac{q}{2})^2}^\infty dp^2 p^{d-3} [f(E_p + \hbar\omega) - f(E_p)]. \end{aligned} \quad (55)$$

Since the real part of the collision integral vanishes in the static limit the relaxation time is directly related to the dc conductivity via

$$\sigma_{dc} = \epsilon_0 \omega_{pl}^2 \lim_{\omega \rightarrow 0} \tau(\omega). \quad (56)$$

From the static limit of (55)

$$\begin{aligned} \lim_{\omega \rightarrow 0} \tau^{-1}(\omega) &= \frac{e^4 \Omega_0^2 n_i 2m}{\hbar^3 n d(2\pi)^d} \int_0^\infty dq q^d V^2(q) S_i(q) \\ &\quad \times \left[\left(\frac{q}{2} \right)^{d-3} f_{\frac{q}{2}} - \frac{d-3}{2} \left(\frac{2m}{\hbar^2} \right)^{\frac{d-3}{2}} \int_{E_{\frac{q}{2}}}^\infty dE_p E_p^{\frac{d-5}{2}} f_p \right], \end{aligned} \quad (57)$$

we find for three-dimensional systems, where the second term of the above expression vanishes,

$$\sigma_{dc}^{3D} = \frac{12\pi^3 \hbar^3 n^2}{e^2 \Omega_0^2 m^2 n_i} \left[\int_0^\infty dq q^3 V^2(q) S_i(q) f(E_{\frac{q}{2}}) \right]^{-1}. \quad (58)$$

This is one of the generalisations of the Ziman formula (Ziman 1961; Faber 1972) which was originally derived for $T = 0$ only. In the two-dimensional case the integrations cannot be reduced to a single one, but an additional Fermi integral remains. However, the $T = 0$ limit yields

$$\sigma_{dc}^{2D} = \frac{8\pi^2 \epsilon_0^2 \hbar^3 n^2}{e^2 m^2 n_i}.$$

The Drude model (e.g. Mahan 1981) is obtained from (53) if the frequency dependent collision term $\Sigma(\omega)$ (54) is approximated by its static limit $\Sigma(0)$ (57). Numerical calculations of the dielectric function (53) with the frequency dependent collision term (54) for the three-dimensional case were presented recently (Reinholz *et al.* 1999; Röpke *et al.* 1999) and will be discussed in the following. The account of the frequency dependence of $\Sigma(\omega)$ leads to deviations from the Drude model for frequencies higher than the plasma frequency. Due to the ω dependence of $\tau(\omega)$, the plasmon peak becomes narrower compared with the Drude expression. Furthermore, due to the finite real part of $\Sigma(\omega)$ it is shifted. It has also been found numerically that the dielectric function in the long-wavelength limit (53) obeys both first moment sum rules (18) within an accuracy of 0.1%. The consistent consideration of both the real and the imaginary part of the frequency-dependent collision term is crucial for the sum rules. Taking into account a frequency dependence in the relaxation time only, i.e. neglecting $\text{Re } \Sigma(\omega)$ in equation (53), leads to a considerable violation of the sum rules of the order of 10%. Of special interest is the third-moment sum rule $C_3^{(-)}(k)$. It is divergent within the Drude model. To obey the third-moment, as well as the compressibility sum rule simultaneously, frequency-dependent local-field factors are required (Iwamoto 1984). Thus, a dielectric function with a frequency-dependent collision term is needed. Evaluating the collision term (54) in the high-frequency limit, the imaginary part of $\epsilon^{-1}(0, \omega)$ behaves as $\omega^{-9/2}$ (Reinholz *et al.* 1999), implying that the third-moment integral converges as desired.

So far we have considered the collision term (54) for arbitrary frequencies ω in the Born approximation. The interaction in the above expressions is a pure Coulombic one. However, the treatment of Coulomb systems in the Born approximation is not satisfactory. The Coulomb interaction is long ranged which leads to divergencies at small values of q . This divergency can be cured if a screened interaction is considered. Static screening will lead to a short-range potential. A more consistent treatment yields dynamical screening, summing up the so-called ring diagrams in the perturbation expansion.

9. Dynamically Screened Born Approximation

From equation (50) with (49) we found in the long-wavelength limit that

$$\begin{aligned}
\langle \dot{J}_k \dot{J}_k \rangle &= \left(\frac{e^2}{m\Omega_0} \right)^2 \sum_{pp'qq'\bar{p}\bar{p}'} p_z p'_z \sum_{jj'} \mathbf{e}^{-i(\mathbf{q} \cdot \mathbf{R}_j - \mathbf{q}' \cdot \mathbf{R}_{j'})} \\
&\quad \times \{ \delta_{\bar{p},p} - \delta_{\bar{p},p+q} \} \{ \delta_{\bar{p}',p'} - \delta_{\bar{p}',p'+q'} \} \\
&\quad \times V(q) \langle c_{\bar{p}-q}^\dagger c_{\bar{p}}; c_{\bar{p}'-q'}^\dagger c_{\bar{p}'} \rangle V(q').
\end{aligned}$$

We perform the summations over p, p' and replace \bar{p} by p :

$$\langle \dot{J}_k \dot{J}_k \rangle = \left(\frac{e^2}{m\Omega_0} \right)^2 \sum_{pp'qq'} q_z q'_z \sum_{jj'} \mathbf{e}^{-i(\mathbf{q} \cdot \mathbf{R}_j - \mathbf{q}' \cdot \mathbf{R}_{j'})} V(q) \langle c_{p-q}^\dagger c_p; c_{p'-q'}^\dagger c_{p'} \rangle V(q').$$

According to (9), the correlation function can be evaluated considering the two-particle Green function $G_{nn}(p-q, p; p'-q', p'; \omega_\mu)$. The Born approximation, which is identical with considering a single bubble diagram, leads to expression (52). We now go beyond this and do a partial summation accounting for all so-called bubble diagrams, replacing within the diagrams

$$G_{vv}(\omega_\mu) = V(q) \sum_{pp'} G_{nn}(p-q, p; p'-q', p'; \omega_\mu) V(q')$$

by the spectral representation of a screened potential

$$G_{vv}(\omega_\mu) = V^s(q, \omega_\mu) - V(q) = \delta_{qq'} V(q) \int \frac{d\bar{\omega}}{\pi} \frac{\text{Im} \epsilon^{-1}(q, \bar{\omega} - i0)}{\omega_\mu - \bar{\omega}}.$$

In order to calculate the correlation function we need to substitute

$$\text{Im} G_{vv}(\omega - i\eta) = \delta_{qq'} V(q) \text{Im} \epsilon^{-1}(q, \omega - i0)$$

into (9) and obtain

$$\langle \dot{J}_k \dot{J}_k \rangle = -i \frac{\hbar}{\beta} \left(\frac{e^2}{m\Omega_0} \right)^2 n_i \Omega_0 \sum_q [q_z]^2 V(q) S_i(q) \int \frac{d\bar{\omega}}{\pi} \frac{\text{Im} \epsilon^{-1}(q, \bar{\omega} - i0)}{(\omega + i\eta - \bar{\omega}) \bar{\omega}}. \quad (59)$$

We use the relation (11) to express the inverse dielectric function by the polarisation function

$$\text{Im} \epsilon^{-1}(q, \omega) = \Omega_0 V(k) \frac{\text{Im} \Pi(q, \omega - i0)}{|\epsilon(q, \omega)|^2}.$$

Since we are looking for the overall second order contribution of (59), we take the dielectric function in the RPA limit (36). Using

$$\text{Im} \Pi^{(0)}(q, \omega - i0) = \pi \sum_p \{ f_p - f_{p-q} \} \delta(E_p - E_{p-q} - \hbar\omega),$$

we can carry out the $\bar{\omega}$ integration in the correlation function (59) and obtain

$$\langle \dot{J}_k \dot{J}_k \rangle = -i \frac{e^4 \hbar n_i}{d m^2 \beta} \sum_{pq} \frac{q^2 V^2(q) S_i(q)}{|\epsilon_{RPA}(q, E_p - E_{p-q})|^2} \frac{f_{p-q} - f_p}{E_{p-q} - E_p - \hbar\omega - i\eta} \frac{1}{E_{p-q} - E_p}. \quad (60)$$

This expression has the same structure as the Born approximation (54) in the long-wavelength limit except the bare Coulomb interaction is screened by the full RPA-expression of the dielectric function. For the collision term $\Sigma(\omega) = \omega_{pe}^2 G(0, \omega)/\omega$, we find

$$\Sigma_{3D}(\omega) = \frac{e^4 \hbar n_i}{d m n} \sum_{pq} q^2 \frac{V^2(q) S_i(q)}{|\epsilon_{RPA}(q, E_p - E_{p-q})|^2} \frac{f_{p-q} - f_p}{E_{p-q} - E_p - \hbar\omega - i\eta} \frac{1}{E_{p-q} - E_p}. \quad (61)$$

Splitting the collision term into real and imaginary part leads to a Drude-like expression for the dielectric function (53) and a frequency dependent relaxation time (55), where the bare Coulomb potential is replaced by the screened one.

Considering the static limit, it can be seen that the frequently used static screening (37) in the Ziman formula (58) is consistent, as long as the ions are considered to be fixed at their sites. For the screened Born approximation, the real part of the collision term in the static limit $\sigma(0)$ vanishes. In general, the conductivity is complex. It has a contribution due to absorption.

For high frequencies ($\omega > \omega_{pl}$), the RPA dielectric function fulfills the limiting relation (21). This leads to an interaction via an unscreened Coulomb potential. Thus, the behaviour of the high-frequency conductivity and the dielectric function is determined by the Born approximation only. Static screening would overestimate the screening effects for high frequencies.

10. Conclusions

This paper has aimed to give a somehow more extended review of the linear response theory, as it has been presented in recent letters to derive a consistent approach for the dielectric function of charged particle systems (Reinholz *et al.* 1999; Wierling *et al.* 1999; Röpke *et al.* 1999). Applications and numerical calculations have been, and will be, presented elsewhere. Starting from a non-equilibrium statistical operator which contains a set of physical relevant observables, we find an expression for the response function of the system (23) which relates the non-equilibrium properties to equilibrium correlation functions and Green functions under the condition that the external electric field is a weak perturbation. A systematic approach to the (\mathbf{k}, ω) -dependent behaviour at finite temperature within a one-moment approach has been given. The RPA was reproduced. A dynamical local-field factor $G(\mathbf{k}, \omega)$ within the first Born approximation (44) was derived, which has also been known from other approaches (Richardson and Ashcroft 1994). The systematic inclusion of collisions into the dynamical local-field factor has been presented. It has been investigated in particular in the long-wavelength limit. As a main result of this paper, an expression for the dielectric function (53) was derived in this limit, which is

similar to the Drude formula but with a complex frequency dependent collision term.

The Drude formula is an empirical relationship which is found to be valid, over a restricted frequency range $\omega \ll \omega_{\text{pl}}$, for most nearly free-electron systems (e.g. Mahan 1981). It also fulfills the conductivity sum rule. Our quantum-statistical derivation leads to a generalisation which defines clearly the validity range of the empirical expression. In general, the relaxation time does depend on the frequency which needs to be taken into account in particular close to the plasmon pole (Röpke *et al.* 1999). The investigation showed that in order to conserve the conductivity sum rule the complex character of the collision term (54) is essential. The frequency dependent relaxation time only leads to a violation of the sum rule.

Having derived a relaxation time within our approach, we looked at an improvement of the second Born approximation to avoid Coulomb divergencies for small q . This can be done by summing up appropriate digrams which lead to a screened interaction potential. For large values of q , the collision integral in the Born approximation, considered in the classical limit, is also divergent. This divergency is cured if strong binary collisions are considered, e.g. summing up the so-called ladder diagrams in the perturbation expansion. In the quantum case, the divergence for large values of q disappears, but also in that case the ladder sum which is equivalent to the solution of the Schrödinger equation will lead to the correct Coulomb logarithm. The inclusion of a t -matrix approximation within the approach presented can be done consistently and will be given in a later paper. The problem of a dynamically screened t -matrix has not been solved so far. However, a convergent effective collision term in the static non-degenerate limit has been proposed by Gould and DeWitt (1967) and Redmer *et al.* (1990). The effect of electron-electron scattering amplitudes on plasmon damping in metals or the dynamical structure factor has been discussed by Hasegawa and Watabe (1969), MacDonald and Geldart (1981) and Green *et al.* (1985).

With the derivation of the general Drude formula within the dielectric response, we have a consistent theory on the same level of approximation as the conductivity. In the static limit, we find a generalised Ziman formula (58) for the dc conductivity. However, it is known that in the non-degenerate limit a correcting prefactor is necessary in order to take into account the effect of electron-electron collisions (Spitzer 1962; Ichimaru *et al.* 1985). Going beyond the one-moment approach and including higher moments of the single-particle density operator according to (28), we automatically get contributions from the electron-electron interaction. The general finding is, the more moments are included, the better the low order perturbation theory works (Reinholz *et al.* 1989, 1995). The inclusion of two-particle density operators has been discussed by Röpke (1988).

The generalisation of our approach for a many-component system is straight forward. In particular, a two-component system consisting of electrons and positively charged ions ($c = e, i$) takes into account ion dynamics beyond a static structure factor. This has been considered for a non-degenerate plasma (Röpke 1998) and calculations for a four-moment approach have been presented by Röpke and Wierling (1998). Generalisations of the Ziman formula, including screening of electrons and ions for a two-component plasma, has previously been discussed by Boercker *et al.* (1982). Electronic bilayers, which are of recent interest, can

also be mapped onto a single two-dimensional layer with two components (Liu *et al.* 1996; Kalman and Golden 1998).

Partially ionised plasma or excitonic semiconductors could be treated by applying a cluster expansion and considering bound states or excitons as a separate component apart from the charged components. Applications to thermodynamic and thermoelectric properties of hydrogen and alkaline systems can successfully explain experimental findings (Reinholz *et al.* 1995; Redmer 1997 and references therein). The influence of two-particle states on the dielectric function was discussed by Röpke and Der (1979) already. It would be interesting to pursue the proposed cluster expansion further to describe the Mott transition on the level of the dielectric response.

Further investigations of the sum rules for the screened Born approximation are necessary to show the consistency of this approximation. Another possibility is the calculation of the dynamical structure factor (15) which is also available from molecular dynamics simulations, cf. Hansen and McDonald (1981) or Moroni *et al.* (1995).

The general formalism of the linear response theory presented is not restricted to Coulomb interactions. Other interaction potentials could be considered in order to account for electron–neutral interactions (e.g. the polarisation potential). Pseudopotentials should be used to allow comparisons with experimental data for dielectric functions or dynamical structure factors in metals. Other experiments for which the presented formalism is relevant comprise optical properties of laser induced plasma (Wierling *et al.* 1999), refraction and absorption index (1), damping of collective excitation due to collisions, and the broadening and shift of plasmon peaks.

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