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Response function including collisions for an interacting fermion gas

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The response function of an interacting fermion gas is considered in the entire $(\vec{k},\omega)$ space. Applying a generalized linear response theory, it is expressed in terms of determinants of equilibrium correlation functions, which allow for a systematic perturbative treatment. The relation to dynamical local-field factors is given. As a special case, the dielectric function is evaluated for two-component (hydrogen) plasmas at arbitrary degeneracies. Collisions are treated in Born approximation leading to a $(\vec{k},\omega)$-dependent collision integral. The link to the dynamical conductivity is given in the long-wavelength limit. Sum rules are discussed.
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The response of an interacting fermion system to an external force is of interest in different fields of physics. In case of small deviations from equilibrium, linear response theory can be used to describe the reaction to a time and space dependent perturbation. As an application we will consider the response of a two-component plasma to an external field.

The many-particle system is investigated under the influence of the potential $U_{\rm ext}(\vec{r},t)=e^{i(\vec{k}\cdot\vec{r}-\omega t)}U_{\rm ext}(\vec{k},\omega)$ + c.c. The total Hamiltonian $H_{\rm tot}(t)=H+H_{\rm ext}(t)$ contains the system Hamiltonian H and the interaction with the external potential

$$H_{\rm ext}(t)=\sum_{p\sigma} U_{\rm ext}(\vec{k},\omega)e^{-i\omega t}n^{\sigma}_{p,-k}+\text{c.c.}, \tag{1}$$

where $n^{\sigma}_{p,k}=c^{\dagger}_{p-k/2,\sigma}c_{p+k/2,\sigma}$ is the Wigner transform of the single-particle density given in terms of creation and annihilation operators in momentum representation. The index σ indicates spin, but can also be extended to further characteristics such as species (electrons, ions) so that $U_{\rm ext}$ could also depend on σ.

As a consequence of the external perturbation, an induced density will arise. In linear response theory, see, e.g., [1], the response function $\chi(\vec{k},\omega)$ relates the induced density to the potential $U_{\rm ext}(\vec{k},\omega)$. It can be expressed in terms of equilibrium correlation functions. In particular, the fluctuation-dissipation theorem relates the response function to the dynamical structure factor $S(\vec{k},\omega)$ according to $\mathrm{Im}\chi(\vec{k},\omega)=-\pi[1-\exp(-\beta\hbar\omega)]S(\vec{k},\omega)/\hbar$.

Considering the special case of the response of an electron system (mass m, charge $-e$) to an electrical field, the dielectric function $\epsilon(\vec{k},\omega)=[1+\chi(\vec{k},\omega)/(\epsilon_0 k^2)]^{-1}$ is related to the polarization function $\Pi(\vec{k},\omega)$ and the dynamic electrical conductivity $\sigma(\vec{k},\omega)$ according to

$$\epsilon(\vec{k},\omega)=1+\frac{i}{\epsilon_0\omega}\sigma(\vec{k},\omega)=1-\frac{1}{\epsilon_0 k^2}\Pi(\vec{k},\omega). \tag{2}$$

The elaboration of a many-particle theory for these quantities is an essential problem in quantum statistics. Evaluating the polarization function in zeroth order with respect to the interaction [2],

$$\Pi^{(0)}(\vec{k},\omega)=\frac{e^2}{4\pi^3}\int d^3p\frac{f_{p+k/2}-f_{p-k/2}}{E_{p+k/2}-E_{p-k/2}-\hbar\omega-i\eta}, \tag{3}$$

the well-known RPA expression for the dielectric function is obtained. Here, $f_p=[\exp(\beta E_p-\beta\mu)+1]^{-1}$ denotes the Fermi distribution function, $\beta=1/(k_BT)$ the inverse temperature, μ the chemical potential fixed by the density n, and $E_p=\hbar^2p^2/(2m)$. The limit $\eta\to 0$ is to be taken after the thermodynamic limit.

The static limit ($\omega=0$) can be improved by using the concept of local-field factors [3]. This treatment has been extended to finite frequencies by introducing dynamical local-field factors $G(\vec{k},\omega)$ according to

$$\Pi(\vec{k},\omega)=\frac{\Pi^{(0)}(\vec{k},\omega)}{1+G(\vec{k},\omega)\Pi^{(0)}(\vec{k},\omega)/(\epsilon_0 k^2)}. \tag{4}$$

Different approximative methods to determine $G(\vec{k},\omega)$ have been developed such as perturbation expansions, see [4], and the parameterization of the dielectric function via sum rules [5–7]. A study of the dynamical local-field factors within a time-dependent mean-field theory neglecting damping effects was reported in [8].

In this Rapid Communication, we consider a systematic quantum statistical approach to the dynamical local-field factors at finite temperatures performing a perturbation expansion for $\Pi^{-1}(\vec{k},\omega)$. Sum rules for the dielectric function are checked. Our approach gives a direct link to the theory of conductivity in Coulomb systems; see [9]. Evaluating correlation functions, a $(\vec{k},\omega)$-dependent collision term is derived.

A generalized linear response theory has been given recently, see [10], leading to the following expression for the response function [11] or density-density correlation function, respectively,

$$\chi(\vec{k},\omega)=\frac{ik^2\beta\Omega_0}{\omega|M_{mn}(\vec{k},\omega)|}\begin{vmatrix} 0 & M_{0n}(\vec{k},\omega) \\ M_{m0}(\vec{k},\omega) & M_{mn}(\vec{k},\omega)\end{vmatrix}. \tag{5}$$

The elements $M_{mn}(\vec{k},\omega)$ of the determinants are given by equilibrium correlation functions of an appropriately chosen set of relevant operators $\{A_1,A_2,\ldots,A_m,\ldots\}$.

Different choices for the set of relevant observables such as finite sets of moments of the n-particle distribution functions are possible. In the present Rapid Communication we will restrict ourselves to the current operator

$$J_k=-\frac{e\hbar}{m\Omega_0}\sum_{p,\sigma}p_z n^{\sigma}_{p,k} \tag{6}$$

of the electron system only. We consider an isotropic system so that the polarization function is a scalar. The vector $\vec{k}=k\vec{e}_z$ is taken in the z direction.

In this first-moment approach [11], Eq. (5) reads

$$\chi(k,\omega)=-i\frac{k^2}{\omega}\beta\Omega_0\frac{(J_k;J_k)^2}{M_{JJ}(k,\omega)}, \tag{7}$$

where the denominator contains the collision term

$$M_{JJ}(k,\omega)=-i\omega(J_k;J_k)+\langle\dot{J}_k;\dot{J}_k\rangle_{\omega+i\eta} -\langle\dot{J}_k;J_k\rangle_{\omega+i\eta}\frac{1}{\langle J_k;J_k\rangle_{\omega+i\eta}}\langle J_k;\dot{J}_k\rangle_{\omega+i\eta}. \tag{8}$$

The correlation functions are defined as

$$(A;B)=\frac{1}{\beta Z}\int_0^{\beta}d\tau\ \mathrm{Tr}[\ \mathrm{e}^{-\beta H+\beta\mu N}A(-i\hbar\tau)B^{\dagger}],$$
$$\langle A;B\rangle_z=\int_0^{\infty}dt\mathrm{e}^{izt}(A(t);B), \tag{9}$$

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

$$(A;B)=-\frac{1}{\beta}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{1}{\omega}\,\mathrm{Im}G_{AB^{\dagger}}(\omega-i\eta),$$
$$\langle A;B\rangle_z=-\frac{i}{\beta}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{1}{z-\omega}\frac{1}{\omega}\,\mathrm{Im}G_{AB^{\dagger}}(\omega-i\eta). \tag{10}$$

The relation to the thermodynamic Green functions $G_{AB^{\dagger}}(z_\mu)$, z_μ being Matsubara frequencies, permits us to perform systematic perturbation expansions.

The correlation function $(J_k;J_k)$ can be related to the commutator of position and linear momentum (cf. [9]),

$$(J_k;J_k)=e^2n/(m\beta\Omega_0). \tag{11}$$

The evaluation of $M_{JJ}(k,\omega)$ using perturbation theory will be given below.

The dynamical local-field factors $G(k,\omega)$, Eq. (4), are directly related to $M_{JJ}(k,\omega)$, Eq. (8), according to

$$G(k,\omega)=i\frac{\epsilon_0\beta m^2\Omega_0\omega}{e^4n^2}M_{JJ}(k,\omega)-\frac{\epsilon_0k^2}{\Pi^{(0)}(k,\omega)}+1. \tag{12}$$

Note that the equivalence of Eqs. (7) and (8) with

$$\chi(k,\omega)=-i\frac{k^2}{\omega}\beta\Omega_0\langle J_k;J_k\rangle_{\omega+i\eta}, \tag{13}$$

the Kubo formula [12], can be shown using partial integrations [11]. Being formally equivalent, different results are obtained within finite order perturbation theory for the correlation functions. On one hand, the perturbation expansion of the Kubo expression at $\vec{k}=0$, $\omega\to0$ to obtain the dc conductivity is involved because divergences arise. On the other hand, the Chapman-Enskog method or the Grad method yielding the conductivity as a ratio of two determinants [9] are exactly reproduced within the generalized linear response theory, Eq. (5), using a finite number of moments of the single-particle distribution function as relevant observables.

For exploratory calculations, we consider a two-component hydrogen plasma in adiabatic limit, where the interacting electrons are moving under the influence of the potential of pointlike ions with charge e, fixed at positions $\vec{R}_j$. The Hamiltonian $H=T+V$ contains the kinetic energy $T=\Sigma_{p,\sigma}E_pc^{\dagger}_{p\sigma}c_{p\sigma}$ and the interaction

$$V=-\sum_{j,qp,\sigma}V(q)\mathrm{e}^{-i\vec{q}\cdot\vec{R}_j}c^{\dagger}_{p+q\sigma}c_{p\sigma} +\frac{1}{2}\sum_{qpp',\sigma\sigma'}V(q)c^{\dagger}_{p+q\sigma}c^{\dagger}_{p'-q\sigma'}c_{p'\sigma'}c_{p\sigma}. \tag{14}$$

$V(q)=e^2/(\epsilon_0\Omega_0q^2)$ denotes the Coulomb potential. The extension to an impurity model accounting for the ion dynamics via a dynamical structure factor is straightforward. In order to generalize for more complex ions, the Coulomb interaction has to be replaced by pseudopotentials.

Within the perturbation expansion of $M_{JJ}(k,\omega)=M^{(0)}_{JJ}+M^{(1)}_{JJ}+M^{(2)}_{JJ}+\cdots$, higher powers of V arise due to the explicit interaction in $\dot{J}_k=\dot{J}^{(T)}_k+\dot{J}^{(V)}_k$, where $\dot{J}^{(T)}_k=i[T,J_k]/\hbar$, and $\dot{J}^{(V)}_k=i[V,J_k]/\hbar$. Higher-order contributions are also due to the perturbative expansion of the correlation functions, e.g., by using a Feynman diagram analysis of the Green functions according to Eq. (10).

Whereas in Eq. (12) the zeroth-order contribution $M^{(0)}_{JJ}(k,\omega)$ is compensated by the term $\epsilon_0k^2/\Pi^{(0)}(k,\omega)$, the first-order contributions contain terms from reducible diagrams compensating the 1. The remaining first-order contributions of $M^{(1)}_{JJ}(k,\omega)$ are due to the explicit V in $\dot{J}^{(V)}_k$ and to terms from $\dot{J}^{(T)}_k$, expanding the correlation functions up to first order (self-energy and vertex corrections). The evaluation of the corresponding Feynman diagrams gives for arbitrary temperatures the result

$$G^{(1)}(k,\omega)=\frac{m^2e^4}{64\pi^6\hbar^4[\Pi^{(0)}(k,\omega)]^2} \times\int d^3p\int d^3p'\ \frac{f_{p+k/2}-f_{p-k/2}}{(\vec{p}-\vec{p}')^2}(f_{p'+k/2} -f_{p'-k/2})\left(\frac{1}{p_z-m\omega/(\hbar k)-i\eta} -\frac{1}{p'_z-m\omega/(\hbar k)-i\eta}\right)^2. \tag{15}$$

At zero temperature, an analytical expression for $G^{(1)}(k,\omega)$ can be found, see [4], and [13] for the static limit $G^{(1)}(k,0)$. The limiting cases are in accordance with the compressibility sum rule, $\lim_{k\to 0} G^{(1)}(k,0) = k^2/(4k_F^2)$, and the relation to the pair distribution at zero distance, $\lim_{k\to\infty} G^{(1)}(k,0) = 1/3$, which are correct within the order of perturbation theory considered here, i.e., comparing with properties of the uncorrelated fermion gas [14]. In higher orders of perturbation theory, the static limit has been investigated by different authors [3]. We will not go in this direction since we are interested in the long-wavelength limit at arbitrary frequencies to give the link to the theory of electrical conductivity in Coulomb systems.

In the long-wavelength limit follows $\lim_{k\to 0} G^{(1)}(k,\omega) \propto k^2$. Thus, no contribution from these exchange terms of first order in V will modify the behavior at $k\to 0$. To include collisions in Born approximation, we have to take into account the second-order term $M_{JJ}^{(2)}(k,\omega)$. The contribution due to the explicit dependence on V^2 from $\dot{J}_k^{(V)}$, caused by the electron-ion scattering, is evaluated as

$$
\begin{aligned}
&G^{(2,V)}(k,\omega) \\
&= \frac{\epsilon_0 m^2 \omega \Omega_0^2}{32\pi^6 e^2 n \hbar^3} \int d^3p \int d^3q V^2(q) S_i(q) \\
&\times \frac{1}{p_z k + \vec{p}\cdot\vec{q}} \frac{f_{p-k/2-q/2} - f_{p+k/2+q/2}}{p_z k + \vec{p}\cdot\vec{q} - m\omega/\hbar - i\eta} \\
&\times \left[q_z^2 + \frac{2e^2 n k}{\hbar\omega \Pi^{(0)}(k,\omega)} \left(\frac{(p_z + q_z/2) q_z}{p_z + q_z/2 - \frac{m\omega}{\hbar k} - i\eta} \right.\right. \\
&\left.\left. - \frac{(p_z - q_z/2) q_z}{p_z - q_z/2 - \frac{m\omega}{\hbar k} - i\eta} \right) \right]. \qquad (16)
\end{aligned}
$$

$S_i(q) = \langle \Sigma_{ij} \exp[i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)]/(n\Omega_0) \rangle$ is the structure factor of the ion system. In the long-wavelength limit to be considered below, terms arising from the electron-electron interaction do not contribute because of momentum conservation. Furthermore, the terms related to $\dot{J}_k^{(T)} = ie\hbar^2 k/(m^2\Omega_0) \Sigma_{p\sigma} p_z^2 n_{p,k}^{\sigma}$ contain a factor k and do not give any contribution.

In the limit $k\to 0$, we find from Eq. (16)

$$
\begin{aligned}
G^{(2)}(0,\omega) &= \frac{\epsilon_0 m^2 \omega \Omega_0^2}{32\pi^6 e^2 n \hbar^3} \int d^3p \int d^3q q_z^2 V^2(q) S_i(q) \\
&\times \frac{1}{\vec{p}\cdot\vec{q}} \frac{f_{p-q/2} - f_{p+q/2}}{\vec{p}\cdot\vec{q} - m\omega/\hbar - i\eta}. \qquad (17)
\end{aligned}
$$

Using the local-field factors $G(k,\omega)$, Eq. (4), the dielectric function (2) can be rewritten as

$$
\epsilon(0,\omega) = 1 - \frac{\omega_{\rm pl}^2}{\omega[\omega + \omega_{\rm pl}^2 \,{\rm Re}\, G(0,\omega)/\omega] + i\omega/\tau(\omega)}, \qquad (18)
$$

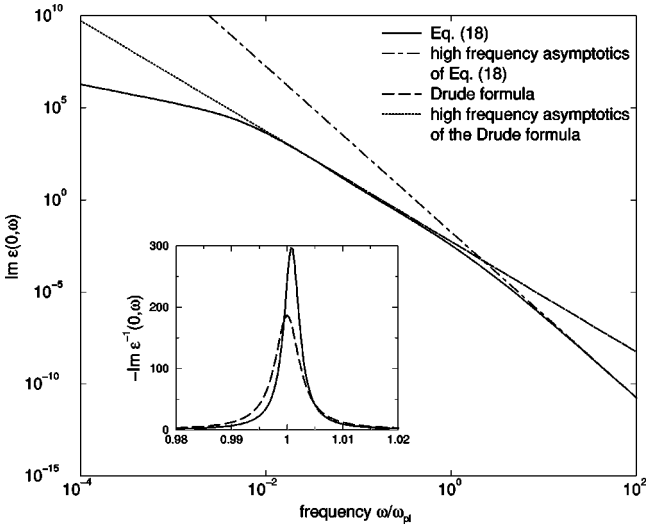

FIG. 1. Imaginary part of the dielectric function in the long-wavelength limit Eq. (18) as a function of ω, compared with the Drude formula. An electron gas at $r_s = 3.5$, $T = 300$ K is considered. The inset displays the imaginary part of the inverse dielectric function near the plasma frequency.

which is a Drude-like expression with the plasma frequency $\omega_{\rm pl}^2 = e^2 n/(\epsilon_0 m)$ and a frequency-dependent relaxation time $\tau^{-1}(\omega) = \omega_{\rm pl}^2 \,{\rm Im}\, G(0,\omega)/\omega$ [15]. According to the discussion above, the first-order term $G^{(1)}(k,\omega)$ does not contribute to the long-wavelength limit. The second-order term, Eq. (17), gives a result for the dielectric function shown in Fig. 1. The Drude formula is obtained replacing $G^{(2)}(0,\omega)/\omega$ by $\lim_{\omega\to 0} G^{(2)}(0,\omega)/\omega$. The high-frequency asymptotics of the Drude formula, ${\rm Im}\epsilon(0,\omega) \propto \tau(0)\omega_{\rm pl}^2/\omega^3$, is also shown in Fig. 1 (dotted line). The account of the frequency dependence of $G^{(2)}(0,\omega)$ leads to deviations from the Drude expressions for frequencies higher than the plasma frequency. Using a saddle-point expansion, the asymptotic behavior $\propto \omega^{-4.5}$ was found (dash-dotted line). The inset shows the behavior of $-{\rm Im}\epsilon^{-1}(0,\omega)$ near 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 $G(0,\omega)$ the peak position is shifted.

For $\omega\to 0$ we get the well-known Born approximation for the dc conductivity $\sigma_{\rm dc} = \epsilon_0 \omega_{\rm pl}^2 \tau(0)$ of a degenerate weakly interacting electron system, cf. [16],

$$
\sigma_{\rm dc} = \frac{12\pi^3 e^2 \hbar^3 n}{m^2 \Omega_0^2} \left[\int_0^\infty dq q^3 V^2(q) S_i(q) f_{q/2} \right]^{-1}. \qquad (19)
$$

The Ziman formula is obtained by introducing a screened potential, which can be done in a systematic way by sum ming up the corresponding ring diagrams [9].

Several exact properties of the dielectric function are known [17], such as sum rules and the high-frequency behavior. In particular, we have

$$
\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^n \,{\rm Im}\,\epsilon^{\pm 1}(k,\omega) = S_n^{(\pm)}(k). \qquad (20)
$$

A numerical check of the *f*-sum rule and the conductivity sum rule, $-S_1^{(-)}(k)=S_1^{(+)}(k)=\omega_{\rm pl}^2$, has been carried out for a two-component plasma with parameters $r_s=3.5$ and $T=300$ K, cf. [5]. It has been found numerically that the dielectric function in the long-wavelength limit (18) obeys both sum rules within an accuracy of 0.1%. The consistent consideration of both the real and the imaginary part of the frequency-dependent collision term $G(0,\omega)$ is crucial for the sum rules. Taking into account a frequency dependence in the relaxation time only, i.e., neglecting $\mathrm{Re}\,G(0,\omega)$ in Eq. (18), leads to a considerable violation of the sum rules of the order of 10%. Until now, a check of the sum rules at finite values of the wave vector has only been performed for a classical, Maxwellian two-component plasma [11] for arbitrary wave vectors *k*.

Of special interest is the third-moment sum rule $S_3^{(-)}(k)$, which 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 [18], i.e., a frequency-dependent collision term is needed. Evaluating the collision term (17) in the high-frequency limit using the saddle-point method, $\mathrm{Im}\epsilon^{-1}(0,\omega)$ behaves as $\omega^{-9/2}$, implying that the third-moment integral converges, whereas higher moments are nonconverging. Note that there are different forms of the asymptotic behavior that are quoted in the literature depending on the approximations made, such as ω^{-5} in [7]. For the degenerate electron gas, due to the electron-electron collisions a high-frequency behavior of the imaginary part of the dielectric function $\propto k^2\omega^{-11/2}$ has been derived for *k* small compared with the Fermi wave number [18].

In conclusion, a systematic approach to the (k,ω)-dependent local-field factors at finite temperatures has been given. Furthermore, we derived a (k,ω)-dependent collision term, and showed that the sum rules are obeyed in the long-wavelength limit. Arbitrary degeneracy is considered, and the direct connection with the theory of dc conductivity is shown.

The single moment Born approximation, Eqs. (7), (15), and (16), can be improved systematically in two directions: (i) Higher order perturbation theory can be applied to determine the correlation functions. As well known for the limiting cases, the dc conductivity should be evaluated by considering a screened interaction or by treating strong collisions introducing a ladder *T* matrix [9]. Also, the local-field factors are improved introducing the pair distribution function. (ii) Taking into account further moments of the single-particle distribution function, see [9,16], the results obtained by perturbation expansion of Eq. (5) are consistent with the Chapman-Enskog or the Grad approach to the dc conductivity.

After improving the Born approximation, a comparison with experimental data for the dielectric function in hydrogenlike plasmas or, in a more specific treatment of the electron system, in condensed matter would be of interest. A possible way to check the present dielectric function is to calculate the dynamical structure factor that is available from molecular dynamics simulations; cf. [19].

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