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Dielectric Properties of Correlated Quantum Plasmas

M. Bonitz[a)], V. Golubnichiy[a)], N.H. Kwong[b)], D. Semkat[a)], D. Kremp[a)], V.S. Filinov[c)], M. Schlanges[d)]

[a)]Fachbereich Physik,Universität Rostock, Universitätspl. 3, D-18051 Rostock
[b)]Optical Sciences Center, University of Arizona, Tucson, AZ 85721, USA
[c)]High Energy Density Research Center Rus.Ac.Sc., Izhorskaya street 13-19, Moscow 127412, Russia
[d)]Institut für Physik der Universität Greifswald, Domstrasse 10a, D-17489 Greifswald
e-mail: michael.bonitz@physik.uni-rostock.de

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Abstract

Results for the dynamic structure factor of a one-component plasma are presented for the situations of strong coupling and weak degeneracy and strong degeneracy and weak coupling. Possibilities to obtain rigorous results when both, coupling and degeneracy are large are discussed.

In dense astrophysical and laboratory plasmas one frequently encounters situations where Coulomb and quantum effects are important simultaneously [1], i.e. where the Coulomb coupling parameter $\Gamma = (4\pi n_e/3)^{1/3} e^2/4\pi\epsilon_0 k_B T$ and the degeneracy parameter $\chi = n_e\lambda_e^3$ [λ_e is the electron thermal wave length $\lambda_e^2 = 2\pi\hbar^2\beta/m_e$] exceed unity. While a rigorous theoretical treatment of the equilibrium properties is now becoming possible, in particular by path integral quantum Monte Carlo (PIMC) techniques [2], comparable results for the *dynamic properties* are still missing. In this paper, we discuss two possible approaches to solve this problem. We focus on the dynamic dielectric function $\epsilon(\omega, q)$ and the dynamic structure factor $S(\omega, q) \sim -\mathrm{Im}\, 1/\epsilon(\omega, q)$ from which all optical and transport properties can be computed.

The central quantity which describes dynamical properties of an N-particle system is the *density fluctuation* $\rho_{\mathbf{q}}$, where $\mathbf{q}$ is the wave vector. In a classical system, it can be computed from Klimontovich's phase space density $\hat\rho_{\mathbf{p},\mathbf{r}}(t) = \sum_{i=1}^N \delta[\mathbf{r} - \hat{\mathbf{r}}_i(t)]\, \delta[\mathbf{p} - \hat{\mathbf{p}}_i(t)]$, where $\hat{\mathbf{r}}_i(t)$ and $\hat{\mathbf{p}}_i(t)$ are classical (random) particle trajectories. Fourier transformation with respect to $\mathbf{r}$ yields the momentum-dependent density fluctuation $\rho_{\mathbf{p},\mathbf{q}}$, and the total fluctuation $\rho_{\mathbf{q}}$ is obtained by a subsequent integration over all momenta,

$$\hat\rho_{\mathbf{p},\mathbf{q}}(t) = \sum_{i=1}^N e^{i\mathbf{q}\hat{\mathbf{r}}_i(t)}\, \delta[\mathbf{p} - \hat{\mathbf{p}}_i(t)], \qquad \hat\rho_{\mathbf{q}}(t) = \sum_{i=1}^N e^{i\mathbf{q}\hat{\mathbf{r}}_i(t)}. \tag{1}$$

The corresponding quantum result is derived from the N-particle wave function $\hat\Psi_N(\mathbf{r}, t) = \sum_s \hat a_s(t)\phi_N^{(s)}(\mathbf{r}, t)$, where $\phi_N^{(s)}$ is a complete set of basis functions, and the coefficients are creation/annihiliation operators obeing (anti-)commutation rules $[\hat a_s^\dagger(t), \hat a_{s'}(t)]_\mp = \delta_{s,s'}$ for bosons (fermions). The quantum generalization of Eq. (1) is then given by ($\hbar = 1$)

$$\hat\rho_{\mathbf{p},\mathbf{q}}(t) = \hat a_{\mathbf{p}}^\dagger(t_2)\, \hat a_{\mathbf{p}+\mathbf{q}}(t_1)\big|_{t_1=t_2=t}, \qquad \hat\rho_{\mathbf{q}}(t) = \sum_{\mathbf{p}} \hat a_{\mathbf{p}}^\dagger(t)\, \hat a_{\mathbf{p}+\mathbf{q}}(t), \tag{2}$$

where the fluctuation $\hat{\rho}_{\mathbf{p},\mathbf{q}}$ describes the annihilation of an electron in momentum state $\mathbf{p}+\mathbf{q}$ at time t_1 and creation in momentum state $\mathbf{p}$ at time t_2. Obviously, the limiting case $q = 0$ of Eqs. (1) and (2) yields the momentum distribution and the density.

The fluctuations $\hat{\rho}_{\mathbf{p},\mathbf{q}}$ and $\hat{\rho}_{\mathbf{q}}$ are random quantities depending on the initial conditions of the equations of motion. To come to measurable quantities, a suitable *average* over the particle ensemble (e.g. over the initial conditions) has to be performed yielding $\rho_{\mathbf{p},\mathbf{q}}(t) \equiv \langle \hat{\rho}_{\mathbf{p},\mathbf{q}}(t) \rangle$ and $\rho_{\mathbf{q}}(t) \equiv \langle \hat{\rho}_{\mathbf{q}}(t) \rangle$. These are already macroscopic observables which are closely related to the dynamic structure factor. There exist two ways to compute $S(\omega, q)$ for a N-particle system in *equilibrium*.

The **first** is to analyze the **equilibrium fluctuations in a field-free system**. In this case, $\rho_{\mathbf{q}}(t) \approx 0$ due to spatial homogeneity. The first non-vanishing average is the density-density correlation function $C_{\rho\rho}$ which is closely related to pair correlations and the Fourier transform of which yields the dynamic structure factor,

$$C_{\rho\rho}(\mathbf{q},\tau) \equiv \langle \hat{\rho}_{\mathbf{q}}(\tau) \hat{\rho}_{-\mathbf{q}}(0) \rangle, \qquad S(\omega,\mathbf{q}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\tau \, e^{i\omega\tau} \, C_{\rho\rho}(\mathbf{q},\tau). \tag{3}$$

$C_{\rho\rho}$ can be computed from equilibrium theories, such as the Bethe Salpeter equation, or nonequilibrium approaches, in particular molecular dynamics simulations (MD). The latter has the advantage that, for a classical system, *correlations of arbitrary strength* are straightforwardly included, e.g. in the frame of Newton's equations. After averaging the resulting trajectories $\hat{\mathbf{r}}_i(t)$ and $\hat{\mathbf{p}}_i(t)$ [over runs with different initial conditions or over time], the dynamic structure factor follows directly from Eqs. (1) and (3).

We have applied this approach to a degenerate electron gas by using an effective quantum pair potential in the classical MD scheme. An appropriate potential was obtained by Kelbg [4] and is rigorous for $\Gamma < 1$ and $\chi < 1$. We have performed extensive simulations in which the influence of quantum effects on the dynamic structure factor and the plasmon spectrum has been investigated [5]. It is found that quantum effects influence the plasmon spectrum predominantly at large wave numbers, but their influence is rather small. Fig. 1.a shows an example of the simulation results and a comparison to mean-field theories.

The **second approach** to dynamic properties is to investigate the **temporal response of the plasma to a weak inhomogeneous field** $U(t)$ with wave number q_o. The field gives rise to collective oscillations of the electrons and thus to a non-vanishing fluctuation $\rho_{\mathbf{q}_o}(t)$ the Fourier transform of which directly yields the dynamic structure factor [3]

$$S(\omega,\mathbf{q}_o) \sim -\frac{1}{n} \frac{\rho_{\mathbf{q}_o}(\omega)}{U_{\mathbf{q}_o}(\omega)}. \tag{4}$$

This expression is much simpler than (3) and well suited for classical MD simulations. On the other hand, using the quantum expressions (2), a kinetic theory of the dynamic properties of *strongly degenerate systems* can be developed. Starting from the Heisenberg equation of motion $i\frac{\partial}{\partial t}\hat{\rho}_{\mathbf{p},\mathbf{q}} - [\hat{\rho}_{\mathbf{p},\mathbf{q}}, \hat{H}^{\rm sys} + \hat{H}^{\rm ext}] = 0$, with the system and external hamiltonians $\hat{H}^{\rm sys} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{q}\neq 0} V(q) \hat{a}^{\dagger}_{\mathbf{k}_1+\mathbf{q}} \hat{a}^{\dagger}_{\mathbf{k}_2-\mathbf{q}} \hat{a}_{\mathbf{k}_2} \hat{a}_{\mathbf{k}_1}$, $\hat{H}^{\rm ext}(t) = \sum_{\mathbf{q}} U(\mathbf{q},t) \sum_{\mathbf{k}} \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}_{\mathbf{k}-\mathbf{q}}$, one can derive an equation of motion for the averaged fluctuation of $\rho_{\mathbf{p},\mathbf{q}}$. However, the most general theory is obtained if one considers the *two-time fluctuations*, cf. Eq. (2), [there are 2 independent functions

due the non-commutivity of the operators $a, a^\dagger$] $G^<_{\mathbf{p}_1,\mathbf{p}_2}(t_1t_2) \equiv i\langle \hat{a}^\dagger_{\mathbf{p}_2}(t_2)\hat{a}_{\mathbf{p}_1}(t_1)\rangle$ and $G^>_{\mathbf{p}_1,\mathbf{p}_2}(t_1t_2) \equiv -i\langle \hat{a}_{\mathbf{p}_1}(t_1)\hat{a}^\dagger_{\mathbf{p}_2}(t_2)\rangle$. The equations of motion for $G^\gtrless$ are the inhomogeneous Kadanoff-Baym equations (KBE) and read

$$\left(i\frac{\partial}{\partial t_1} - \epsilon_{\mathbf{k}_1}\right) G^\gtrless_{\mathbf{k}_1,\mathbf{k}_2}(t_1t_2) = \sum_{\mathbf{q}} U(-\mathbf{q},t_1) G^\gtrless_{\mathbf{k}_1-\mathbf{q},\mathbf{k}_2}(t_1t_2) + \sum_{\bar{\mathbf{k}}} \Sigma^{HF}_{\mathbf{k}_1,\bar{\mathbf{k}}}(t_1t_1) G^\gtrless_{\bar{\mathbf{k}},\mathbf{k}_2}(t_1t_2) + I^\gtrless_{\mathbf{k}_1,\mathbf{k}_2}(t_1t_2), \quad (5)$$

and are to be supplemented with the adjoint equation. The Coulomb potential V gives rise to mean-field and short-range correlation effects which are contained in the Hartree–Fock selfenergy Σ^{HF} and the collision integrals I, respectively.

Eqs. (5) are very general and include the response from a nonequilibrium state as well as the nonlinear response in case of a strong external field. But here our interest is in the linear response to a weak field resulting in Eq. (4). This limit is obtained by considering Eqs. (5) for a monochromatic excitation $U(\mathbf{q},t) = U_0(t)\delta_{\mathbf{q},\mathbf{q}_o}$ of small amplitude U_0 which allows for a linearization. The result are coupled equations for the spatially homogeneous and monochromatic components $G^\gtrless_{00} \sim G^\gtrless_{\mathbf{k},\mathbf{k}}(t_1t_2)$ and $G^\gtrless_{10} \sim G^\gtrless_{\mathbf{k}+\mathbf{q}_o,\mathbf{k}}(t_1t_2)$, respectively, where $|G^\gtrless_{00}| \sim U^0_0 \gg |G^\gtrless_{10}| \sim U^1_0$, for details, cf. Ref. [3]. After solving this system, the total fluctuation follows according to $\rho_{\mathbf{q}_o}(t) = -i\sum_p G^<_{\mathbf{p}+\mathbf{q}_o,\mathbf{p}}(t,t)$, the Fourier transform of which yields the structure factor (4). This is illustrated in Fig. 2, middle and lower figures.

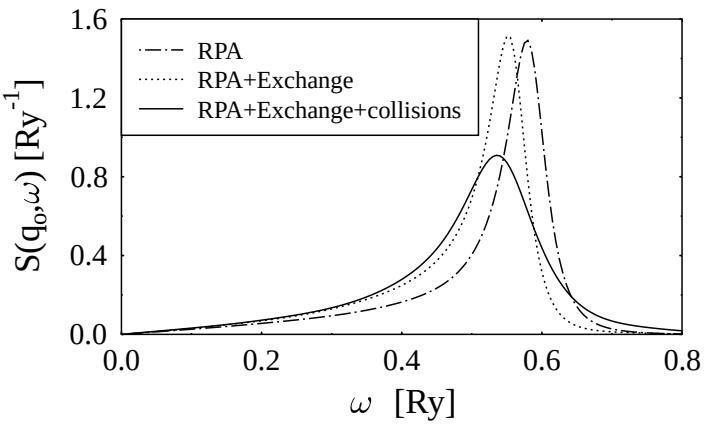

Fig. 1: Dynamic structure factor for an electron gas. **a:** Using Eq.(3) with molecular dynamics simulations with the Coulomb and Kelbg potential compared to the RPA and Vlasov theories for weak degeneracy, $n\lambda^3 = 0.5$, $\Gamma = 1$, $q\bar{r} = 0.6$. **b:** Quantum kinetic theory results for S, Eq.(4), comparing RPA, RPA plus exchange and RPA with exchange and collisions in Born approximation for strong degeneracy, $r_s = 4, T = 0.16E_R$, $q = 0.6k_F$. $\bar{r}, r_s, E_R$ and k_F denote the mean interparticld distance, Brueckner parameter, Hydrogen binding energy and Fermi momentum, respectively.

Equations (5) contain all important limiting cases of a quantum electron plasma: i) neglect of Σ^{HF} and I yields just the spectrum of single-particle excitations; ii) inclusion of Σ^H (Hartree mean field) is equivalent to the RPA (or - in the classical limit - the Vlasov response); iii) inclusion of $\Sigma^{HF} = \Sigma^H + \Sigma^F$ yields the RPA corrected by exchange (time-dependent Hartree-Fock) and, finally, iv) addition of $I^\gtrless$ yields RPA with exchange and correlations. Numerical results comparing cases ii)–iv) are shown in Fig.1.b.

Most remarkably, consistency problems (e.g. sum rule preservation) often encountered in theories incorporating collisions in the dielectric response functions, are completely avoided due to the conservation properties of the Kadanoff-Baym equations.

In fact, choice of density conserving collision integrals is sufficient to preserve the f-sum rule. Moreover, the KBE easily allow to fully conserve the total energy, i.e. all functions $G^{\gtrless}_{00}, G^{\gtrless}_{10}$ are *full* renormalized Greens functions and are thus appropriate to describe the response from a correlated equilibrium or nonequilibrium state of the plasma. Interestingly, the solution of the KBE in the time domain allows to account for very complex correlation effects by using very simple (compared e.g. to the Bethe Salpeter theory) selfenergies in the collision integrals, and it automatically yields all necessary vertex corrections. The numerical result in Fig.1.b used the static Born approximation, thereby fulfulling the f-sum rule to better than 0.1%.

To extend these calculations to plasmas with *strong correlations and strong degeneracy*, one has two possibilities: 1. Generalize MD simulations to nonequilibrium quantum systems, e.g. [6]. 2. Include strong correlation effects into the collision integrals of the quantum kinetic equations. Alternatively, one can use, instead of the selfenergies, pair correlation functions from independent calculations [7], such as path integral Monte Carlo [2]. This should allow to obtain first-principle dynamic response functions in the near future.

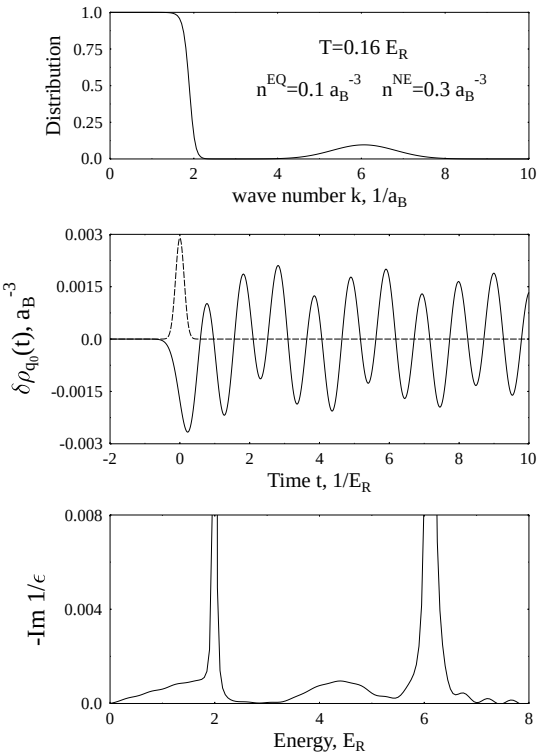

Fig. 2: Quantum kinetic results including RPA and exchange for a strongly degenerate electron gas in an optically excited n-doped semiconductor. **upper fig.**: momentum distribution, with equilibrium (density n^{EQ}, temperature T) and nonequilibrium electrons (n^{NE}). **Middle fig.**: time-dependent total density fluctuation (full line) excited by a monochromatic external field (dashed line). **Lower fig**: structure factor with an optical (high frequency) and a weakly damped acoustic plasmon which emerges out of the pair continuum.

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