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Correlations and spectral function in strongly coupled Coulomb systems

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Abstract

The formation of bound states and their modifications within a dense medium is an important aspect of strongly coupled Coulomb systems. In particular, within the concept of a partially ionized plasma, the plasma is considered as a mixture of electrons and ions in free and bound states. The account of the interaction with the medium by self-energy shifts for the free and bound states becomes less founded at high densities. Within the framework of a systematic Green's function approach, the spectral function is investigated. It is demonstrated how a band is formed if additional contributions which describe hopping between bound states are taken into account. In this way, the connection to condensed matter approaches can be made directly which has not been shown before.

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1. Strongly coupled Coulomb systems

Coulomb systems where the properties are governed by the Coulomb interaction between the charged components occur under different circumstances. In particular we will consider ionic plasmas, but similar effects can be found also in electron–hole plasmas formed in excited semiconductors. The equilibrium state of a system of charged particles is characterized by the temperature T and the particle density n (in the case of a charge-neutral electron–ion plasma $n_e = n_i = n$) or correspondingly, by the coupling parameter $\Gamma = e^2/(4\pi\epsilon_0 k_B T)(4\pi n/3)^{1/3}$ and the degeneration parameter $\Theta = 2m_e k_B T/\hbar^2(3\pi^2 n)^{-2/3}$. At low densities, the model of a partially ionized plasma (PIP) is an appropriate concept to explain the physical properties of the charged particle system. The system is considered to consist of distinguishable components of (quasi-)particles such as free electrons, ions and atoms. Important correlations are the

formation of bound states and, at low temperatures, the possible formation of a quantum condensate, see [1].

At high densities, a disordered Anderson–Hubbard model (DAH model) [2, 3] is appropriate. The properties are determined by the motion of electrons in a potential formed by the disordered system of ions, similar to amorphous solids or liquids, which can be described by a dynamical structure factor. Electron correlations can be included within the Hubbard model which accounts for the single-site electron–electron Coulomb repulsion.

At intermediate densities, the transition from dielectric to metallic behaviour may occur. Different mechanisms have been suggested to explain this metal–insulator transition (MIT) in strongly coupled Coulomb systems, such as the Mott transition due to the screening by free charge carriers in the PIP model, or the closure of the correlation gap in the Hubbard model. The aim of the present work is to discuss a unified description of dense plasmas including the PIP model as well as the DAH model.

2. Greens function and spectral function

We consider a charged particle system with components c (mass m_c , charge e_c) described by the Hamiltonian

$$H = \sum_{\mathbf{p},c} E_c(\mathbf{p}) a_{\mathbf{p},c}^\dagger a_{\mathbf{p},c} + \frac{1}{2} \sum_{\mathbf{p}\mathbf{p}'\mathbf{q},cc'} V_{cc'}(\mathbf{q}) a_{\mathbf{p}-\mathbf{q},c}^\dagger a_{\mathbf{p}'+\mathbf{q},c}^\dagger a_{\mathbf{p}',c} a_{\mathbf{p},c} \quad (1)$$

with $E_c(\mathbf{p}) = \hbar^2 p^2 / (2m_c)$ being the kinetic energy, \mathbf{p} the wave number and $V_{cc'}(\mathbf{q}) = e_c e_{c'} / (\epsilon_0 \Omega_0 q^2)$ the Coulomb interaction. Ω_0 denotes the normalization volume. We will restrict ourselves to a two-component system consisting of fermionic ions (protons) and electrons so that $c = e, i$. If not explicitly denoted, the spin variable will be included in the index c . The creation or annihilation operators for particles in the momentum–spin state $\{\mathbf{p}, c\}$ are denoted by $a_{\mathbf{p},c}^\dagger$ and $a_{\mathbf{p},c}$, respectively.

Physical properties can be expressed in terms of correlation functions [4, 5]. We will focus on the equilibrium single-particle correlation function $\langle a_{k',c'}^\dagger(t') a_{k,c}(t) \rangle$ because all thermodynamic properties can be derived from it. Here, $|k, c\rangle$ denotes an arbitrary, complete orthonormal basis of single-particle states of species c . Usually the momentum representation $k \rightarrow \mathbf{p}$ is chosen. The time dependence in the correlation function is due to the Heisenberg picture. The quantum statistical average is taken using the grand canonical statistical operator $\exp\{-\beta(H - \sum_c \mu_c N_c)\} / Z$ with the inverse temperature $\beta = 1/(k_B T)$, the chemical potential μ_c of species c and $N_c = \sum_k a_{k,c}^\dagger a_{k,c}$ being the particle number operator of species c . The single-particle correlation function is related to the spectral function $A_c(k, k', \omega)$ according to

$$\langle a_{k',c'}^\dagger(t') a_{k,c}(t) \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} f_c(\omega) A_c(k, k', \omega) \quad (2)$$

where $f_c(\hbar\omega) = [\exp \beta(\hbar\omega - \mu_c) + 1]^{-1}$ is the Fermi distribution function. The diagonal element of the spectral function obeys a sum rule $\int (d\omega/2\pi) A_c(k, k, \omega) = 1$. The particle number density follows from the particle number operator as $n_c(\beta, \mu_c) = (1/\Omega_0) \sum_k \langle a_{k,c}^\dagger a_{k,c} \rangle$. Thermodynamic potentials such as the pressure or the free energy can be obtained via further integration, see [1]. Introducing the density of states

$$D_c(\omega) = \frac{1}{\Omega_0} \sum_k A_c(k, k, \omega) \quad (3)$$

the particle number density can also be written as $n_c(\beta, \mu_c) = \int \frac{d\omega}{2\pi} f_c(\omega) D_c(\omega)$.

As is well known [4, 5], the spectral function $A_c(k, k', \omega)$ can be related to the thermodynamic Green function according to

$$A_c(k, k', \omega) = \text{Im}[G_c(k, k', \omega + i0) - G_c(k, k', \omega - i0)] \quad (4)$$

where the analytical continuation of the thermodynamic Green function from the discrete Matsubara frequencies $z_1 = i\pi\nu/\beta + \mu_c$, $\nu = \pm 1, \pm 3, \dots$, into the complex z plane has to be performed, see [4, 5].

For the calculation of the Green function $G_c(\mathbf{p}, z_1)$ (being diagonal in the momentum representation for homogeneous systems), perturbation theory can be applied. Considering the zeroth order, the propagation of free particles is described. All interaction effects can be taken into account by a self-energy $\Sigma_c(\mathbf{p}, z_1)$ introduced by a Dyson equation

$$G_c(\mathbf{p}, z_1) = \frac{1}{z_1 - [E_c(\mathbf{p})] - \Sigma_c(\mathbf{p}, z_1)}. \quad (5)$$

Then, the spectral function (4) is directly related to the self-energy according to

$$A_c(\mathbf{p}, \omega) = \frac{\text{Im} \Sigma_c(\mathbf{p}, \omega)}{[\omega - E_c(\mathbf{p}) - \text{Re} \Sigma_c(\mathbf{p}, \omega)]^2 + [\text{Im} \Sigma_c(\mathbf{p}, \omega)]^2}. \quad (6)$$

Within a perturbation expansion, the self-energy has to be treated via consistent approximations, which can be expressed by Feynman diagrams. In first order with respect to the interaction, a quasi-particle concept can be introduced considering the Hartree–Fock approximation. Possible divergences due to the long-range character of the Coulomb potential are avoided if the interaction is screened, using appropriate summations of diagrams. In the present work, we are especially interested in the formation of bound states. These are obtained from the two-particle T-matrix approximation to the self-energy as given in the next section. This way we get a systematic expansion in the low-density limit. Within a virial expansion the next order in density is determined by a three-particle T-matrix and will be considered here. As a new result we obtain the formation of energy bands applying this technique. These approximations are limited to weakly coupled plasmas, $\Gamma < 1$. As shown in [1] the region of applicability can be extended to higher densities, where screening and degeneracy effects are of importance. These effects are relevant for highly ionized plasmas, but will not be discussed here.

3. Bound state contribution to the density of states

We will consider an approximation which describes the formation of bound states as well as interaction and hopping processes between bound states at different positions [6]. The self-energy is taken from the two- or three-particle ladder T-matrix summing up the interaction between an electron and one or two ions, respectively, to any order (the single-particle states are denoted as $1 = \{\mathbf{p}_1\sigma_1c_1\}$):

$$\begin{aligned} \Sigma_e^{L,2}(1, z_1) + \Sigma_e^{L,3}(1, z_1) &= \sum_{2, z_2} \frac{1}{z_2 - E_2} T_2^L(12, 12, z_1 + z_2) \\ &+ \sum_{23, z_2 z_3} \frac{1}{z_2 - E_2} \frac{1}{z_3 - E_3} [T_3^L(123, 123, z_1 + z_2 + z_3) - T_2^L(12, 12, z_1 + z_2)] \end{aligned}$$

$$\begin{aligned}
&= \sum_2 f_2(E_2) \sum_{n_2} \frac{(E_1 + E_2 - E_{n_2})^2}{z_1 + E_2 - E_{n_2}} |\psi_{n_2}(12)|^2 \\
&+ \sum_{23} f_2(E_2) f_3(E_3) \left[\sum_{n_3} \frac{(E_1 + E_2 + E_3 - E_{n_3})^2}{z_1 + E_2 + E_3 - E_{n_3}} |\psi_{n_3}(123)|^2 \right. \\
&\left. - \sum_{n_2} \frac{(E_1 + E_2 - E_{n_2})^2}{z_1 + E_2 - E_{n_2}} |\psi_{n_2}(12)|^2 \right]. \tag{7}
\end{aligned}$$

Note that the last term reflects the subtraction of disconnected diagrams. To find the solution $E_{n_2}, \psi_{n_2}(12); E_{n_3}, \psi_{n_3}(123)$ of the respective Schrödinger equation, we will use the adiabatic approximation which can be applied because of the large difference between the masses of the electrons and the ions, $m_e/m_i \ll 1$. Whereas for the electron–ion system, $\psi_{n_2}(12)$, the well-known hydrogen states result, the solution for an electron moving in the potential of two ions at distance R can be given within the tight-binding approximation (TBA) by the superposition of hydrogen (ground state) orbitals at the corresponding positions of the ions. The overlap term $S(R) = \int d^3\mathbf{r} \psi_{1s}^*(\mathbf{r}) \psi_{1s}(\mathbf{r} - \mathbf{R})$ as well as the expressions for the Coulomb and exchange interaction are well known from the literature.

Considering only the contribution of the hydrogen ground state, from the self-energy the following expressions for the spectral function and the density of states are obtained reflecting the validity of the sum rule:

$$\begin{aligned}
A_e(1, \omega) &= 2\pi \delta(\omega - E_1) \left[1 - \frac{2\Omega_0 e^{\beta\mu_i}}{\Lambda_i^3} |\psi_{1s}(p_1)|^2 \left(1 + 2\pi \frac{N_p}{\Omega_0} \int_0^\infty dR R^2 \right. \right. \\
&\quad \times \left. \left. \left[\sum_{s,a} \frac{1 \pm \frac{\sin(p_1 R)}{p_1 R}}{1 \pm S(R)} - 2 \right] \right) \right] + 2\pi \frac{2\Omega_0}{\Lambda_i^3} e^{\beta\mu_i} |\psi_{1s}(p_1)|^2 \left\{ \delta(\omega - E_{1s}) \right. \\
&\quad \left. + 2\pi \frac{N_p}{\Omega_0} \int_0^\infty dR R^2 \left[\sum_{s,a} \delta(\omega - E_{1s}^{s/a}(R)) \frac{1 \pm \frac{\sin(p_1 R)}{p_1 R}}{1 \pm S(R)} - 2\delta(\omega - E_{1s}) \right] \right\} \tag{8}
\end{aligned}$$

$$\begin{aligned}
D_e(\omega) &= \frac{(2m_e)^{3/2}}{\pi \hbar^3} \omega^{1/2} + \frac{8\pi}{\Lambda_i^3} e^{\beta\mu_i} \left\{ \delta(\omega - E_{1s}) + 2\pi \frac{N_p}{\Omega_0} \int_0^\infty dR R^2 [\delta(\omega - E_{1s}^s(R)) \right. \\
&\quad \left. + \delta(\omega - E_{1s}^a(R)) - 2\delta(\omega - E_{1s}) \right\}. \tag{9}
\end{aligned}$$

We considered a quasi-classical approximation, N_p denotes the total number of protons. In the density of state D_e the renormalization of the free electron contribution due to the bound states was discarded.

Figure 1 shows the two-site contribution of equation (9) which has two singularities. The first one occurs at the low-energy band edge. The related energy value is the binding energy of the hydrogen molecule ion (≈ -1.26 Ry) given by the minimum of $E_{1s}^s(R)$ at the equilibrium distance $R_0 \approx 2.49a_B$. The other singularity is related to the hydrogen atom. The hydrogen molecule H_2 is not explicitly included. Since correlation terms between the electrons are not considered, the molecule follows as double occupation of the symmetric or antisymmetric orbitals. The finite bandwidth is due to the two-site integrals in $E_{1s}^{s/a}(R)$. For higher energies we do not find a sharp upper band edge because the energy values for decreasing distances R are divergent. In order to calculate the equations of state, e.g. n_e , we have to include the

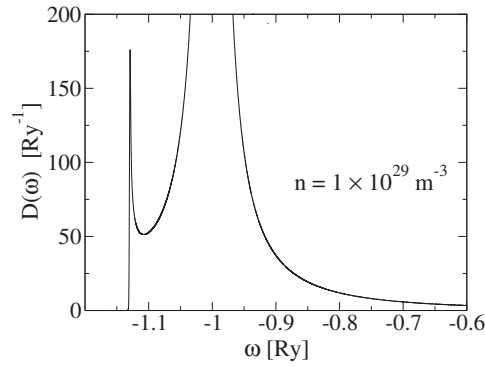


Figure 1. Two-site contribution (molecule ion) of equation (9) to the density of states.

single-site contributions to the density of states, too. In the quasi-classical limit we find

$$n_e = 2 \frac{e^{\beta\mu_e}}{\Lambda_e^3} + 4 \frac{e^{\beta\mu_i}}{\Lambda_i^3} e^{\beta\mu_e} e^{-\beta E_{1s}} \times \left\{ 1 + (n_i + n_a) \frac{1}{2} \int d^3\mathbf{R} [e^{-\beta(E_{1s}^s(R) - E_{1s})} + e^{-\beta(E_{1s}^a(R) - E_{1s})} - 2] \right\}. \quad (10)$$

The particle density is decomposed into a free and a bound part. The bound part itself consists of atomic bound electrons and molecular bound ones.

4. Chemical picture and band structure

In the low-density limit where systematic expansions with respect to the density are possible, the chemical picture can be applied to describe a partially ionized plasma consisting of free particles and bound states (see [1, 7] and references therein). In thermal equilibrium, the abundance of the different components follows from a mass action law. Such an approach can be extended to higher densities if medium modifications are taken into account. In particular, the different energy shifts of free particles and bound states due to screening effects lead to the Mott effect where the bound states merge with the continuum of scattering states. As a consequence, the transition from a dielectric to metallic behaviour (MIT) happens when the lowest bound state disappears, see [1]. In a more systematic approach, medium modifications are produced not only by free particles, but also by bound states. In the second Born approximation the polarization potential between bound and free particles as well as the van der Waals interaction between bound states is obtained, see [7]. This approach is based on the systematic application of the chemical picture where the single particle and bound states are treated on the same footing so that the polarization function of free particles in the screened Coulomb interaction has to be complemented by the contribution of bound states. The behaviour of the single particle and bound states in a medium which is a mixture of single particle and bound states has to be solved self-consistently, see [8].

At high densities, models known from liquid metals or disordered solids (Anderson–Hubbard model) have been used to describe the electron structure in dense plasmas. The quantum mechanics is given by the Hamiltonian

$$H = \sum_{m\sigma} E_m a_{m,\sigma}^\dagger a_{m,\sigma} + \sum_{mm'\sigma} T_{mm'} a_{m',\sigma}^\dagger a_{m,\sigma} + \frac{U}{2} \sum_{m\sigma} a_{m,\sigma}^\dagger a_{m,\sigma} a_{m,-\sigma}^\dagger a_{m,-\sigma}. \quad (11)$$

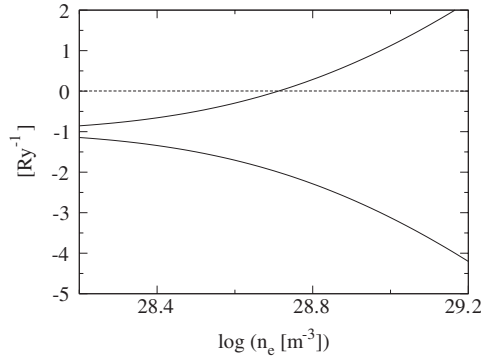


Figure 2. Band edges for a hydrogen lattice in the TBA: broad ground state (solid line) and continuum edge (dashed line).

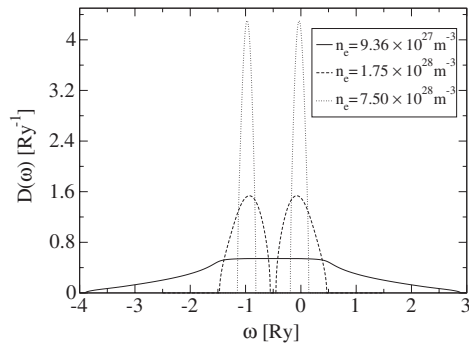


Figure 3. Normalized density of states for a hydrogen lattice in Hubbard approximation.

The first term reflects the binding energy of an electron with spin σ at the ion position \mathbf{R}_m . Due to local fluctuations of the mean field produced by the surrounding medium this binding energy will vary. $T_{mm'}$ is the two-site contribution due to the electron hopping between sites m and m' . Last we have the electron–electron correlation term, indicated by the Hubbard parameter U for the single-site Coulomb repulsion.

To characterize some typical aspects of the Anderson–Hubbard model, we discuss different limiting cases. Bound states and hopping of electrons between them can be described within a tight-binding approximation ($U = 0$). In the case of periodically (simple cubic) ordered systems with a lattice constant a , the solution of the eigenvalue problem can be given in the nearest neighbour approximation as $E_{\mathbf{k}}(a) = 2T(a)[\cos k_x a + \cos k_y a + \cos k_z a]$, where $T(a)$ is the hopping integral between two neighbouring sites. The related density of states is characterized by its band edges, shown in figure 2 for a simple model calculation. The systematic inclusion of electron–electron correlations remains a problem which is treated only in certain approximations such as the Hubbard approximations [3] ($U \neq 0$) and its generalizations, leading to a correlation gap in the density of states as shown in figure 3. The Hubbard transition is related to the correlation-gap closure in a half-filled band if the ratio of bandwidth and correlation energy exceeds a critical value. As a consequence, a transition from dielectric to metallic behaviour (MIT) occurs, see [9].

Both, the chemical picture, which describes partially ionized plasmas with medium modifications of the eigenvalues of the different components, and the Anderson–Hubbard

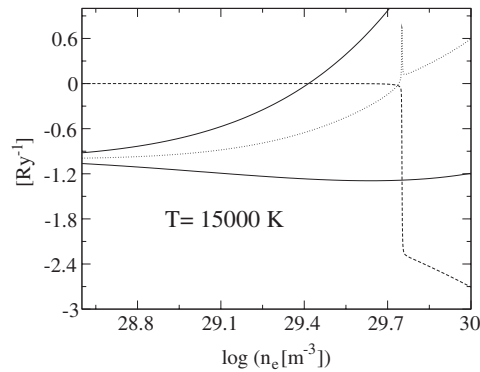


Figure 4. Band edges for in-medium hydrogen atoms in the AA model: broad ground state (solid), scattering states (dashed) and chemical potential (dotted).

model, shortly outlined above, represent different concepts in describing strongly correlated dense plasmas. It is a challenge to unify both concepts within a systematic Green's function approach. For this, we have to analyse the spectral function. In the present work we have shown that the formation of a band structure can be found when considering higher-order correlations, such as those described by the three-particle T-matrix, see figure 1. The influence of Hubbard type electron–electron correlations on the energy bands can be derived within an adiabatic approximation and will be given in a forthcoming paper.

5. Alternative approaches

Considering the adiabatic approximation, an appropriate starting point to describe an electron–ion plasma would be electrons moving in a disordered distribution of ions. A simple model reflecting only the variation of the binding energies and the hopping matrix elements ($U = 0$ in equation (11)) is the Anderson model, see [2]. The energy bands are smeared out. A Green function technique for disordered systems leading to the density of states was developed in [10]. The generalization by including electron–electron correlations leads to the Anderson–Hubbard model. Because of the disorder the correlation gap vanishes and is replaced by a pseudo-gap formed by mobility edges.

Another approach to describe the modification of the bound states by the medium is the average atom (AA) model, see [11]. The Schrödinger equation is solved in a Wigner–Seitz sphere for a self-consistently determined potential, with special boundary conditions at the surface of the sphere. A band is formed with edges given by the zero of the wavefunction (upper band edge) or zero first derivative (lower band edge). As an example, the shifts of scattering states and the modification of bound states for hydrogen are shown in figure 4. Calculations including exchange and correlation effects can be improved by using methods of the density functional theory, see, e.g., [12]. Here a combination of the broadening of the bound states and the shift of free electrons leads to the Mott effect.

It would be desirable to develop an approach which contains all these different pictures in a consistent way. The Green function approach shown here is believed to bridge the gap between the chemical picture and electron structure calculations known from condensed matter physics. A highly delicate question, the disappearance of two-particle bound states, is related to the Mott effect. Whereas in the chemical picture screening is responsible for this effect, in the AA model it is the broadening of single-particle bands which leads to a closure of the

band gaps. In the Hubbard model it is related to the closure of the correlation gap due to the broadening of energy levels. Only the simultaneous consideration of all these effects may consistently describe the Mott effect.

6. Macroscopic properties

The properties of dense plasmas, especially at the MIT in hydrogen [13], are a subject of recent experimental investigations. A consistent description of macroscopic properties in such plasmas should be given in terms of the spectral function. For example, the dc conductivity is related to the abundance of charge carriers in delocalized, extended states. The corresponding expressions for a partially ionized plasma can be found in [7, 8]. As discussed recently, [9], the conductivity near the MIT is determined not only by the free charge components. In particular, a strong increase of the conductivity is expected due to the closure of the correlation gap as known from the Hubbard model [3]. More generally, in order to determine the conductivity, the evaluation of a two-particle Green's function is necessary where the mobility edges have to be taken into account, see [10]. We infer that for a unified description of free electrons and hopping processes, both contributing to the conductivity, a more detailed investigation of the density of states is necessary as outlined in this paper.

Besides the dc conductivity optical properties are of special interest. Thus the inverse bremsstrahlung is given by the free particle contribution [14], whereas the discrete line spectrum is determined by the transitions between bound states. Systematic evaluation of the spectral line shape including the interaction with the medium yields shift and broadening of spectral lines [1]. An interesting quantity is the reflectivity [15]. The corresponding calculations are based on a chemical picture which is applicable in the low-density region. In order to describe metallization we have to go beyond the chemical picture and include the formation of electron bands as discussed in this paper. The treatment of optical absorption in the region of MIT should be based on a spectral function, taking into account the formation of bound states, energy bands and correlation effects. For this, the use of the improved treatment of the spectral function, given in this paper, is a task of future work.

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