Internal vs. External Conductivity of a Dense Plasma: Many-particle theory and simulations

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In the long-wavelength limit \( \mathbf{k} = 0 \), the response function has been investigated with respect to the external and internal fields which is expressed by the external and internal conductivity, respectively. Molecular dynamics (MD) simulations are performed to obtain the current-current correlation function and the dynamical collision frequency which are compared with analytical expressions. Special attention is given to the dynamical collision frequency and the description of plasma oscillations in the case of \( \mathbf{k} = 0 \). The relation between the external and internal conductivity and to the current-current correlation function is analyzed.

Keywords: linear response theory, dielectric function, dynamical collision frequency, molecular dynamics simulations, dynamical conductivity, internal conductivity, dense plasma

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I. INTRODUCTION

The treatment of strongly correlated Coulomb systems is a challenge for many-particle theories. It has applications in different fields such as dense ionic plasmas and the electron-hole plasma in excited semiconductors. Within a quantum statistical approach, the methods of equilibrium and non-equilibrium Green functions have successfully been utilized to calculate the properties of dense plasmas, see [1]. However, a problem is the validity of perturbative approximations when using the Green function approach for strongly correlated systems.

With increasing computer capacities, simulation techniques such as molecular dynamics (MD) simulations have been developed to obtain physical quantities from correlation functions, see [2, 3, 4, 5, 6, 7]. The MD approach allows the application to large coupling parameters. On the other hand, quantum effects are difficult to include. This shortcoming is partially cured by considering pseudopotentials which effectively take into account the uncertainty principle by a short distance modification of the Coulomb interaction within the range of the thermal wavelength, see [1]. More rigorous methods to include quantum effects are wave packet MD simulations [8] or path integral Monte Carlo calculations [9].

Other points are the finite particle number and the limited accuracy when solving the equations of motion. The latter will not be discussed any further. The transition from a finite system to the thermodynamic limit of an infinite system can be performed by periodic boundary conditions. The total force on a given particle from all the other particles in a basic cell, as well as from the infinite array of their periodic images, can be obtained using the standard Ewald procedure [2, 8].

In the present paper, the long-wavelength limit \( \sigma(\omega) = \lim_{k \rightarrow 0} \sigma(k, \omega) \) of the dynamical conductivity is considered for a two-component plasma. According to the fluctuation-dissipation theorem (FDT), this transport quantity can be expressed in terms of equilibrium correlation functions, in particular the auto-correlation function (ACF) of the electrical current or the ACF of the electrical charge density. In the literature [10], see also [11], the internal as well as the external conductivity are introduced, relating the electrical current density to the internal or the external electrical field strength, respectively. We will present the corresponding relations in the following Section II. An important quantity related to the dynamical conductivity is the dynamical collision frequency \( \nu(\omega) \). Analytical expressions can be derived in different approximations within a perturbative approach, see [12].

Section III defines the current in the context of MD simulations, and the connection to the collision frequency is shown. While results from MD simulations and analytical approaches for the structure factor and other frequency dependent quantities at finite wavenumber \( k \) are in good agreement, see e.g. [2, 6], we will discuss the zero-wavenumber...
case of MD simulations which is relevant for the dielectric function $\epsilon(k = 0, \omega)$ or the dynamical conductivity $\sigma(\omega)$. Calculations are presented without and including a mean field contribution which lead to the external and internal conductivity, respectively.

Details of the MD simulations are reported in Section IV. Results for the current ACF and the dynamical collision frequency at parameter values of a strongly coupled plasma are shown and compared with results of the analytical approach. The inclusion of a mean field when performing MD simulations is considered in Section V. The controversy between the internal and external conductivity in calculating the collision frequency is resolved. Conclusions are drawn in Section VI.

II. DYNAMICAL CONDUCTIVITY OF THE TWO-COMPONENT PLASMA

We consider a two-component fully ionized neutral plasma, such as a H plasma consisting of electrons and protons, at temperature $T$ and density $n$ of each component. The interaction is given by the Coulomb potential, and the plasma is characterised by the nonideality parameter $\Gamma = e^2(4\pi n_e/3)^{1/3}/(4\pi\epsilon_0 k_B T)^{-1}$ and the degeneracy parameter $\Theta = 2m_n k_B T h^{-2}(3\pi^2 n)^{-2/3}$. The linear response to external perturbations in general is presented in various references, see e.g. [1, 12]. In Eq. (4), the dynamical collision frequency is found from the generalized Drude formula Eq. (4) if the collision frequency is considered to be a real constant equal to the inverse of the relaxation time $\tau$ in momentum phase space.

In analogy to the internal conductivity, a so-called external conductivity [10] can be introduced from the response function [11]

$$
\sigma^{\text{ext}}(k, \omega) = \frac{i\omega}{k^2} \chi(k, \omega) = \beta \Omega_0 \left\langle J_k^{\text{long}}(t), J_k^{\text{long}}(0) \right\rangle_{\omega+i\eta}.
$$

This quantity is directly related to the longitudinal current ACF. Note that it is not the dynamical conductivity defined by Eq. (4). Instead, it is related to the dynamical collision frequency in the following way
The transverse part of the dielectric tensor can also be related to a conductivity according to

\[ \hat{\epsilon}(k, \omega) = 1 + \frac{i}{\epsilon_0 \omega} \hat{\sigma}(k, \omega). \tag{7} \]

The transverse conductivity is defined in analogy to the longitudinal (4) as

\[ \sigma^{\text{trans}}(k, \omega) = \frac{i \omega}{k^2} \Pi^{\text{trans}}(k, \omega) = \frac{\epsilon_0 \omega_{\text{pl}}^2}{-i \omega + \bar{\nu}(k, \omega)}, \tag{8} \]

where \( \bar{\nu}(k, \omega) \) is commonly called memory function [2]. However, in this case, the Kubo-Greenwood formula [2, 4, 11, 13, 14] relates the polarization function directly to the transverse current ACF,

\[ \sigma^{\text{trans}}(k, \omega) = \beta \Omega_0 \langle J_{k}^{\text{trans}}; J_{k}^{\text{trans}} \rangle_{\omega+i\eta}. \tag{9} \]

Within a Green function approach, a diagram representation is possible [12]. In contrast to \( \chi(k, \omega) \) and the transverse polarization, which are given by diagrams containing Coulomb interaction in any order, the respective current ACF \( \Pi^{\text{long}}(k, \omega) \) is given only by the irreducible diagrams. In the long-wavelength limit, transverse and longitudinal conductivities lead to the same response of the system,

\[ \lim_{k \to 0} \sigma^{\text{trans}}(k, \omega) = \lim_{k \to 0} \sigma^{\text{long}}(k, \omega). \tag{10} \]

### III. CURRENT AUTO-CORRELATION FUNCTION

Within MD simulations [3, 4, 11, 13], the normalized current ACF

\[ K(t) = \frac{\langle J_k(t) J_k \rangle}{\langle J_k^2 \rangle} \tag{11} \]

is calculated. Here, the long-wavelength limit \((k \to 0)\) of the current

\[ J_{k=0}(t) = \frac{1}{\Omega_0} \sum_c \sum_{i=1}^N c v_{i,c}^z(t) \tag{12} \]

is considered, where \( N \) is the number of electrons and singly ionized ions, and \( v_{i,c}^z \) is the speed in \( z \)-direction of the \( i \)th particle of component \( c \), denoted by \( \{i, c\} \). For convenience, we will drop the index \( k \) in the following. Due to isotropy, the normalizing factor is equal to

\[ \langle J^2 \rangle = \frac{e^2}{3 \Omega_0} N \langle v^2 \rangle = \frac{e^2}{\Omega_0} N \frac{k_B T}{m} = \frac{\epsilon_0 \omega_{\text{pl}}^2}{\Omega_0 \beta}. \tag{13} \]

The Laplace transform of the current ACF reads

\[ \langle J; J \rangle_{\omega+i\eta} = \langle J^2 \rangle \int_0^\infty e^{i(\omega+i\eta)t} K(t) dt. \tag{14} \]

On the basis of this quantity, two different results for the conductivity

\[ \sigma(\omega) = \epsilon_0 \omega_{\text{pl}}^2 \int_0^\infty e^{i(\omega+i\eta)t} K(t) dt \tag{15} \]

are derived depending on whether the current densities are considered to be long-wavelength limit of the longitudinal or transverse case.

Firstly, within the transverse response, the Kubo-Greenwood formula (9) is utilized. The conductivity (15) is then related to the memory function \( \bar{\nu}(\omega) \) [2, 4, 11, 13, 14] via the Drude like formula (8) and we find

\[ \frac{\bar{\nu}(\omega)}{\omega_{\text{pl}}} = \frac{\epsilon_0 \omega_{\text{pl}}}{\sigma^{\text{trans}}(\omega)} + i \frac{\omega}{\omega_{\text{pl}}}. \tag{16} \]
If we assume a constant memory function (collision frequency) \( \tilde{\nu}(\omega) = \tilde{\nu} \), the Laplace transformation of \( \sigma^{\text{trans}}(\omega) \) back to \( K^{\text{trans}}(t) \) using the functional dependence given by Eq. (15), leads to a monotonically decreasing \( K^{\text{trans}}(t) = \exp(-\tilde{\nu}t) \). This behaviour is observed indeed in simulations for \( \Gamma \leq 1 \). Secondly, within longitudinal response, we have to distinguish between the external and the internal conductivity. Inserting Eqs. (14) and (13) into (5), this implies that expression (15) is the external conductivity. The internal conductivity can be calculated via

\[
\sigma^{\text{long}}(\omega) = \frac{\sigma^{\text{ext}}(\omega)}{1 - i\sigma^{\text{ext}}(\omega)/(\epsilon_0\omega)}. \tag{17}
\]

and due to the generalized Drude formula (4) the collision frequency is, in contrast to (16),

\[
\nu(\omega) = \frac{\epsilon_0\omega{\text{pl}}}{\sigma^{\text{ext}}(\omega)} + i \left( \frac{\omega}{\omega{\text{pl}}} - \frac{\omega{\text{pl}}}{\omega} \right). \tag{18}
\]

Using a constant collision frequency \( \nu(\omega) = \nu \) in the respective relationship (6) for the external conductivity, we find for the longitudinal current ACF via a Laplace transformation

\[
K^{\text{long}}(t) = \exp \left\{ -\frac{\nu}{2} \right\} \left[ -\frac{\nu}{2z} \sin(zt) + \cos(zt) \right], \quad z = \sqrt{\omega^2_{\text{pl}} - \frac{\nu^2}{4}}. \tag{19}
\]

This shows that an oscillating behaviour is expected for the ACF. The oscillation frequency tends to \( \omega_{\text{pl}} \) in the limit \( \nu \to 0 \).

If in the long-wavelength limit both \( \nu(\omega) \) and \( \tilde{\nu}(\omega) \) coincide, the current ACF for the longitudinal and transverse response cannot be identical. In the following Sections IV, V we will resolve the contradiction between the internal conductivity as obtained from the current ACF according to (17) and (5) and the transverse conductivity obtained from the current ACF according to (16) and (4).

**IV. SIMULATION TECHNIQUE**

In the MD simulation scheme, the Newtonian equations of motion are solved for a system consisting of \( N \) singly charged ions and \( N \) electrons exerting Coulomb forces on each other. The \( i \)-th particle of component \( c \) shall be denoted as \( \{i, c\} \). This is a classical treatment where the trajectories of each particle are determined. The original Coulomb interaction can be replaced by a pseudopotential, where the short-range part of the interaction is modified reflecting the quantum character of the interaction. A systematic derivation of a pseudopotential which reproduces the equilibrium properties has been given by Kelbg, see [2, 13, 14] on the basis of the Slater sum. In particular, we use the so-called “corrected Kelbg” potential (19):

\[
V_{cd}(r) = \frac{e_c e_d}{4\pi\epsilon_0 r} \left[ F \left( \frac{r}{\lambda_{cd}} \right) - r \frac{k_B T}{e_c e_d} \tilde{A}_{cd}(\xi_{cd}) \exp \left( -\left( \frac{r}{\lambda_{cd}} \right)^2 \right) \right]. \tag{20}
\]

where

\[
\lambda_{cd} = \frac{\hbar}{\sqrt{2m_{cd}k_B T}}, \quad \frac{1}{m_{cd}} = \frac{1}{m_c} + \frac{1}{m_d}, \quad \xi_{cd} = -\frac{e_c e_d}{k_B T \lambda_{cd}},
\]

\[
F(x) = 1 - \exp(-x^2) + \sqrt{\pi x} (1 - \text{erf}(x)),
\]

\[
\tilde{A}_{ee}(\xi_{ee}) = \sqrt{\pi} |\xi_{ee}| + \ln \left[ 2\sqrt{\pi} |\xi_{ee}| \int_0^\infty \frac{y \exp(-y^2) dy}{\exp(\pi |\xi_{ee}|/y) - 1} \right],
\]

\[
\tilde{A}_{ci}(\xi_{ci}) = -\sqrt{\pi} \xi_{ci} + \ln \left[ \sqrt{\pi} \xi_{ci}^2 \left( \zeta(3) + \frac{1}{4} \zeta(5) \xi_{ci}^2 \right) + 4\sqrt{\pi} \xi_{ci} \int_0^\infty \frac{y \exp(-y^2) dy}{1 - \exp(-\sqrt{\pi} \xi_{ci}/y)} \right],
\]

where \( \zeta(n) \) are the Riemann-Zeta functions. This interaction potential corresponds to the Coulomb potential at large distances and provides the exact value of the Slater sum and its first derivative at \( r = 0 \).

Initially, all the particles are gathered in a cubic box with the edge size \( L \). The number of particles \( N \) in this basic cell is obtained from a given mean plasma density \( n \) via \( N = nL^3 \). To simulate an infinite homogeneous plasma,
images of this charge-neutral basic cell are considered shifting the basic cell by integer multiples of \( L \) in different directions. This extended system has a constant mean plasma density \( n \). Artefacts may occur due to the periodicity of the particle positions, but they are suppressed if the basic cell size is increased.

The dynamics of both electrons with charge \(-e\), mass \( m_e \) and ions with charge \( e \), mass \( m_i \), is considered. Because of the continuous expansion of such plasma, the nearest image method is applied to the force calculation procedure. Here, the force \( \vec{F}_{i,c} = \vec{F}_{i,c}^{\text{short}} + \vec{F}_{i,c}^{\text{long}} \) on a particle \( \{i, c\} \) is considered to consist of two contributions. The interaction forces between particle \( \{i, c\} \) and the nearest neighbour images of all other particles found in the basic cell centered around the position \( \vec{r}_{i,c} \) of the considered particle \( \{i, c\} \) is the short-range contribution \( \vec{F}_{i,c}^{\text{short}} \). The contribution \( \vec{F}_{i,c}^{\text{long}} \) is originated from the remaining images, which are not in the basic cell.

The short-range part of the force is calculated as

\[
\vec{F}_{i,c}^{\text{short}} = \sum_d \sum_{j(\neq i)}^{N} \vec{F}_{cd}(r^{n.n.}_{j,d} - \vec{r}_{i,c}), \quad \vec{F}_{cd}(\vec{r}) = -\frac{\vec{r} \cdot dV_{cd}(r)}{r}.
\]  

(21)

The time argument \( t \) is suppressed. According to this method it is assumed that the particle \( \{i, c\} \) doesn’t interact with original particles which at large \( t \) may be found far away due to the motion in space beyond the basic cell, but with their next neighbours’ images obtained by periodically shifting their coordinates into the basic cell centered around the particle \( \{i, c\} \). Thus, the position of each original particle \( \vec{r}_{i,c} \) is replaced by the position of an image \( \vec{r}_{j,d} \)

\[
r^{n.n.\alpha}_{j,d} = x^{\alpha}_{j,d} - mL, \quad |r^{n.n.\alpha}_{j,d} - \vec{r}_{i,c}| \leq \frac{L}{2},
\]  

(22)

where \( \alpha = x, y, z \) and \( m \) is an integer. It should be noted that this procedure is repeated for each particle at \( \vec{r}_{i,c} \).

This method implies that each particle is always surrounded by \( 2N - 1 \) other particles with a constant mean density and the plasma is homogeneous in scales larger than the simulation cell.

The forces \( \vec{F}_{i,c}^{\text{long}} \) due to the interaction with images outside the basic cell centered around the position \( \vec{r}_{i,c} \) of the particle \( \{i, c\} \) are treated in a different way. If the dimension \( L \) of the basic cell is large in comparison to the screening length, the contributions of all images except the nearest one can be neglected. In particular, this is justified in the case of a nonideal plasma where the effective interaction potential decreases exponentially with distance due to screening. The influence of the far images can be taken into account considering Ewald sums. They are expected to give only a small contribution to \( \vec{F}_{i,c}^{\text{short}} \) provided \( N \) is high enough. They are not relevant with respect to our considerations.

For explicit MD simulations, we consider a model plasma consisting of singly charged ions and electrons with density \( n = 3.8 \times 10^{21} \text{ cm}^{-3} \) at a temperature of \( T = 33000 \text{ K} \). This corresponds to recent experiments in dense xenon plasmas [16]. The plasma parameters introduced in Sec. II take the value \( \Gamma = 1.28, \Theta = 3.2 \). It is a nondegenerate, strongly coupled plasma. The computations of the current ACF for the ion-electron mass ratios \( m_i/m_e = 1836 \) and \( m_i/m_e = 100 \) show no considerable difference. Thus the ratio \( m_i/m_e = 100 \) is selected for better convergence when averaging over the configurations of ions. The total number of particles \( N = 250 \) was found to be enough for \( \Gamma \approx 1 \). Further increase of the number of particles makes the current ACF performance change to the dynamically averaged value, equilibrium correlation functions and others. The equilibrium state of the plasma at the given temperature was obtained using a special procedure described in [18].

The current ACF is calculated directly from the velocities of the particles in subsequent moments of time according to Eqs. [11] and [12], where \( \Omega_0 = L^3 \) with \( L \) the length of the basic cell. The averaging of the ACF is performed over \( 1 - 5 \cdot 10^5 \) initial configurations. These configurations are obtained from a long MD trajectory at different time moments. As shown in [18], two configurations are statistically independent if they are taken at times separated by the dynamical memory time. In our case about \( 5 \cdot 10^5 \) initial configurations are already fully statistically independent for electrons. The dynamical memory time for ions increases with the ion mass [18]. Thus the smaller mass ratio the better averaging for ions is obtained.

Results are shown in Fig. [1] with circles. The relatively small ion-electron mass ratio \( (m_i/m_e = 100) \) was chosen for computational reasons since the calculation with greater mass ratio shows exactly the same results for the current ACF. The current ACF \( K(t) \) decreases monotonously as it was also obtained in previous MD simulations [2, 4, 6]. It indicates that the conductivity obtained numerically from \( K(t) \) according to [15] should be treated as the transverse conductivity [15]. The dimensionless dynamical conductivity \( \sigma(\omega)/(\epsilon_0 \omega_{pl}) \) is shown in Fig. [2] with circles. As \( \omega \to 0 \), the real part has a finite value and the imaginary part vanishes, as expected from Eq. [16]. According to the latter expression, we then deduct a memory function or collision frequency \( \tilde{\nu}(\omega) \) as shown in Fig. [3] with circles.

Details of different approximations for the dynamical collision frequency within a generalized linear response theory can be found in [12]. The dynamical collision frequency in Born approximation with respect to the statically screened
potential (Debye potential) taken in the non-degenerate case and within the long-wavelength limit, is given here

\[ \nu^{\text{Born}}(k = 0, \omega) = -i \gamma n \int_0^\infty dy \frac{y^4}{1 + \frac{y^2}{\alpha^2}} \left[ \tilde{V}(q) \frac{16m_e k_B T \Omega_0 \epsilon_0}{e^2 \hbar^2} \right]^2 \int_{-\infty}^{\infty} dx e^{-(x-y)^2} \frac{1 - e^{-4xy}}{xy(xy - \nu - i\eta)}, \]  

(23)

where

\[ q = \frac{y}{\hbar} \sqrt{16m_e k_B T}, \quad \bar{n} = \frac{\hbar^2 ne^2}{8\epsilon_0 m_e (k_B T)^2}, \quad g = \frac{e^2 \beta^3/2}{4\sqrt{\pi} \epsilon_0^3 m_e^{1/2}}, \quad \tilde{\nu} = \frac{\hbar \omega}{4 \kappa k_B T}. \]  

(24)

In the case of the Fourier transform of the Coulomb interaction \( \tilde{V}(q) = e^2/(\Omega_0 \epsilon_0 q^2) \) the square brackets become \( 1/y^2 \).

We will now compare the MD simulations with this analytical treatment of the dynamical collision frequency within perturbation theory, see Figs. [4]. Firstly, we consider a system with statically screened Coulomb interaction \( \tilde{V}(q) = e^2/(\Omega_0 \epsilon_0 q^2) \) according to Eq. (24). The results are presented as dotted line. The Born approximation can be improved by taking into account the effects of dynamically screening, strong collisions (T matrix) and higher moments by introducing a renormalization factor \( [12] \) in the generalized Drude formula Eq. (4). This approximation is shown as solid line. Details of the calculation are given in \( [12] \). It can be seen that both real and imaginary part are in good agreement with the simulation results for \( \omega < \omega_{\text{pl}} \). This means that in this region the quantum mechanical treatment of the Coulomb potential and the classical simulations based on the corrected Kelbg potential are consistent.

At frequencies \( \omega \gg \omega_{\text{pl}} \) the asymptotic expansion of the analytical expression for the collision frequency is possible using the Fourier transform of the corrected Kelbg potential \( [20] \)

\[ \tilde{V}_{\text{cd}}(q) = \frac{e \epsilon_0 \lambda_{\text{cd}}}{\epsilon_0 \Omega_0 q} \left[ \sqrt{\frac{2}{\lambda_{\text{cd}}^2 q^2}} \text{Erf} \left( \frac{\lambda_{\text{cd}}}{2} q e^{-\frac{\lambda_{\text{cd}}^2}{4q^2}} - \frac{\lambda_{\text{cd}}^2 k_B T \pi^{3/2}}{4 \epsilon_0^3 m_e^{1/2}} A_{\text{cd}}(\xi_{\text{cd}}) q e^{-\frac{\lambda_{\text{cd}}^2}{4q^2}} \right) \right]. \]  

(25)

For the high frequency behaviour of the real part is found \( \Re \nu(\omega) \sim \omega^{-3.5} \) which is given in Fig. [4] as dashed line. There is good agreement between the simulation data and the analytically derived high frequency behaviour. The presented analytical treatment was also confirmed by MD calculations of the dynamical structure factor at finite \( k \) in \( [7] \) where the Deutsch potential was used.

V. LONGITUDINAL CONDUCTIVITY

We now investigate the evaluation of the longitudinal conductivity by MD simulations. The current ACF \( K^{\text{trans}} \) discussed in the previous Section cannot be taken since this current ACF yields the correct collision frequency only if the external conductivity is related to a Drude ansatz. However, this is not consistent. Instead we have to derive the internal conductivity, from which a collision frequency can be obtained via the Drude formula. Therefore, the current ACF \( K^{\text{ions}} \) has to be calculated differently than the ACF \( K^{\text{trans}} \). It will be shown how to obtain the longitudinal current ACF in the long-wavelength limit. However, we note that for finite wavevector \( k \) excellent agreement for the dynamical structure factor from MD simulation and analytical expressions has been found \( [7] \). The condition \( k > 2\pi/L \) means that any charge density wave occurs already within the basic simulation cell and the corresponding mean electric field is accurately taken into account. The limit \( k \to 0 \) is not trivial. For any small \( k \), the system is nearly homogeneous, but charge densities (or surface densities) are present at large distances, which can also be considered as a mean field.

For this, we follow the procedure to construct an infinite system by periodic images of a basic cell. We consider this as a limiting case of a finite number of images. Denoting the images in z-direction by \( N_{\text{images}} \), then a surface of our system is obtained at \( z_- = -(2N_{\text{images}} + 1) \cdot L/2 \) and \( z_+ = (2N_{\text{images}} + 1) \cdot L/2 \). When considering the force calculation procedure, there are contributions to the forces originating from a surface charge density. This occurs if positive and negative charges are moving at different rates across the surface of the basic cell. The introduction of a finite number of images compensates this effect at the interfaces, but not at the surface of the whole system including all the images. A large dipole moment follows connected with a finite polarization of the system. This surface charge density will produce an electrical field which has to be taken into account even in the limit when the number of images goes to infinity. If the surface is far away, it produces a homogeneous electrical field \( \bar{E}(t) \) within the simulation box. Following this reasoning, it is necessary to include a mean field in the long-wavelength limit as shown below. As a consequence, plasma oscillations are obtained in the current ACF.

On the macroscopic level, the Maxwell equations relate this mean field \( \bar{E}(t) \) to the average current density \( \bar{J}(t) \), which is oriented in z-direction according to the conventions in Sec. II,

\[ \frac{d\bar{E}(t)}{dt} = -\frac{1}{\epsilon_0} \langle \bar{J}(t) \rangle. \]  

(26)
Taking the current density according to Eq. (12) as an average over the basic simulation cell and the initial condition \( \vec{E}(0) = 0 \), the integration of Eq. (26) leads to

\[
\vec{E} = \frac{1}{L^3} \left( -e \sum_{i=1}^{N} \vec{r}_{i,e} + e \sum_{i=1}^{N} \vec{r}_{i,i} \right)
\]

(27)

In this approach, the long-range interaction forces are given by \( \vec{F}_{i,e}^{\text{long}}(t) = e_c\vec{E}(t) \). In particular, the equation of motion for an electron includes two parts

\[
m_e \frac{d\vec{v}_{i,e}}{dt} = \vec{F}_{i,e}^{\text{short}} - e\vec{E}.
\]

(28)

The interaction forces \( \vec{F}_{i,e}^{\text{short}} \) originate from close partners in the Debye sphere within the basic cell. It is fluctuating around a nearly zero mean value. Nevertheless, the amplitude of these fluctuations are much higher than the fluctuations of \( e\vec{E} \).

In the MD method, if no mean field term is taken into account, the total energy

\[
\mathcal{E}_{\text{tot}} = \mathcal{E}_{\text{pot}} + \mathcal{E}_{\text{kin}} = \frac{1}{2} \sum_{c,d} \sum_{i \neq j}^{N} V_{cd}(\vec{r}_{j,d} - \vec{r}_{i,c}) + \frac{m_e}{2} \sum_{i=1}^{N} v_{i,e}^2 + \frac{m_i}{2} \sum_{i=1}^{N} v_{i,i}^2
\]

(29)

is conserved. If the particle trajectories are calculated including the mean field force, the energy \( \mathcal{E}^\prime_{\text{pot}} + \mathcal{E}^\prime_{\text{kin}} \) is not conserved. Nevertheless, the conservation law can be fulfilled by including the mean field energy \( \mathcal{E}_{\text{field}} = L^3 \epsilon_0 E^2/2 \) so that the total energy \( \mathcal{E}^\prime_{\text{tot}} = \mathcal{E}^\prime_{\text{pot}} + \mathcal{E}^\prime_{\text{kin}} + \mathcal{E}_{\text{field}} \) is conserved. This is illustrated by simulations below.

The occurrence of plasma oscillations can be demonstrated in the following way. If the mass ratio between electrons and ions \( m_i/m_e \) is large the ion current can be neglected in Eq. (12). After that the derivative of the total current density is obtained from

\[
\frac{d\vec{J}(t)}{dt} = -\frac{e}{L^3} \sum_{i=1}^{N} \frac{d\vec{v}_i}{dt} = \frac{eN}{mL^3}(e\vec{E} - \vec{\zeta}),
\]

(30)

\[
\vec{\zeta} = \frac{1}{N} \sum_{i=1}^{N} \vec{F}_{i,e}^{\text{short}} = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \vec{F}_{ij}.
\]

(31)

The force \( \vec{\zeta} \) includes only electron-ion interaction forces as all electron-electron interaction forces are compensated since they do not change the total momentum of the electrons. Although the force \( \vec{F}_{i,e}^{\text{short}} \) on each electron is typically much greater than the force \( e\vec{E} \) from the mean electric field, the average over all electrons is of the same order of magnitude as \( e\vec{E} \). If we now differentiate Eq. (28) and substitute the derivative of the current using (30), we obtain the equation for the mean field

\[
\frac{d^2 \vec{E}}{dt^2} + \omega_{\text{pl}}^2 \vec{E} = \frac{\omega_{\text{pl}}^2}{e} \vec{\zeta}.
\]

(32)

On an average, \( \vec{\zeta} \) vanishes, so that plasma oscillations are described. The corresponding oscillations in the current ACF are obtained from MD simulations as the results below show.

We now present MD simulations based on the solution of the equations of motion (28) in comparison to the MD simulations as presented in the previous Sec. IV where the contribution of the mean field \(-e\vec{E}\) was not taken into account. The energy conservation is demonstrated in Fig. 5 according to Eq. (29). It can also be seen that the field energy \( \mathcal{E}_{\text{field}} \) is rather small compared to the particle energy \( \mathcal{E}_{\text{pot}}^\prime + \mathcal{E}_{\text{kin}}^\prime \).

Results for the longitudinal and transverse current ACF are shown in Fig. 1. After including the mean field into the MD simulations, the plasma oscillations in \( K(t) \) become well pronounced in contrast to a monotonously decreasing behaviour. It should be stressed that the amplitude of these oscillations does not depend on \( N \).

The conductivity calculated according to Eq. (13) is shown in Fig. 2. In comparison to the transverse case, the conductivity shows a qualitatively different behaviour. The real part following from the MD simulations including mean field is zero for zero frequency as is expected from the expression for the external conductivity (9). For the case without mean field, \( \text{Re} \sigma \) has a finite value. In the high frequency limit, both curves coincide. The dynamical collision frequencies \( \nu(\omega) \) and the memory function \( \tilde{\nu}(\omega) \) calculated from the simulation data for the ACFs are shown...
in Fig. 3. As pointed out, the results for the Laplace transform of the ACF differ significantly (Figs. 2). Nevertheless, if Eq. (18) is used for the collision frequency $\nu(\omega)$ and Eq. (16) for the memory function $\tilde{\nu}(\omega)$ in order to calculate the collision frequency, the results for both coincide quite clearly (Fig. 3).

Therefore, our analysis showed that the contradiction between the transverse conductivity which should be identical with the internal conductivity in the long-wavelength limit and the external conductivity could be resolved if the mean field is taken into account. The difference between Im $\nu(\omega)$ and Im $\tilde{\nu}(\omega)$ in the low frequency limit is caused by the numerical error of Im $\nu(\omega)$ due to subtraction of two large terms in Eq. (18).

VI. CONCLUSION

Molecular dynamics simulations of strongly coupled plasmas were performed using the quasiclassical Kelbg interaction potential. The current auto-correlation function was computed for a non-degenerate two-component plasma. Whereas for finite $k$ the dynamical structure factor and the plasma oscillations are reproduced by MD simulations, see [2, 4, 7], the original methods do not allow to consider $k$ values with $k < 2\pi/L$. On the other hand $k = 0$ should be possible to investigate with MD simulations in a finite volume.

We presented calculations for the transverse current ACF as well as for the longitudinal one. Although in the limit $k \to 0$ the transverse and longitudinal dielectric function and conductivities, respectively, coincide, the current ACF behave differently in this limiting case. It was shown that the results of MD simulations without a mean field in the long wavelength limit provide the monotonously decreasing transverse ACF. Its Laplace transform is to be directly related to the transversal conductivity.

In MD simulations for the longitudinal case, a mean-field term has to be included into the equations of motion in addition to the short range forces inside the Debye sphere. This mean-field term originates from surface charges not taken into account in the usual procedure of force calculation by the nearest image method. Simulations with these altered equations of motion show well pronounced plasma oscillations in the longitudinal current ACF. The results for the collision frequency as obtained in both simulation methods using the corresponding relations for the internal or external conductivities do coincide.

Additionally, the dynamical collision frequency inferred from the simulation data was compared with analytical results, which were derived using a generalized linear response theory. We found good agreement in the low and high frequency limits for a moderate nonideality. In particular, for $\omega < \omega_{pl}$, classical MD simulations using the corrected Kelbg potential are able to reproduce the quantum behaviour of Coulomb plasmas.

VII. ACKNOWLEDGEMENTS

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[1] W.-D. Kraeft, D. Kremp, W. Ebeling, G. Röpke, Quantum Statistics of Charged Particle System (Plenum, New York, 1986) [or Akademie Verlag, Berlin 1986].
[2] J. P. Hansen and I. R. McDonald, Phys. Rev. A 23, 2041 (1981); L.Sjögren, J.P. Hansen and E.L. Pollock, Phys. Rev. A 24, 1544 (1981).
[3] J. P. Hansen and I. R. McDonald, Theory of simple liquids (London, Academic Press, 1976)
[4] J. P. Hansen in Strongly Coupled Plasma Physics, eds. F.J. Rogers, H.E. DeWitt, Plenum, New York 1987, p.111.
[5] I.V. Morozov, G.E. Norman and A.A. Valuev, Dokl. Akad. Nauk 362, 752 (1998) [Doklady Physics 43, 608 (1998)].
[6] I.V. Morozov, G.E. Norman and A.A. Valuev, Phys. Rev. E 63, 036405 (2001).
[7] A. Selchow, G. Röpke, A. Wierling, H. Reinholz, T. Pschigu, G. Zwicknagel, Phys. Rev. E 64, 056410 (2001).
[8] D. Klakow, C. Toepffer, P.-G. Reinhard, J. Chem. Phys. 101, 10766 (1994); M. Knaup, P.-G. Reinhard, C. Toepffer, Contrib. Plasma Phys. 41, 159 (2001).
[9] B. Millitzer, S.M. Ceperley, Phys. Rev. Lett. 85, 1890 (2000).
[10] V.M. Adanyan, T. Meier, I.M. Tkachenko, Fiz. Plasm. (in Russian) 11, 826 (1985); V. M. Rylyuk, I.M. Tkachenko, Phys. Rev. A 44, 1287 (1991).
[11] G. D. Mahan, Many-Particle Physics (Plenum, New York, 1990).
[12] H. Reinholz, R. Redmer, G. Röpke, A. Wierling, Phys. Rev. E 62, 5648 (2000).
FIG. 1: Current auto-correlation function (ACF) for $\Gamma = 1.28$, $m_i/m_e = 100$; total number of averages $5 \times 10^5$; MD trajectory length of $2.5 \times 10^4 \tau_e$, $\tau_e = 2\pi/\omega_{pl}$ – period of electron plasma oscillations: MD simulations without (circles) and including (triangles) an additional mean-field term in the equations of motion.
FIG. 2: Real and imaginary parts of the Laplace transformation of the current ACF; MD simulations without (circles) and including (triangles) an additional mean-field term in the equations of motion.
FIG. 3: Real and imaginary parts of the dynamic collision frequency or memory function from MD simulations without (circles) and including (triangles) an additional mean-field term in the equations of motion.
FIG. 4: Dynamical collision frequency within different methods; points – MD simulations; analytical approximations: dotted line – Born approximation Eq. (23) with Coulomb potential, solid line – same approach including dynamically screening and strong collisions (T matrix) and higher moments via renormalization factor [12], dashed line – high frequency asymptote for Born approximation Eq. (23) with corrected Kelbg potential.
FIG. 5: Conservation of the total energy in MD simulations; curve 1 – total energy of the particles $E_{\text{tot}}' = E_{\text{pot}}' + E_{\text{kin}}'$ according to Eq. (29), curve 2 – total energy $E_{\text{tot}}'$ including the mean field energy.