Warm dense matter conductivity including electron-electron collisions

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The controversy with respect to the role of electron-electron collisions in the dynamic conductivity of dense plasmas is resolved. In particular, the dc conductivity is analyzed in the low-density, non-degenerate limit where the Spitzer theory is valid and electron-electron collisions lead to the well-known reduction of the result for a Lorentz plasma. With increasing degeneracy, the contribution of electron-electron collisions to the dc conductivity is decreasing and can be neglected for the liquid metal domain where the Ziman-Faber theory is applicable. We show how electron-electron collisions have to be implemented in calculations based on the Kubo-Greenwood formula which is prevalently applied in simulations for the frequency-dependent conductivity in the warm dense matter region, i.e. for arbitrary degeneracy.

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I. INTRODUCTION

Physical properties of warm dense matter (WDM) have become an emerging field of research. New techniques such as intense ultra-short pulse laser irradiation or shock wave compression allow to produce states of matter with high energy density in the laboratory that are of relevance for astrophysical processes. In the density-temperature plane of strongly coupled Coulomb systems, the region of degenerate, non-ideal plasmas is now accessible.

The calculation of properties of WDM is a challenging task. Transport properties, in particular the dc conductivity, are well investigated for a fully ionized plasma in the classical, low-density limit as given by Spitzer and Härm [1] within kinetic theory (KT), see also [2] and references given therein. The evolution of the electron velocity distribution function is described by a Fokker-Planck kinetic equation. The linearized kinetic equations are solved with a Landau collision integral, that includes both the electron-ion ($e-i$) and electron-electron ($e-e$) collisions.

Alternatively, the conductivity of strongly degenerate electron systems such as liquid metals has been obtained by Ziman and Faber [3] using the relaxation time approach. The treatment of $e-i$ interaction has been improved by Dharma-wardana [4] and others [5,7] who used expressions for the pseudopotentials and ionic structure factors that are appropriate for the particular ions under consideration. Lee and More [8] extended this approach to the non-degenerate regime. However, to recover the Spitzer result for the conductivity, $e-e$ collisions have to be taken into account. This is not consistently possible within the relaxation time approach [9], but has been done by Stygar [10] and Fortov et al. [11] using interpolation procedures. We present in this work a general approach using linear response theory (LRT) that allows also for a systematic treatment of $e-e$ collisions.

The investigation of time-dependent fields is somehow difficult in KT, too. Often, a combination of the collisionless kinetic equation with the relaxation time ansatz is used, see Landau and Lifshits [12], Dharma-wardana [4], or Kurilenko et al. [13,14]. According to Landau and Lifshits [12] it should be emphasized that such an approach is only applicable in the low frequency limit. The high-frequency region, relevant for describing bremsstrahlung, can be treated in LRT, see [15]. In the present work, we focus on the static conductivity for a response to an electric field that is constant in time and space (dc conductivity).

Originally, the Ziman formula was obtained treating the $e-i$ interaction in Born approximation. The strong coupling case, but also the deviation from the zero-temperature Fermi distribution function has been treated to determine the contribution of $e-i$ interactions. Recently, the Kubo-Greenwood formula [16,17] was considered as a promising approach to the dynamical conductivity in dense, strongly interacting systems at arbitrary degeneracy. Progress in calculating the $e-i$ pseudopotentials (e.g. within density functional theory (DFT)) and the structure factor makes this approach very successful. Based on the rich experience in electronic structure calculations for solids, liquids and complex molecules using DFT and the enormous progress in computing power, ab initio simulation techniques have been developed that allow to treat a large number of constituents with individual atomic structure. Most successful so far has been a combination of DFT for the electron system and classical molecular dynamics (MD) simulations for the ions which we will refer to as the DFT-MD method in what follows; for details, see [18,20]. This method relies on the Born-Oppenheimer approximation which allows to determine the electronic structure for a given configuration of ion positions. Simultaneously, the Hellmann-Feynman theorem yields the forces on the ions for every time step.
of the MD simulation so that neither two-particle potentials nor cross sections have to be used which are of limited validity for applications in WDM. As will be discussed below, the evaluation of the Kubo-Greenwood formula using optimal single electron states in the static mean-field potential of the ion subsystem, gives the full account of \( e - i \) interaction, but does not contain \( e - e \) collisions. The inclusion of the \( e - e \) collision into DFT-MD calculations based on the Kubo-Greenwood formula \cite{18,20}, as well as relaxation time approaches \cite{4,8,10} remains a puzzle in recent calculations of transport properties of WDM.

To solve this problem, we apply in the present work a generalized approach to non-equilibrium processes according to Zubarev et al. \cite{21,22}. Within this generalized linear response theory (gLRT) transport properties are related to equilibrium correlation functions such as current-current or force-force correlation functions. Different expressions for the conductivity are deduced that are equivalent if they are exactly calculated, as shown performing partial integration. However, they are differently suited in performing calculations. In particular, expressions that are consistent with KT (Spitzer result for the dc plasma conductivity) are compared with the Ziman-Faber theory, the Kubo-Greenwood formula, and the rigorous results for the Lorentz model. In the Lorentz model, non-interacting electrons are considered that are moving under the influence of the potential of the ions with given configuration (adiabatic limit).

Transport theory for WDM benefits from different sources. On one hand, the conductivity of liquid metals and disordered solids that is well described in the weak scattering limit (Fermi’s golden rule) by the Ziman formula if the conducting electrons are degenerate, see also the Ziman-Faber approach \cite{3} where alloys at finite temperature are considered \cite{23}. Main ingredients are the element-specific electron-ion pseudopotential and the (dynamical) ion structure factor that are adequately described using the Kubo-Greenwood formula where the \( e - i \) interaction is considered in any order. Evaluating the correlation functions within DFT-MD \cite{18,20,22} no perturbation expansion is performed. On the other hand, the conductivity of plasmas is described by KT so that in the low-density, non-degenerate limit the Coulomb interaction between \( e - i \) as well as \( e - e \) pairs leads to the Spitzer result. At higher densities, gLRT can be applied that considers correlation functions to be evaluated analytically using the method of thermodynamic Green functions \cite{22,25,28} or, non-perturbatively in the non-degenerate case, by MD simulations, see \cite{29}.

Bridging between both, the transport theory of condensed matter and plasma kinetic theory, the contribution of \( e - e \) collisions that is clear in KT remains unclear in the Ziman-Faber or Kubo-Greenwood approach \cite{4}. We solve this problem within gLRT that incorporates the Kubo formula as well as the KT as particular special cases, see \cite{15,22}. A simple expression is derived that accounts for the contribution of \( e - e \) interactions provided that the contribution of the \( e - i \) interaction is known. We show that the dc conductivity of WDM is reduced in the non-degenerated region due to \( e - e \) collisions. This reduction becomes smaller with increasing degeneracy. Exemplarily, we present exploratory calculations for aluminum in the WDM region. Further properties such as the optical conductivity and general thermoelectric transport coefficients will be considered in subsequent work.

II. LINEAR RESPONSE THEORY AND EQUILIBRIUM CORRELATION FUNCTIONS

A. Generalized response equations

We consider a charge-neutral Coulomb system consisting of ions of charge \( Z e \) and particle density \( n \), and electrons of charge \(-e\), mass \( m \), and particle density \( Z n \). The interaction with an external, spatially uniform electric field \( E^{\text{ext}}(t) \) is given by

\[
H_F(t) = -e \sum_i \mathbf{r}_i \cdot E^{\text{ext}}(t)
\]

with \( \mathbf{r}_i \) the position operator of the different electrons of the considered sample. In the adiabatic limit, the contribution of the ions can be neglected because of the large mass ratio. The current density is given by (homogeneous case, only electron contribution)

\[
\mathbf{j} = \frac{e}{m \Omega} \sum_i \mathbf{p}_i = \frac{e}{m \Omega} \mathbf{P},
\]

\( \Omega \) denotes the volume of the sample, and \( \mathbf{P} \) the total momentum of the electron subsystem. Without loss of generality we consider periodic time dependence of the field with frequency \( \omega \). In LRT the average value of the current has the same periodic time dependence, \( \langle \mathbf{j} \rangle = \text{Re}\{\mathbf{j}(\omega) \exp(-i \omega t)\} \). Similarly, an inhomogeneous external field can be decomposed into Fourier components with wave vector \( \mathbf{k} \). In the spatially homogeneous (\( \mathbf{k} \to 0 \)) and isotropic case considered here, the dynamical electric conductivity is defined as

\[
\mathbf{j}(\omega) = \chi(\omega) E^{\text{ext}}(\omega) = \sigma(\omega) \mathbf{E}(\omega),
\]
where \( \mathbf{E}(\omega) = \mathbf{E}^{\text{ext}}(\omega)/\epsilon(0, \omega) \) so that \( \mathbf{E} \) is the local, screened electric field, and \( \epsilon(k, \omega) \) the dielectric function. Consequently, the response function \( \chi(\omega) = \lim_{\eta \to 0} \chi(k, \omega) \) that relates the current density to the external field, is connected with the dielectric function and the dynamical conductivity \( \sigma(\omega) \) according to \( \sigma(\omega) = \chi(\omega) \epsilon(0, \omega) \).

There is a fundamental theory for transport coefficients that relates those to equilibrium correlation functions [15, 21, 22]. We outline this theory in App. A. A main ingredient is the possibility to extend the relevant statistical operator considering a set \( \{B_n\} \) of relevant observables that characterize the non-equilibrium state of the system. The currents of the deviation of the single-particle occupation numbers from the equilibrium value could be considered. If the averages of these observables are already correctly taken into account, they don’t have to be calculated dynamically so that the corresponding non-equilibrium state is observed in shorter time. As shown in App. A, response equations are derived to eliminate the Lagrange parameters \( F_n \) according to self-consistency conditions. Assuming linearity with respect to the external field, a system of linear equations follows where the coefficients are equilibrium correlation functions.

\[
\langle A; B \rangle_z = \int_0^\infty dt \, e^{izt} \langle A(t), B \rangle = \int_0^\infty dt \, e^{izt} \int_0^1 d\lambda \, \text{Tr} \{ A(t - i\hbar\beta\lambda)B^\dagger \rho_0 \} . \tag{4}
\]

The time dependence \( A(t) = e^{iHt/\hbar}A e^{-iHt/\hbar} \) is given by the Heisenberg picture with respect to the system Hamiltonian \( H \), and \( A = i[H, A]/\hbar \).

### B. Different choices of relevant observables and corresponding response functions

The fluctuation-dissipation theorem (FDT) relates transport coefficients to equilibrium correlation functions [1]. They can, in principle, be calculated because we know the equilibrium statistical operator. Thus, the FDT seems to be very convincing and promising to evaluate transport coefficients in dense, strongly correlated systems like WDM. However, the evaluation of the correlation functions is a quantum statistical many-body problem that may be treated by perturbation theory or numerical simulations. We discuss first the analytical approach where the interaction between the charged constituents of the system \( (e, i) \) is considered as perturbation. We discuss three different choices for the set of relevant observables \( B_n \) to characterize the non-equilibrium state, in addition to the conserved observables energy \( H \) and particle number \( N \) of the system, see [22].

i) The empty set of relevant observables is considered. It is equivalent to the grand canonical ensemble, see Eq. (A1). All non-equilibrium distributions are formed dynamically. As the result we obtain the Kubo formula [16].

\[
\chi^{\text{Kubo}}(\omega) = \frac{e^2}{3m^2\Omega} \langle \mathbf{P}; \mathbf{P} \rangle_{\omega+i\eta} \tag{5}
\]

where \( \lim_{\eta \to 0} \) has to be taken after the thermodynamic limit. The response function is given by the correlation function of the electrical current, see Eq. (2). It coincides with the conductivity \( \sigma(\omega) \) if only the irreducible part of the current-current correlation function is taken. In contrast to the very compact, comprehensive and intuitive expression for a transport coefficient, its evaluation contains a lot of difficulties. In particular, it is not suited for perturbation expansions of the dc conductivity because it is diverging in zeroth order. We come back to this item in Sec. [11] and App. [13].

ii) Relevant observables can be considered on the level of single-particle occupation numbers \( n_p \). The non-equilibrium state is characterized by the single-particle distribution function \( f(p, t) \). In order to derive expressions in parallel to KT we choose the fluctuations \( \delta n_p \) of the single-particle occupation number as relevant observables \( B_n \). The modification of the single-particle distribution function can be calculated straightforwardly according to

\[
\text{Tr} \{ \rho_{\text{rel}}(t) \delta n_p \} = \sum_{p'} (\delta n_{p}, \delta n_{p'}) F_{p'}(t) = \delta f(p, t) . \tag{6}
\]

The Lagrange multipliers \( F_{p}(t) = F_{p} \exp(-i\omega t)/2 + c.c. \) are determined from the response equations Eq. (A3). These response equations are generalized linear Boltzmann equations that contain the drift term and the collision term in the form of correlation functions so that many-particle effects can be included. A comprehensive discussion is found in Ref. [15]. For the solution, different methods are known. Below we present a solution using the Kohler variational principle as standard in KT.

The non-equilibrium single-particle distribution function \( \delta f(p) \) in the case of a time independent, constant external field is known if we have information about all moments of the distribution function, i.e. the averages over the observables

\[
P_n = \sum_p \hbar p E_p^{(n-1)/2} n_p . \tag{7}
\]
For instance, $P_1 = P$ is related to the electrical current, and $P_3$ to the heat current. The Kohler variational principle considers only a limited number $L$ of such functions of the single-particle distribution function. Within this space of functions, the response function is approximated by a ratio of two determinants

$$\chi^{(L)}(\omega) = -\frac{e^2}{3m^2\Omega} \begin{vmatrix} 0 & N_{11} & \ldots & N_{1L} \\ N_{11} & d_{11} & \ldots & d_{1L} \\ \vdots & \vdots & \ddots & \vdots \\ N_{L1} & d_{L1} & \ldots & d_{LL} \end{vmatrix} / \begin{vmatrix} d_{11} & \ldots & d_{1L} \\ \vdots & \ddots & \vdots \\ d_{L1} & \ldots & d_{LL} \end{vmatrix}. \quad (8)$$

$N_{mn} = (1/3)(P_m, P_n)$ and $d_{mn} = (1/3)(P_m; P_n)_{\omega+i0}$ are correlation functions [3] for thermodynamic equilibrium.

The identical expression is obtained within the gLRT if the finite number of moments $P_n$ with $n \leq L$ is taken as the set of relevant observables $\{B_n\}$, see [15, 22, 31, 32]. We conclude that with increasing number of moments, $L \to \infty$, the solution $\chi^{(KT)}(\omega)$ of the KT is reproduced. With a complete set of moments we have

$$\chi^{(KT)}(\omega) = \lim_{L \to \infty} \chi^{(L)}(\omega). \quad (9)$$

Note that the conductivity is increased if more moments are taken into account as a consequence of the variational principle. Convergence issues have been discussed in detail elsewhere, see [28, 33, 34].

To calculate the conductivity, the correlation functions have to be evaluated. The Kubo scalar products can be given analytically for the electron gas as

$$N_{mn} = \frac{1}{3}(P_m, P_n) = N_e \frac{\Gamma((m+n+3)/2) I_{(m+n-1)/2}(\beta \mu_{ei}^d)}{\Gamma(5/2) I_{1/2}(\beta \mu_{ei}^d)}, \quad (10)$$

with $\beta = (k_BT)^{-1}$, the ideal part of the electron chemical potential $\mu_{ei}^d$ and the Fermi integrals $I_\nu(y) = \frac{1}{\Gamma(\nu+1)} \int_0^\infty e^{-t} t^\nu dt$. The correlation functions $d_{mn}$ can be evaluated by perturbation theory using thermodynamic Green’s functions, see [15] and Sec IIIA. From the definition $\hat{P}_n = (i/\hbar)[H, P_n]$ with $H = T + V_{ei} + V_{ee}$, it is evident that $d_{mn}$ is of second order in the interaction (the kinetic energy $T$ commutes with $P_n$). Since the potential energy contains the electron-ion ($V_{ei}$) pseudo potential and the electron-electron ($V_{ee}$) Coulomb interaction, $\hat{P}_n$ entering the correlation function $d_{mn}$ is decomposed in the contributions due to the $e-i$ and the $e-e$ interaction. The evaluation of the correlation functions

$$d_{mn} = d_{mn}^{ei} + d_{mn}^{ee} = -\frac{1}{\hbar} \{ \langle [V_{ei}, P_m]; [V_{ei}, P_n] \rangle_{\omega+i0} + \langle [V_{ee}, P_m]; [V_{ee}, P_n] \rangle_{\omega+i0} \} \quad (11)$$

in Born approximation for the screened Coulomb potential is given for the static case in Sec. IIIA, see [15] for arbitrary $\omega$. It should be mentioned that for the dc conductivity a perturbation expansion is possible starting with a non-diverging term in lowest order, in contrast to the Kubo formula [5]. The contribution of $e-e$ collisions to the electrical conductivity is represented by the term $d_{mn}^{ee}$.

iii) The current operators are taken as relevant observables. This is the level of thermodynamics of irreversible processes where the state of the system is also described by currents. Corresponding generalized forces are introduced which are identified as the response parameters $F_n$. Details of the distribution functions beyond the average of momentum (shifted Fermi or Boltzmann distribution) are formed dynamically. In a first step, we consider the total momentum $P$ as relevant observable since $j(\omega) = eP / (m\Omega)$, which is also the first moment of the single-particle distribution function. The response function ist then derived as

$$\chi_{\text{Ziman}}(0, \omega) = e^2 \frac{(P, P)^2}{3m^2\Omega} - i\omega(P, P) + (P, P)_{\omega+i\eta}. \quad (12)$$

Expressing $(P, P) = 3N_e m$ with the electron number $N_e = Zn\Omega$, we obtain the generalized Drude expression

$$\sigma_{\text{Ziman}}(\omega) = \frac{e_0\omega_{pl}^2}{-i\omega + \nu_{\text{Ziman}}(\omega)} \quad (13)$$

with the plasmon frequency $\omega_{pl} = \sqrt{e^2 Zn / (\epsilon_0 m)}$. The dynamical collision frequency

$$\nu_{\text{Ziman}}(\omega) = (P, P)_{\omega+i\eta}/3N_e m \quad (14)$$
is given in terms of the force-force correlation function. For $\omega = 0$ this expression \cite{12} is known as Ziman-Faber formula. Within a perturbation expansion, the lowest order (Born approximation) is finite. It can be improved if dynamical screening and strong collisions are included.

In the Ziman-Faber formula, the $e-e$ interaction does not contribute because the total momentum of electrons is conserved, $[P, V_{ee}] = 0$. Thus, in the Ziman-Faber formula for the dc conductivity no contribution from $e-e$ collisions is obtained.

Note that for $L = 1$ the force-force correlation function is recovered from the general approach \cite{35}. It represents the first moment approach in KT. Adopting a generalized Drude form also for the solution of the conductivity in KT,

$$\sigma(\omega) = \frac{\epsilon_0\omega^2_{pl}}{-i\omega + \nu(\omega)},$$

we can take this as definition of the dynamical collision frequency $\nu(\omega)$. To relate this full dynamical collision frequency to the dynamical collision frequency in the one-moment approach as a reference value, we can introduce a renormalization function $r(\omega)$,

$$\nu(\omega) = r(\omega)\nu^{\text{Ziman}}(\omega) = r(\omega)\frac{1}{(\mathbf{P}, \mathbf{P})} (\mathbf{P}, \dot{\mathbf{P}})_{\omega + i\eta}.$$  \hspace{1cm} (16)

If the solution for the KT is approximated within a finite number $L$ of moments, also the complex renormalization function $r^{(L)}(\omega)$ is obtained in the corresponding approximation. Using higher order moments $P_n$, Eq. (7), of the distribution function, converging expressions are obtained for the transport coefficients \cite{31, 35}. Taking higher order moments into account, the change of the dynamical conductivity can be represented by a complex function $r^{(L)}(\omega)$ so that, see Refs. \cite{32, 36, 37},

$$\sigma^{(L)}(\omega) = \frac{\epsilon_0\omega^2_{pl}}{-i\omega + r^{(L)}(\omega)\nu^{\text{Ziman}}(\omega)}.$$  \hspace{1cm} (17)

In particular, higher moments are needed in order to take into account $e-e$ collisions. As a special case, the two-moment approach with $P_1, P_3$ as relevant observables (i.e. particle current and energy current) is given in Ref. \cite{15}. The account of these two functions in $p$ space allows for a better variational approach to the single-particle distribution function. The corresponding renormalization function $r^{(2)}$ is given in Sec. IIIA for the static case $\omega = 0$.

\section{C. The Kubo-Greenwood formula: DFT-MD calculations of correlation functions in warm dense matter}

Recent progress in the numerical treatment of many-particle systems allows to calculate correlation functions in WDM by simulation techniques. This gives an alternative to evaluate the Kubo formula but also other relations that express the conductivity in terms of equilibrium correlation functions. In classical systems, MD simulations have been performed for sufficiently large systems using effective two-particle potentials in order to obtain correlation functions that can be compared with analytic results, see \cite{29}. In warm dense matter, it is inevitable to treat quantum effects and strong correlations in the region of degenerate electrons. This can be done, for example, within DFT-MD simulations based on finite-temperature density functional theory (FT-DFT). More explicitly this method uses Kohn-Sham (KS) single-electron states. To treat a disordered system of moving ions in adiabatic approximation, in addition to the general periodic boundary conditions for the macroscopic system, the ion positions are fixed for every time step in a finite supercell ($\text{volume } \Omega_c$) so that the KS potential is periodic with respect to this supercell. We can introduce Bloch states $u_{\mathbf{k}\nu}(\mathbf{r})$ where $\mathbf{k}$ is the wave vector (first Brillouin zone of the supercell) and $\nu$ is the band index \cite{19, 20, 35}. Subsequently, the MD step is performed by moving the ions according to the forces imposed by the electron system using the Hellmann-Feynman theorem. This procedure can be repeatedly performed many thousand times until thermodynamic equilibrium is reached and physical observables such as equation of state data (pressure, internal energy), pair distribution functions, and diffusion coefficients can be extracted. In this way the ion dynamics can be treated properly, allowing to resolve even the collective ion acoustic modes \cite{39, 40}.

Starting point is the Kubo formula \cite{5}. The equilibrium statistical operator $\rho_0$ contains the Kohn-Sham (KS) Hamilton operator $H_{KS}$. Single-electron states are introduced solving the Schrödinger equation for a given ion configuration within the KS approach. The time-dependent operators $\mathbf{P}_n$ within the Heisenberg picture are defined as

$$\mathbf{P}_n(t - i\hbar \tau) = e^{\hat{\mathbf{H}}(t - i\hbar \tau)H_{KS}} \mathbf{P}_n e^{-\hat{\mathbf{H}}(t - i\hbar \tau)H_{KS}}.$$  \hspace{1cm} (18)
The electric current operator reads in second quantization
\[ J_c = \frac{e}{m_e} \sum_{k,k',\nu,\nu'} \langle k\nu | p | k'\nu' \rangle a_{k\nu}^\dagger a_{k'\nu'} . \] (19)

For the single-particle KS Hamiltonian, the averages with the equilibrium statistical operator are evaluated using Wick’s theorem. With
\[ \langle k\nu | p | k'\nu' \rangle = \delta_{k,k'} \left( \frac{2}{\Omega} \int_{\Omega} d^3r \bar{u}_{k\nu}(r) \bar{u}_{k'\nu'}(r) \right), \] (20)
and the broadened \( \delta \) function
\[ \delta_\eta(x) = \frac{1}{\pi} \frac{\eta}{x^2 + \eta^2}, \] (21)
we find for the conductivity
\[ \text{Re} \chi_{\alpha\beta}^{\text{KG}} (\omega) = \frac{2\pi e^2}{3\Omega m_e^2 \omega} \sum_{k,k',\nu,\nu'} \langle k\nu | p | k'\nu' \rangle \cdot \langle k'\nu' | p | k\nu \rangle (f_{k\nu} - f_{k'\nu'}) \delta_\eta (E_{k\nu} - E_{k'\nu'} - \hbar \omega). \] (22)

For instance, extensive DFT-MD simulations have been performed for warm dense hydrogen \[20, 24\] using up to \( N = 512 \) atoms in a supercell (depending on the density) and periodic boundary conditions so that \( N \) discrete bands appear in the electronic structure calculation for the cubic supercell. The relation
\[ \text{Re} \sigma_{\alpha\beta}^{\text{KG}} (\omega) = \frac{2\pi e^2 \hbar^2}{3\Omega m_e^2 \omega} \sum_k W(k) \sum_{\nu'\nu} \sum_\alpha (|\langle \Psi_{k\nu'} | \nabla_\alpha | \Psi_{k\nu} \rangle|^2 (f_{k\nu} - f_{k\nu'}) \delta_\eta (E_{k\nu} - E_{k\nu'} - \hbar \omega) \] (23)
is been evaluated numerically, where \( f_{k\nu} = f(E_{k\nu}) \) describes the occupation of the \( \nu \)th band, which corresponds to the energy \( E_{k\nu} \) and the wave function \( \Psi_{k\nu} \) at \( k \). The \( \delta_\eta \) function has to be broadened because a discrete energy spectrum results from a finite simulation volume. An integration over the Brillouin zone is performed by sampling special \( k \) points, where \( W(k) \) is the respective weighting factor \[18, 24\]. The imaginary part can be calculated using the Kramers-Kronig relation.

This approach solves the electron-ion \((e-i)\) part (strong interaction with the ions) and the strong ion-ion correlations (structure factor) in an adequate way. As shown in App. [3], the broadening of the \( \delta \) function \[21\] is necessary to obtain convergent results. These results are identical to the use of a energy-dependent relaxation time in KT. However, the contribution due to electron-electron \((e-e)\) collisions is missing. The \( e-e \) interaction is considered only in the quasi-particle mean-field potential of the KS Hamiltonian (in particular the density functional). Collisions are obtained going beyond a mean-field description.

The Lorentz gas model has been introduced in plasma physics with a Hamiltonian that contains only the \( e-i \) interaction. The \( e-e \) interactions are neglected, only a homogeneous charged background is considered to compensate the ion charges. In the adiabatic limit where the collisions of the electrons with the ions can be considered as elastic, the linearized Boltzmann equation in KT is solved with the relaxation time ansatz. As shown in App. [3] the evaluation of the Kubo formula given here is equivalent to the relaxation time ansatz where the collision of the electron quasiparticles with the total ion subsystem with given structure factor is considered. The evaluation of the Kubo formula for WDM given here corresponds with calculations for the conductivity in the Lorentz model, with \textit{ab initio} calculations for the \((e-i)\) pseudo-potential interaction and the ion-ion structure factor.

D. Perturbation theory for the dynamic conductivity and convergence

We derived expressions for the conductivity \[6, 8, 9, 12\] that look differently, but can be proven to be identical performing integrations by part, see \[15, 22\]. They have, however, different properties when considering the time behavior of the respective equilibrium correlation functions and systematic perturbation expansions, including quantum statistical Green functions approaches.

Version (i), the Kubo formula and the current-current correlation function. As well-known, in lowest order of perturbation theory, the Lindhard RPA expression for the polarization function is obtained. It gives \( \epsilon(0, \omega) = 1 - \omega^2 / \omega^2 \) so that the dynamical conductivity is purely imaginary for finite frequencies. The dc conductivity diverges for \( \omega \to 0 \).
The same follows also directly from the Kubo formula containing the current-current correlation function, because the momentum of the electrons is conserved in zeroth order of the interaction with the ions and the Laplace transform is diverging for \( \omega \to 0 \). More explicitly we have in lowest order

\[
\chi^\text{Kubo}(\omega) = \frac{e^2 N_e}{m \Omega} \frac{1}{i \omega + \eta}
\]

what diverges for \( \lim_{\eta \to 0} \) at \( \omega = 0 \). Version (i) of the previous subsection is not appropriate to calculate the dc conductivity by perturbation expansion. The use of the Kubo formula \([8]\) to calculate the dc conductivity needs some additional steps like partial summations in perturbation theory or \( \delta \eta \) functions with finite width in the Kubo-Greenwood approach.

Version (iii), the Ziman-Faber formula and the force-force correlation function. If \( \nu(\omega) \) behaves regular for \( \lim \omega \to 0 \) one can also perform the limit \( \omega \to 0 \) in the expression \([15]\). In particular, if a Drude-like behavior \([15]\) is assumed at high frequencies, with a real relaxation time \( \tau = 1/\nu \) not depending on \( \omega \), one can estimate the dc conductivity as extrapolation of the ordinary Drude formula, \( \sigma(0) = n_e e^2 \tau / m \), with \( n_e = Z n \).

The Ziman-Faber formula \([12]\) is sometimes also denoted as second fluctuation-dissipation theorem where the inverse transport coefficients are related to the force-force correlation function. For \( \nu(\omega) \) inverse transport coefficients are related to the force-force correlation function. For \( \omega \to 0 \) in the expression (15). In particular, if a Drude-like behavior (13) is assumed for increasing numbers of moments are included, see \([28, 33]\). Going beyond \( P \) the single-particle distribution function improves the result also for the Born approximation. The solution converges to the Spitzer formula if increasing numbers of moments are included, see \([28, 33]\). Going beyond \( P \) the electron-electron collisions will contribute. Another way to avoid singular expansions is to enlarge the number of relevant observables corresponding to the Kohler variational principle as given by version (ii) \([13]\).

The evaluation of the Kubo-Greenwood formula corresponds to the Lorentz model where the pure \( P \) collisions are rigorously solved similar to the relaxation time ansatz for elastic scattering of electrons by the fixed ion potential (that is a single-particle approach containing \( e - e \) interaction in mean-field approximation, but no \( e - e \) collision terms).

### III. DC CONDUCTIVITY AND \( e - e \) COLLISIONS

#### A. Renormalization function

To show the influence of \( e - e \) collisions on the conductivity we consider in the following the dc conductivity of WDM that depends on the temperature \( T \), the ion density \( n \), and the effective ion charge \( Z \). In the non-degenerate limit, the dynamical conductivity was discussed in \([15]\). We calculate the corrections of the dc conductivity for arbitrary degeneracy that is expressed by a renormalization factor \( r(\omega = 0) \). For this, we have to evaluate the correlation functions \( d_{mn} = d_{mn}^{ei} + d_{mn}^{ee} \) that can be performed by perturbation expansion. In screened Born approximation we have

\[
d_{mn}^{ei} = \pi \beta \hbar Z^2 \sum_{k|p|q} \int_{-\infty}^{\infty} \frac{d \omega}{\epsilon_{RPA}(q, \omega)} \left| \frac{V(q)}{\epsilon_{RPA}(q, \omega)} \right|^2 f_k'(1 - f_{[k+q]}') f_p'(1 - f_{[p-q]}) \\
\times \delta(h\omega - E_{[k+q]}') \delta(h\omega - E_p') (K_n(\vec{k}, \vec{q}) K_m(\vec{k}, \vec{q})), \tag{25}
\]

\[
d_{mn}^{ee} = \frac{\pi \beta \hbar}{2} \sum_{k|p|q} \int_{-\infty}^{\infty} \frac{d \omega}{\epsilon_{RPA}(q, \omega)} \left| \frac{V(q)}{\epsilon_{RPA}(q, \omega)} \right|^2 f_k'(1 - f_{[k+q]}') f_p'(1 - f_{[p-q]}) \\
\times \delta(h\omega - E_{[k+q]}') \delta(h\omega - E_p') (K_n(\vec{k}, \vec{q}) + K_n(\vec{p}, -\vec{q}))(K_m(\vec{k}, \vec{q}) + K_m(\vec{p}, -\vec{q})), \tag{26}
\]
where $E_k^e = h^2k^2/(2m_e)$ and $K_n(k,q) = k/(\beta E_k^e)^{(n-1)/2} - (k + q_e)(\beta E_{k+q}^e)^{(n-1)/2}$. Exchange terms in $d_{mn}^{e,e}$ are small and not given here. The Coulomb interaction $V(q) = e^2/(\epsilon_0\Omega q^2)$ is screened in the static case with $e^{RPA}(q,0) = 1 + \kappa^2/q^2$, where $\kappa^2 = (Z + Z^2)e^2/(\epsilon_0k_BT)$ is related to the Debye screening length, $Z$ is the average charge of the ions, and $Zn$ the electron density.

Whereas the use of the screened Coulomb potential for the $e-e$ interaction is a reasonable approximation leading to a convergent result for the correlation function, the use of a screened Coulomb potential for the interaction of electrons with ions (effective charge $Z$) is only possible in the low-density limit. For WDM at higher densities, the interaction at short distances is of relevance where the Coulomb potential has to be replaced by a pseudo-potential, and the ion contribution to the screening has to be replaced by the ion-ion structure factor. This will modify the result for $d_{mn}^{e}$. In the high density region, but has no significant influence on the renormalization function $r(\omega = 0)$ since in that region $r(\omega = 0) \approx 1$, the corrections due to $e-e$ collisions become small.

The evaluation of the correlation functions $d_{mn}^{e}$ is given in App. C, where also simple interpolation expressions are given. We give results for the dc conductivity within a two-moment approach, using the moments $P_1, P_3$. The limit of non-degenerate electrons is discussed in the following subsection. There also the accuracy of this two-moment approach, considering the electrical and heat current, is discussed.

Using higher order moments $P_n$ of the distribution function, see Eq. [7], converging expressions are obtained for the transport coefficients [31, 35]. In particular, higher moments are needed in order to take into account electron-electron collisions. Taking higher order moments into account, the change of the dynamical conductivity can be represented by a complex function $r(\omega)$ so that $\nu(\omega) = r(\omega)\nu_{RPA}(\omega)$, see Eqs. [13] - [17].

As a special case, the two-moment approach with $P_1, P_3$ as relevant observables (i.e. particle current and energy current) is given in Ref. 15. The account of these two functions in $p$ space allows for a better variational approach to the single-particle distribution function.

An improved calculation is necessary that evaluates the correlation functions occurring in $r(\omega)$ equivalently to $d_{11}$, using pseudopotentials and ion-ion structure factor. Also the $e-e$ contribution will be modified using Kohn-Sham orbitals instead of free electron states. However, in a first step one can use the renormalization factor $r(\omega)$ obtained for the fully ionized plasma that should work in the low-density limit. At high densities, the influence of the renormalization factor is fading ($r(\omega) \rightarrow 1$).

Let us consider the simplest non-trivial approximation that is this two-moment approach with $P_1, P_3$. As shown in [15], we have in the non-degenerate case $(P_1, P_3)/3 = Nm/\beta$, $(P_1, P_3)/3 = (P_3, P_1)/3 = 2Nm/\beta$, and $(P_3, P_1)/3 = 2Nm/\beta$. For the general case, see Eq. [10]. Using Cramer’s rule, the response parameters $F_1, F_2$ are expressed in terms of the electrical field $E$ and correlation functions. For the dynamical conductivity, see [15], we find after algebraic manipulations the expression Eq. [17]. In the static (dc) case we have for the renormalization factor in the two-moment approach

$$r(2)(0) = \frac{\langle \hat{P}_3; \hat{P}_3 \rangle \langle \hat{P}_1; \hat{P}_1 \rangle}{\langle \hat{P}_1; \hat{P}_1 \rangle} + \frac{(P_3, P_3)^2}{(P_3, P_3)^2} \frac{\langle \hat{P}_3; \hat{P}_3 \rangle}{\langle \hat{P}_1; \hat{P}_1 \rangle} - \frac{(P_1, P_3)}{(P_1, P_1)} \frac{\langle \hat{P}_3; \hat{P}_3 \rangle}{\langle \hat{P}_3; \hat{P}_3 \rangle} - \frac{(P_3, P_3)}{(P_3, P_3)} \frac{\langle \hat{P}_3; \hat{P}_3 \rangle}{\langle \hat{P}_1; \hat{P}_1 \rangle}.$$  \tag{27}

These correlation functions contained in expression [27] have to be evaluated on the same level, i.e. the same electron-ion pseudopotentials and the same ion-ion structure factor. In a certain approximation, we can also take the renormalization factor obtained for a Coulomb system.

Evaluation of the correlation functions occurring in the renormalization factor $r(\omega)$ in Born approximation is given for a plasma with singly charged ions in [15]. For the dc case, we derive the results for the two-moment approach in Born approximation $r^{(2, \text{Born})}(0; \Gamma, \Theta, Z)$ in App. C see also Fig. 1.

The introduction of the renormalization factor solves two problems: First, the correct solution is obtained for the Lorentz model corresponding to kinetic theory where the solution with the relaxation time ansatz is possible, and second, the proper inclusion of $e-e$ collisions.

B. Non-degenerate plasma with singly-charged ions

We present results for the fully ionized hydrogen plasma ($Z = 1$) in the low-density limit, see [25, 31, 33, 44]. For the charge-neutral Coulomb system consisting of electrons and singly charged hydrogen ions, we introduce instead of $n_e = n, T$ two dimensionless parameters, the plasma parameter $\Gamma = e^2(4\pi n_e/3)^{1/3}/(4\pi n_e k_BT)$ and the electron degeneracy parameter $\Theta = (2mk_BT/h^2)(3\pi^2n_e)^{-2/3}$; the general definition is given for plasmas with arbitrary $Z$ by using $Z$ and $n_e = Zn$. 
The dc conductivity $\sigma(n, T)$ can also be related to a dimensionless function $\sigma^*(\Gamma, \Theta)$ according to

$$\sigma(n, T) = \frac{(k_B T)^{3/2}(4\pi\epsilon_0)^2}{m^{1/2}e^2} \sigma^*. \quad (28)$$

Using the results of Ref. 15 we obtain the following expansions for collision integrals in the low-density, non-degenerate limit $\Gamma^2 \Theta \gg 1, \Gamma \ll 1$:

$$d_{mn}^{\text{ei}} = d(n/2 + m/2 - 1)! \left( -\ln \sqrt{6\Gamma^3} + A(n + m) - \epsilon_n^{\text{ei},s} \right), \quad (29)$$

$$d_{mn}^{\text{ee}} = d\sqrt{2}b_{nm} \left( -\ln \sqrt{6\Gamma^3} + f_{nm} - \epsilon_n^{\text{ee},s} \right), \quad (30)$$

where $\epsilon_n^{\text{ei},s} = 0.1148$ and $\epsilon_n^{\text{ee},s} = -0.8894$. These coefficients are slightly corrected in comparison earlier evaluations 16. With $d = (4/3)(2\pi)^{1/2}n^2\Omega m^{1/2}3^{1/2}e^4/(4\pi\epsilon_0)^2$ we have 14 $b_{11} = b_{13} = b_{31} = 0$ and $b_{33} = 1$. This shows explicitly that in the lowest order approach $L = 1$, i.e., using only $P_1$ (force-force correlation function in screened Born approximation) the direct contribution of $\epsilon - \epsilon$ collisions vanishes, but appears already in the next order $L = 2$ using $P_1$ and $P_3$. Values for the constants $A, c, f$ are given in Ref. 34. It can be dropped in the low-density limit.

The term $d_{mn}^{\text{ee}}$ is missing in the force-force correlation function approach 12. It can be taken into account by a renormalization factor 15, see below.

Note that already the electron-ion contribution, calculated with relation 5, deviates from the Ziman-Faber formula for finite temperatures where higher moments are of relevance. This is well-known from the Lorentz model where $\epsilon - \epsilon$ collisions are neglected. The relaxation time ansatz gives the correct result for the dc conductivity, known from semiconductor physics as Brooks-Herring formula 47.

The evaluation of the dc conductivity within the two-moment approach (8) yields

$$\sigma^{(2),\text{KT}} = 0.577 L_{\text{Sp}}^{-1}. \quad (31)$$

Kinetic theory for the fully ionized plasma in the high-temperature, low-density limit ($\Gamma \ll 1, \Theta \gg 1$) leads to the Spitzer result 11 $\sigma^{\text{KT}} = 0.591 L_{\text{Sp}}^{-1}$, with the Spitzer Coulomb logarithm $L_{\text{Sp}}^{-1} = \frac{1}{2} \ln(\frac{2}{3}\pi^{-1} \Gamma^{-1})$. The $\epsilon - \epsilon$ collisions are taken into account. We conclude that the two-moment approach is a reasonable approximation to the numerical value given by Spitzer. It can be improved taking higher moments into account 28, 33, 34.

For the Lorentz model of electrons interacting only with the ions by the statically screened Coulomb interaction, the contributions $d_{mn}^{\text{ee}}$ do not occur in kinetic theory 8. Then, the two-moment approach gives

$$\sigma^{(2),\text{Lorentz}} = 0.97 L_{\text{BH}}^{-1} \quad (32)$$

which has to be compared with the exact solution of the Boltzmann equation using the relaxation time ansatz. The low-density conductivity is given in Born approximation by the Brooks-Herring formula 47.

$$\sigma^{\text{KT}} = 2^{5/2}\pi^{-3/2}L_{\text{BH}}^{-1} = 1.016 L_{\text{BH}}^{-1},$$

$$\sigma^{\text{Lorentz}} = \frac{2^{3/2}}{3^{3/2}} \frac{1}{2} \ln(\frac{3}{2}\pi^{-1} \Gamma^{-1} \Theta^2) + C = 0.5772 \ldots$$

is Euler’s constant. The two-moment approach gives a good approximation to the exact value given by Brooks and Herring. It can be improved taking higher moments into account. In particular, the exact result is reproduced if the moment $P_3$ is included in the set of relevant observables.

All these expressions contain a different Coulomb logarithm $L$ that has the identical low-density limit $L^{-1} = -\frac{1}{2} \ln(n) + O(n^0)$, where the contributions $O(n^0)$ are depending on $T$ and are determined by the treatment of screening and strong collisions, see 23, 31, 44. We discuss here only the prefactor of this leading term that is different in both cases. We see that the neglect of $\epsilon - \epsilon$ collisions increases the dc conductivity. It is the main result of the present work to show that the dc conductivity is reduced if the $\epsilon - \epsilon$ collisions are taken into account. In the non-degenerate limit, in the case of the singly charged fully ionized plasma this reduction amounts the value

$$R^{\text{ee},\text{KT}} = \lim_{n_e \to 0} \frac{\sigma^{\text{KT}}}{\sigma^{\text{Lorentz}}} = 0.591 \frac{\pi^{3/2}}{2^{5/2}} = 0.582,$$

to be compared with the result in the two-moment approach $R^{\text{ee},(2),\text{KT}} = 0.594$. This reduction of the dc conductivity is due to the contribution of $\epsilon - \epsilon$ collisions.

For completeness we also discuss the Ziman-Faber formula 8 that arises from evaluating the force-force correlation function in Born approximation,

$$\sigma^{\text{Ziman}} = \frac{3}{4} (2\pi)^{-1/2} L^{-1} L_{\text{Ziman}} = 0.299 L_{\text{Zi}}^{-1}, \quad (34)$$

where $L_{\text{Zi}}$ is the Ziman-Faber logarithm.
with the Ziman Coulomb logarithm

\[ L_{Zi} = \frac{3\pi^{1/2}}{4} \Theta^{3/2} \int_{0}^{\infty} dq \, q^3 f_e(q/2) \left| \frac{V_{ei}(q)}{\epsilon_e(q)} \right| \frac{c_0^2}{e^2} S_{ei}(q). \]  

(35)

We discuss also the prefactor of the leading term of the low-density limit that is different from the previous cases. It is clear that the Ziman formula \([34]\) with the prefactor \(\frac{1}{2}(2\pi)^{-1/2}\) that can be applied for the strongly degenerate electron gas is no longer exact for higher temperatures. As discussed above, the force-force correlation (version iii) in Born approximation cannot reproduce the details of the distribution function. Higher moments of the distribution function have to be included that leads to the solution of the kinetic equation.

The prefactor \(2^{5/2} \pi^{-3/2}\) in the Brooks-Herring formula \([32]\) results from solving a kinetic equation, what can be done in the Lorentz model using the relaxation time ansatz because of missing \(e-e\) collisions. Thus, this result corresponds the evaluation of the conductivity according to version (iii) by taking into account arbitrary numbers of moments. However, the electron-electron interaction cannot be treated within the relaxation time ansatz because the electrons can change the energy when scattering.

The inclusion of \(e-e\) scattering leads to the prefactor 0.591 in the Spitzer formula \([31]\). This result is reproduced from Eq. \([5]\), the convergence with increasing rank \(L\) is shown e.g. in \([28, 31, 33]\). As a special case, the two-moment approach with \(P_1, P_3\) as relevant observables (i.e. particle current and energy current) is given in the following subsection for arbitrary degeneracy, see also Ref. \([15]\). The account of these two functions in \(p\) space allows for a better variational approach to the single-particle distribution function as shown for the low-density, nondegenerate limit in the present section.

IV. RESULTS

A. The correction factor for arbitrary degeneration

After discussing the limit of non-degenerate hydrogen-like plasmas, we give results for arbitrary degeneracy that is relevant for WDM. If arbitrary degeneracy is considered, the influence of \(e-e\) collisions is also changing. If we compare with a calculation \(\sigma^{\text{Lorentz}}\) that takes only \(e-i\) collisions into account, the influence of \(e-e\) collisions leads to a reduction of the conductivity so that

\[ \sigma^{\text{KT}} = \frac{\sigma^{\text{Lorentz}}}{\sigma^{\text{KT}}} = \frac{R^{ee,KT}}{\sigma^{\text{Lorentz}}} \sigma^{\text{KT}}. \]  

(36)

This reduction factor \(R^{(2),ee,KT}\) for the two-moment approach follows from the expressions for the renormalization functions \([27]\), with the expressions given in the App. \([C]\). It depends mainly on the degeneracy of the electron system \(\alpha = \mu/(k_B T)\) and \(Z\), see Fig. 1. The correction factor \(R^{(2),ee,KT}(\alpha)\) introduced in Eq. \((36)\) can be approximated as

\[ R^{(2),ee,KT}(\alpha, Z) = \frac{R^{(2),\text{Lorentz}}(\alpha)}{R^{(2),\text{KT}}(\alpha, Z)} \approx 1 - \frac{1 - 0.594 Z^{0.26}}{e^{0.914(\alpha-1.014 Z^{-0.45})} + 1} \].

(37)

We considered here only the leading terms in the density \(n_e\) (virial expansion) so that only the dependence on \(\alpha\) and \(Z\) appears. Within a more refined calculation, we have to investigate the effects of dynamical screening, ion-ion structure factor, and strong collisions, see Refs. \([31, 32, 34, 44, 46]\). They affect the the \(e-e\) and \(e-i\) correlations in a different way, but can be neglected for the first estimation of the influence of \(e-e\) collisions because the reduction factor isqual to 1 in the high-density case and where these corrections are of significance. At low densities, they contribute only to the higher orders in the virial expansion.

To get this correction factor as function of temperature and density, one has to determine \(\alpha\). In the simplest approximation, the chemical potential of the free electrons, density \(n_e\), follows from

\[ n_e(T, \alpha) = \frac{2}{(\frac{\pi}{2})^3} \int d^3k \frac{1}{e^{E_k/k_B T - \alpha} + 1}. \]  

(38)

The inclusion of further effects such as dynamical screening, ion-ion structure factor, and strong collisions demands further more detailed investigations, but are not of relevance for the correction due to \(e-e\) collisions in the high-density limit where \(\lim_{\alpha \to \infty} R^{ee,KT}(\alpha) = 1\) as well as in the low-density limit where they appear only in higher orders of the virial expansion, so that they may be considered as corrections.

Examplarily, we consider the experimental data for Al plasmas that were analyzed using the Kubo-Greenwood formula by Dejarlais et al. \([18]\), see also \([19]\). The results are shown in Fig. 2.
FIG. 1: Correction factor $R^{(2),ee;KT}(\alpha)$ of the conductivity, calculated without electron-electron collisions ($e - i$ collisions determining the energy-dependent relaxation time), if $e - e$ collisions are included as function of degeneracy $\alpha = \beta\mu$. Comparison with the fit formula [36].

FIG. 2: Variation of the QMD aluminum dc conductivity as function of density for two isotherms: 10 000 K (blue) and 30 000 K (red), see [19]. Calculation results from Ref. [18] are shown in circles; the corresponding data at 10 000 K and 30 000 K from exploding wire experiments [48] are shown in blue (inverted triangle) and red (triangle). Further calculations according to [4] (cross), data from [49] (star). The value $\Theta = 1$ where degeneracy effects appear occurs at 0.3 g/cm$^3$ for $T = 30 000$ K and 0.05 g/cm$^3$ for $T = 10 000$ K. The inclusion of $e - e$ collisions (full line) reduces the values obtained in Ref. [18].
The calculated DFT-MD values for the conductivity (only $e - i$ collisions, Kubo-Greenwood formula) are reduced by a factor of about 0.5 in the low-density, nondegenerate limit. Exemplarily we used the correction factor $R^{(2), ee, KT}(\alpha, Z)$ for $Z = 1$. With increasing electron density, the reduction becomes smaller if the electron system becomes degenerate. In the dense, metallic region, where the electron system is highly degenerate, the influence of $e - e$ collisions on the dc conductivity disappears. As shown in Fig. 2 this reduction of the conductivity due to $e - e$ collisions gives a better agreement between theory and experimental data in the low-density region. It should be mentioned that also other contributions, in particular the collisions with neutral atoms in a partially ionized plasma, will lead to a further correction of the dc conductivity, in particular at low temperatures. A more sophisticated treatment of the correction factor should take into account the concentration of free electrons as given by the ionization degree or the effective ion charge what is the subject of future work. At present we only show the tendency that the conductivity values obtained from the Kubo-Greenwood approach will be reduced if $e - e$ collisions are included.

B. The contribution of $e - e$ collisions

In Ref. [4], the inverse of the transport relaxation time $1/\tau(k)$ has been calculated using the single-center T matrix and the total ion-ion structure factor, both calculated with the quantum HNC approach. Comparison with data for aluminum and gold give good coincidence in the region of a degenerate electron system. Here, Fermi’s golden rule obtained from the Kubo-Greenwood approach will be reduced if $e - e$ collisions are included.

In Ref. [4], there is also a general discussion about the role of $e - e$ interaction for the electrical conductivity. It is trivial that for the one-component electron plasma no resistivity can be observed because the total current is conserved under the $e - e$ interaction. The conclusion that also in the general case of a two-component plasma the $e - e$ interaction cannot contribute to the resistivity arising from the electron current is not stringent. It is not only the indirect influence by screening the electron-ion pseudopotential interaction that arise within a mean-field treatment, but also collisions that are entropy producing. The umklapp processes in crystalline solids [23] is not relevant in a plasma without long-range order. It is correct that the interaction with the ion subsystem is necessary to have any change in the total electron current, but it cannot be concluded that $e - e$ interactions play no part in the static or dynamic conductivity at all.

The Spitzer-Härm result contains the contribution of $e - e$ collisions to the conductivity. This is due to the flexibility of the single-momentum distribution $f_1(k)$ that is sensitive to the contribution of $e - e$ collisions. The same is also obtained introducing moments of the distribution function as done in the variational approach [31, 32]. It is claimed that the Spitzer result is a benchmark for the low-density limit of a classical plasma. The conclusion drawn in [4] that this does not establish the validity of results of the Spitzer-Härm type is not justified. The same holds also for the argument that good agreement between experimental data and calculations neglecting $e - e$ contributions shows that the direct role of $e - e$ interactions, taken for granted in the plasma literature, needs to be seriously reconsidered. It is a particular case of highly degenerate WDM states where the contribution of $e - e$ collisions to the conductivity becomes small, as also seen from the correction factor $R^{ee, KT}(\alpha)$ that approaches the value 1 for $\alpha \rightarrow \infty$.

V. CONCLUSIONS

We conclude that electron-electron collisions have to be included in the low-density, nondegenerate region of warm dense matter. Compared with calculations of the dc conductivity that take into account only $e - i$ collisions, such as the use of the Kubo-Greenwood formula or the relaxation time ansatz, the contribution of the $e - e$ collisions can be represented by a renormalization factor $R^{ee, KT}(\alpha)$ that depends mainly on the degeneration $\alpha = \beta \mu$. Whereas in the case of the strongly degenerate electron gas ($\alpha \rightarrow -\infty$) the contribution of $e - e$ collisions can be neglected (only umklapp processes are of relevance in solids), in the non-degenerate limit $\alpha \rightarrow \infty$ the $e - e$ collisions lead to a reduction of the dc conductivity by a factor of about 0.5.

The generalized linear response theory allows to evaluate the transport coefficients of WDM in a wide region, joining the limits of strong degeneration known from liquid metals and low densities as known from standard plasma physics. The present work considers free electrons interacting with ions having an effective charge $Z$ that changes with temperature $T$ and ion density $n$. Fit formulae given in the Appendix to calculate the influence of $e - e$ collisions on the conductivity allow for a better implementation in codes and other applications.

Future work will concern the composition of WDM in the low-density, low-temperature limit where a chemical model is applicable, the ionization degree and composition are derived from a mass action law. Additional scattering with neutrals will reduce the conductivity at low temperatures.
Appendix A: Generalized linear response theory

In the case of a charged particle system considered here, described by the Hamiltonian $H$, under the influence of an external field, $H_{F}(t)$, the nonequilibrium statistical operator has to be determined. According to Bogoliubov and Zubarev [32, 50–52], one can start with a relevant statistical operator

$$
\rho_{rel}(t) = \frac{1}{Z_{rel}(t)} e^{-\beta(H - \mu N) + \sum F_{n}(t) B_{n}}, \quad Z_{rel}(t) = \text{Tr} \left\{ e^{-\beta(H - \mu N) + \sum F_{n}(t) B_{n}} \right\},
$$  \hspace{1cm} (A1)

as a generalized Gibbs ensemble which is derived from the principle of maximum of the entropy. This relevant distribution is characterized by a set of relevant observables $\{B_{n}\}$ (in addition to $H, N$). The Lagrange parameters $\beta, \mu, F_{n}(t)$, which are real valued numbers, are introduced to fix the given averages

$$
\text{Tr} \{ B_{n} \rho(t) \} = \langle B_{n} \rangle = \text{Tr} \{ B_{n} \rho_{rel}(t) \}.
$$  \hspace{1cm} (A2)

This self-consistency condition means that the observed averages $\langle B_{n} \rangle$ are correctly reproduced by the hermitean $\rho_{rel}(t)$. Similar relations are used in equilibrium to eliminate the Lagrange parameters $\beta$ and $\mu$. Starting with the relevant statistical operator, the stationary non equilibrium state is formed dynamically, and this process converges the faster the more relevant observables $B_{n}$ are included to characterize the initial state. The selection of the set of relevant observables has no influence on the result if the calculations are performed rigorously, but will influence the result if approximations such as perturbation expansions are performed.

In linear response, the response parameters $F_{n}(t)$ are considered to be small so that we can solve the implicit relation \[ \rho_{rel}(t) \]. The response parameter are determined after expanding up to the first order with respect to the external field $E^{\text{ext}}(0, \omega)$ and the response parameters $F_{n}$, where $F_{n}(t) = \text{Re}\{F_{n}e^{-i\omega t}\}$. We arrive at the response equations \[ [15] \]

$$
\sum_{m} \left\{ \langle B_{n}; \dot{B}_{m} \rangle + \langle \dot{B}_{n}; B_{m} \rangle \right\} z - i\omega \left\{ \langle B_{n}; B_{m} \rangle + \langle \dot{B}_{n}; \delta B_{m} \rangle \right\} z = F_{m} = \beta \frac{e}{m} \left\{ \langle B_{n}; \vec{P} \rangle + \langle \dot{B}_{n}; \vec{P} \rangle \right\} \cdot E^{\text{ext}}(0, \omega),
$$  \hspace{1cm} (A3)

with $z = \omega + i\eta$ ($\lim_{\eta \to +0}$), the total momentum of electrons $\vec{P} = \sum_{p} \hbar \vec{p} n_{p}$, and the Laplace transform of the correlation functions, Eq. [7].

Considering $N_{B}$ relevant observables $B_{n}$, Eq. (A3) is a system of $N_{B}$ linear equations to determine the response parameters $F_{n}$ for a given external field $E^{\text{ext}}(0, \omega)$. It is the most general form of LRT, allowing for arbitrary choice of relevant observables $B_{n}$ and corresponding response parameters $F_{n}$. Comparing with kinetic theory [15], the first term on the left hand side can be identified as a collision term, while the right hand side represents the drift term due to the external perturbing field.

The set of relevant observables $B_{n}$ to characterize the non-equilibrium state can be chosen arbitrarily, and the result calculating non-equilibrium properties is independent on this choice if no approximations like perturbation expansions are performed. At least, the set of relevant observables $B_{n}$ should contain conserved quantities that determine the equilibrium state. It should also contain long-living fluctuations in the system that are hardly produced by the dynamical evolution (such as bound state formation) so that a perturbation expansion is not quickly converging. Different expressions and results can be understood as approximations, working in a Markov approximation and describing the system on different level of sophisticated. Results that are obtained in lowest order are improved summing up (sometimes divergent) terms that occur in higher order perturbative expansions. Alternatively, we can suggest the different choices of the set of relevant observables $B_{n}$ like a variational approach (Kohler variational principle), see [15].

Starting with the occupation numbers $n_{p}$ of the single-particle states $|p\rangle$ as set of relevant observables $B_{n}$, we arrive at the generalized linear Boltzmann equations \[ [15] \] \hspace{1cm} (A4)

$$
\sum_{p'} \left\{ \langle \delta n_{p'} \rangle + \langle \dot{n}_{p'} \rangle \right\} z - i\omega \left\{ \langle \delta n_{p}, \delta n_{p'} \rangle + \langle \dot{n}_{p}, \delta n_{p'} \rangle \right\} z = \frac{\hbar}{m} \beta \sum_{p''} \left\{ \langle \delta n_{p}, n_{p''} \rangle + \langle \dot{n}_{p}, n_{p''} \rangle \right\} z \cdot E^{\text{ext}}(0, \omega).
$$

The time derivative of the position operator in $H_{\text{ext}}^{t}$ leads to the total momentum $\sum_{i} \hbar \vec{p}_{i} = m \sum_{i} \vec{r}_{i}$ and subsequently to the right hand side of Eq. (A4).
Appendix B: Broadening of the $\delta$-function

Another topic is the broadening of the $\delta$-function to make the transition to $\omega \rightarrow 0$ smooth. In the calculations \cite{19}, for the use of Eq. (23) it was pointed out: "In practice, because of the finite simulation volume and resulting discrete eigenvalues, the $\delta$-function must be broadened. We use a Gaussian broadening of the $\delta$-function that is as small as feasible without recovering the local oscillations in the optical conductivity resulting from the discrete band structure".

To discuss the result \cite{23}, we consider a finite value for $\eta$,

$$\delta_\eta(z) = \frac{\eta}{\eta^2 + z^2}. \quad (B1)$$

The finite width of the $\delta$ functions can be interpreted as an additional damping to overcome the level spacing. The finite value of $\eta$ that should go to zero only after the other expansions have been performed. This corresponds to the van Hove limit ($V^2/\eta \rightarrow 0$), see \cite{32}. Then, one can expand with respect to the collision frequency.

With the perturbation expansion

$$\langle k_1|p|k_2 \rangle = k_1\delta_{k_1,k_2} + \frac{\langle k_1|V|k_2 \rangle}{E_1 - E_2}(k_1 - k_2) \quad (B2)$$

we have with $k_2 = k_1 + q$ and $\langle k_1|V|k_2 \rangle = V_q$

$$\text{Re} \chi_{KG}(0) = \frac{\pi e^2 \hbar \beta}{3m^2 \Omega} \sum_{k,q} \frac{\partial f(E_k)}{\partial E_k} \left( k_0, \frac{V_q}{E_k - E_{k+q}}q + \ldots \right)^2 \frac{\eta}{\eta^2 + (E_k - E_{k+q})^2}. \quad (B3)$$

In the nondegenerate case and taking the screened interaction with uncorrelated ion, $V_q^2 = N \tilde{Z}^2 e^4/|\epsilon_0 \Omega |(q^2 + \kappa^2)^2$, a term

$$\text{Re} \chi_{KG}(0) = \frac{\pi e^2 \hbar \beta}{3m^2} \int \frac{d^3 k}{(2\pi)^3} f(E_k) \left( k_0 \frac{1}{\eta} + \int \frac{d^3 q}{(2\pi)^3} \frac{n \tilde{Z}^2 e^4}{|\epsilon_0(q^2 + \kappa^2)|^2(E_k - E_{k+q})^2 \eta} \frac{\eta}{\eta^2 + (E_k - E_{k+q})^2} + \ldots \right). \quad (B4)$$

Before the last term is interpreted as a delta function, we estimate the denominator $E_k - E_{k+q}$ by the broadening parameter $\eta$ of the $\delta_\eta$ function so that

$$\text{Re} \chi_{KG}(0) = \frac{\pi e^2 \hbar \beta}{3m^2} \int \frac{d^3 k}{(2\pi)^3} f(E_k) k^2 \tau_{KG}(k) + \ldots \quad (B5)$$

with

\[
\tau_{KG}(k) = \frac{1}{\eta} + \frac{1}{k^2} \int \frac{d^3 q}{(2\pi)^3} \frac{n \tilde{Z}^2 e^4}{|\epsilon_0(q^2 + \kappa^2)|^2(E_k - E_{k+q})^2} \frac{q^4}{\eta} \frac{\eta}{\eta^2 + (E_k - E_{k+q})^2} + \ldots
\]

\[
= \frac{1}{\eta} + \frac{1}{k^2} \frac{n \tilde{Z}^2 e^4}{\epsilon_0^2 \hbar^2} \int_0^\infty dq \frac{q^4}{(2\pi)^2 (q^2 + \kappa^2)} \left( \frac{m}{\hbar^2 k^2} \right)^3 \int_1^1 dz \frac{\eta m/|kq|}{(z + q/2)^2 + \pi^2} \frac{1}{z + q/2^2}
\]

\[
= \frac{1}{\eta} + \frac{1}{k^2} \frac{n \tilde{Z}^2 e^4}{\epsilon_0^2 \hbar^2} \int_0^\infty dq \frac{q^4}{(2\pi)^2 (q^2 + \kappa^2)} \left( \frac{m}{\hbar^2 k^2} \right)^3 \frac{h^2 k q}{\eta m} \left( \frac{1}{1 - (q/2k)^2} + \pi \frac{h^2 k q}{\eta m} \right)^2
\]

\[
= \frac{1}{\eta} + \frac{1}{\eta^2} \frac{n \tilde{Z}^2 e^4 m \pi}{\epsilon_0^2 \hbar^2} \int_0^{2k} dq \frac{q^3}{(2\pi)^2 (q^2 + \kappa^2)} + O \left( \frac{e^4}{\eta} \right). \quad (B6)
\]

In principle, one has to sum the leading divergent terms $\propto (1/\eta) (e^4/\eta)^n$. We give here only the first contributions,

$$\frac{1}{\eta} + \frac{1}{\eta^2} A + \ldots = \frac{1}{\eta} \left[ 1 + \frac{1}{\eta} A + \ldots \right] = \frac{1}{\eta} \left[ 1 - \frac{1}{\eta} A + \ldots \right]. \quad (B7)$$

Now the limit $\eta \rightarrow 0$ can be performed with the result $-1/A$.

For comparison, see \cite{15}, with the golden rule for the transition rates and $S(q) \approx 1$, $|V_{ci}(q)|^2 \approx N \tilde{Z}^2 V^2(q)$, the energy dependent relaxation time can be calculated

$$\frac{1}{\tau_k} = -\frac{2\pi^2}{\hbar} \sum_q N \tilde{Z}^2 V^2(q) \delta(E_k - E_{k+q}) \frac{|E \cdot q|}{|E \cdot k|}. \quad (B8)$$
The dynamically screened Coulomb potential will be replaced by the static Debye potential. The effect of dynamical
plane. It is convergent only in the case of a screened Coulomb potential. Using the statically screened Debye potential
in addition to the single-electron Hamiltonian considered. Thus, electron-electron interaction has to be included, not on the level of the total force that vanishes where the semiconductor conductivity for the screened electron-hole interaction is considered. It is also possible for the ion configuration.

We introduce the average relaxation time $\tau_{Lorentz}$ and the static collision frequency $\nu_{Lorentz} = 1/\tau_{Lorentz}$. The approach can also be applied for a pseudopotential describing the $e-i$ interaction and an ion structure factor describing the ion configuration.

The Lorentz model is solved if using the relaxation time ansatz. It corresponds to the Brooks-Herring result where the semiconductor conductivity for the screened electron-hole interaction is considered. It is also possible for interacting electrons? However, secular divergent terms related to $e-i$ interactions arise if higher moments are considered. Thus, electron-electron interaction has to be included, not on the level of the total force that vanishes because of momentum conservation, but in higher orders. We have to calculate the correlation functions that arise if, in addition to the single-electron Hamiltonian $H_{KS}$ that defines the basis set of single-electron states in the statically screened potential of ions, also the $e-i$ interaction is considered.

Appendix C: Evaluation of the correlation functions and renormalization factor for degenerated warm dense matter

We evaluate Eq. (26) in the lowest non-vanishing order, with the electron Fermi functions. Because of total momentum conservation, $d^{ee}_{11} = d^{ee}_{13} = 0$, and

$$d^{ee}_{33} = \frac{\pi \beta \hbar}{2} \int \frac{d^3 q}{2 \pi} \int \frac{d^3 q}{2 \pi} \int \frac{d^3 k}{2 \pi} \left| \frac{\hbar}{\epsilon_0 q^2 / (q^2 + \kappa^2)} \right|^2 f^e(E_k)(1 - f^e(E_k + \hbar \omega)) f^e(E_p)(1 - f^e(E_p - \hbar \omega)) \times \delta(\hbar \omega - E^e_{k+q} + E^e_k) \delta(\hbar \omega - E^e_{p} + E^e_{p-\vec{q}}) [k_z \beta E_k - (k_z + q_z)(\beta E_k + \beta \hbar \omega) + p_z \beta E_p - (p_z - q_z)(\beta E_p - \beta \hbar \omega)]^2. \tag{C1}$$

The dynamically screened Coulomb potential will be replaced by the static Debye potential. The effect of dynamical screening that leads to the Lenard-Balescu expression for the conductivity has been discussed elsewhere. For the evaluation, we introduce spherical coordinates with $q = q(0, 0, 1), k = k(\sin \theta_k \cos \phi_k, \sin \theta_k \sin \phi_k, \cos \theta_k), p = p(\sin \theta_p \cos \phi_p, \sin \theta_p \sin \phi_p, \cos \theta_p)$, so that with $\kappa^2 = (Z^2 + Z^2)\epsilon^2/(\epsilon_0 k_BT)$ and $a_z = (a_x^2 + a_y^2 + a_z^2)/3 = a_z/3$ in isotropic expressions

$$d^{ee}_{33} = \frac{\pi \beta \hbar \Omega^3}{2 \times 3(2\pi)^3} \int d^3 q \int \frac{d^3 q}{2 \pi} \int \frac{d^3 k}{2 \pi} \left| \frac{e^2}{\epsilon_0 q^2 / (q^2 + \kappa^2)} \right|^2 f^e(E_k)(1 - f^e(E_k + \hbar \omega)) f^e(E_p)(1 - f^e(E_p - \hbar \omega)) \times \delta(\hbar \omega - \hbar^2 kq \cos \theta_k \cos \theta_p - \hbar^2 q^2 / m) \delta(\hbar \omega - \hbar^2 pq \cos \theta_p - \hbar^2 q^2 / m) \times \beta^2 \left[ q^2 (E_p - E_k)^2 + 2q \cdot (p - k - 2q)(E_p - E_k)\hbar \omega + (p - k - 2q)^2 \hbar^2 \omega^2 \right]. \tag{C2}$$

The square brackets are in spherical coordinates

$$\left[ \frac{\hbar^4}{2^4 m^2} q^2 (p^2 - k^2)^2 + \frac{\hbar^2}{2m} (pq \cos \theta_p - qk \cos \theta_k - 2q^2)(p^2 - k^2) \hbar \omega \right. \tag{C3}$$

$$\left. + (p^2 + k^2 - 4q^2 - 4pq \cos \theta_p + 4kq \cos \theta_k - 2pk(\cos \theta_p \cos \theta_k + \sin \theta_p \sin \theta_k)(\cos \phi_p \cos \phi_k + \sin \phi_p \sin \phi_k)) \hbar^2 \omega^2 \right]$$
The last parentheses can be rewritten as \( \cos \phi_p \cos \phi_k + \sin \phi_p \sin \phi_k = \cos(\phi_p - \phi_k) \). \( \phi_p - \phi_k \) can be introduced as new variable, the integral vanishes. We have now

\[
d_{33}^{ee} = \frac{\pi^3 \hbar e^4 \Omega}{6 \sqrt{(2\pi)^9 \beta^3 2 \hbar^4}} \int_0^\infty dq \int_0^\infty dh\omega \int_0^\infty dk \int_{-1}^1 dz_k \int_0^\infty dp \int_{-1}^1 dz_p \frac{1}{(q^2 + \kappa^2/2)^2} f^*(E_k)(1 - f^*(E_k + \hbar \omega)) f^*(E_p)(1 - f^*(E_p - \hbar \omega)) \frac{1}{kq} \delta(z_k + \frac{q_2}{2k}) \frac{m\omega}{hkq} \delta(z_p - \frac{q}{2p} - \frac{m\omega}{hpq}) \times \left[q^2 \frac{\hbar^4}{4m^2} (p^2 - k^2)^2 + 2(qp z_p - qk z_k - 2q^2) \frac{\hbar^2}{2m} (p^2 - k^2) \hbar \omega + (p^2 + k^2 + 4q^2 - 4pq z_p + 4kq z_k - 2pk z_p z_k) \hbar^2 \omega^2 \right].
\]

Introducing dimensionless variables \( q = Q/\sqrt{2mk_B T}/\hbar, k = x/\sqrt{2mk_B T}/\hbar, p = y/\sqrt{2mk_B T}/\hbar, \omega = \nu Q/(\beta \hbar) \), and performing the integrals over \( z_p, z_k \), we have with \( \alpha = \beta \mu \)

\[
d_{33}^{ee} = \frac{4 \pi e^4 \Omega m^{7/2}}{3 \sqrt{2\pi}^6 \beta^3 \hbar^6} \int_0^\infty dQ \frac{Q^3}{(Q^2 + \hbar^2 \beta \kappa^2/2m)^2} \int_{-\infty}^\infty d\nu \int_{-\infty}^\infty d\bar{\nu} \int_0^\infty dx \int_{-\infty}^\infty dy \int_0^\infty \frac{1}{e^{2 - \alpha} + 1 + e^{-2 - \nu Q/\alpha} e^{2 - \alpha} + 1 + e^{y^2 - \nu Q + \alpha}} \times \left[(y^2 - x^2)^2 - 2(y^2 - x^2)\nu Q + 2(y^2 + x^2)\nu^2 - 4(\frac{\nu^2}{2} - \frac{Q^2}{8})\nu^2 \right].
\]

Now we transform \( x^2 = \hat{x} + \nu^2/2 - \nu Q/2 + Q^2/8 \), \( y^2 = \hat{y} + \nu^2/2 + \nu Q/2 + Q^2/8 \)

\[
d_{33}^{ee, \text{clas}} = \frac{\pi e^4 \Omega m^{7/2}}{3 \sqrt{2\pi}^6 \beta^3 \hbar^6} \int_0^\infty dQ \frac{Q^3 e^{-Q^2/4\epsilon^2\alpha}}{(Q^2 + \hbar^2 \beta \kappa^2/2m)^2} \int_{-\infty}^\infty d\nu \int_{-\infty}^\infty d\bar{\nu} \int_0^\infty dx \int_{-\infty}^\infty dy \frac{1}{e^{\hat{x} + \nu^2/2 - \nu Q/2} + e^{\alpha - Q^2/8} 1 + e^{-\hat{x} - \nu^2/2 - \nu Q/2 + \alpha - Q^2/8} e^{\hat{y} + \nu^2/2 + \nu Q/2 + e^{\alpha - Q^2/8} 1 + e^{-\hat{y} - \nu^2/2 + \nu Q/2 + \alpha - Q^2/8}} \times \left[(\hat{y} - \hat{x})^2 + 2\nu^2(\hat{y} + \hat{x}) \right].
\]

In the non-degenerate case, the four Fermi distribution functions are replace by \( e^{-\nu^2 + 2\alpha} \), and the integral is evaluated as

\[
d_{33}^{ee, \text{clas}} = d\sqrt{2} \int_0^\infty dQ \frac{Q^3}{(Q^2 + \hbar^2 \beta \kappa^2/2m)^2} e^{-Q^2/4\epsilon^2\alpha}.
\]

In Eq. \( \text{(C6)} \) the dependence of the last integrand on \( Q \) is weak. For instance, the expansion with respect to \( Q \) gives \( 0.47682 + 0.009719 Q^2 + \ldots \) at \( \alpha = 0 \). Neglecting the dependence on \( Q \) in the last integrand, the ratio is approximated in the following way:

\[
d_{33}^{ee}/d_{33}^{ee, \text{clas}} = \frac{1}{2\sqrt{\pi}} \int_0^\infty dx \int_{-\infty}^\infty d\hat{x} \int_{-\infty}^\infty d\hat{y} \frac{1}{e^{\hat{x} + \nu^2/2 + \alpha} 1 + e^{-\hat{x} - \nu^2/2 + \alpha} e^{\hat{y} + \nu^2/2 + \alpha} 1 + e^{-\hat{y} - \nu^2/2 + \alpha}} \times [(\hat{y} - \hat{x})^2 + 2\nu^2(\hat{y} + \hat{x})] \approx \frac{1}{e^{1.05886(\alpha + 0.092698) + 0.02956(\alpha + 0.092698)^2 + 0.005151(\alpha + 0.092698)^3 + 1}}.
\]

see Fig. \( \text{[3]} \) A simple fit is given by the expression \( 1/[e^\alpha + 1] \).

The ratio \( d_{33}^{ee}/d_{33}^{ee, \text{clas}} \) depends mainly on \( \alpha \). (The screening parameter gives an additional dependence on \( T, n, \)) Also the other contributions in Eq. \( \text{(C7)} \) depend mainly on \( \alpha \), the interaction cancels approximately if considering the Born approximation.

The evaluation of the \( \epsilon - i \) contributions is much easier. Within the two-moment approach, we have the expressions

\[
\frac{(P_1, P_3)}{(P_1, P_1)} = \frac{5}{2} \frac{I_{3/2}(\alpha)}{I_{1/2}(\alpha)}
\]
FIG. 3: Dependence of the ratio with full degeneration $d_{ee}^{\alpha}/d^{1}$ on $\alpha = \beta \mu$. Numerical data compared with the fit formula \[(C8)\] and the simple fit $1/[e^{\alpha} + 1]$.

In leading order of the virial expansion (term $\propto \ln n$), the correlation functions give the following ratios

\[\frac{\langle \hat{P}_1; \hat{P}_3 \rangle_{ie}}{\langle \hat{P}_1; \hat{P}_1 \rangle_{ie}} = I_0(\alpha)(1 + e^{-\alpha}),\] (C10)

from the $e - i$ interaction

\[\frac{\langle \hat{P}_3; \hat{P}_3 \rangle^{ei}_{ie}}{\langle \hat{P}_1; \hat{P}_1 \rangle^{ei}_{ie}} = 2I_1(\alpha)(1 + e^{-\alpha}),\] (C11)

and from the $e - e$ interaction

\[\frac{\langle \hat{P}_3; \hat{P}_3 \rangle^{ee}_{ie}}{\langle \hat{P}_1; \hat{P}_1 \rangle^{ee}_{ie}} = \frac{1}{Z} \sqrt{d_{ee,cl}^{33}} (e^{\alpha} + 1).\] (C12)

The result for the renormalization function is approximated by the following fit formula ($Z = 1$) that relates the kinetic theory to the result given by the Ziman-Faber formula. According to Eq. (17) we have for the conductivity in the kinetic theory the renormalization function

\[\frac{1}{\rho^{(2),KT}(\alpha)} = 1 + \frac{0.93198}{\exp(0.65(\alpha - 2.218) - 0.04(\alpha - 2.218)^2 + 0.001(\alpha - 2.218)^3) + 1},\] (C13)

where (2) denotes the two-moment approach.

For comparison the renormalization factor for a Lorentz plasma, neglecting $e - e$ collisions, is calculated. The corresponding fit is

\[\frac{1}{\rho^{(2),Lorentz}(\alpha)} = 1 + \frac{2.25}{\exp(0.65(\alpha - 0.962) - 0.04(\alpha - 0.962)^2 + 0.001(\alpha - 0.962)^3) + 1}.\] (C14)

[1] J. L. Spitzer, and R. Härm, Phys. Rev 89, 977 (1953).
