

Interpolation formula for the electrical conductivity of nonideal plasmas

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On the basis of a quantum-statistical approach to the electrical conductivity of nonideal plasmas we derive analytical results in the classical low-density regime, in the degenerate Born limit, and for the contribution of the Debye-Onsager relaxation effect. These explicit results are used to construct an improved interpolation formula of the electrical conductivity valid in a wide range of temperature and density which allows to compare with available experimental data of nonideal plasmas.

1 Introduction

Optical and transport properties of plasmas are governed by the mutual Coulomb interaction and depend strongly on temperature and the electron and ion density. Experimental efforts for the measurement of the electrical conductivity up to high densities revealed the importance of collective excitations and many-body effects such as Pauli blocking, dynamic screening and self-energy, structure factor, the Debye-Onsager relaxation effect, formation of bound states etc. [1]. Although different methods have been proposed for the evaluation of plasma transport properties [2, 3, 4, 5, 6], it still remains a theoretical challenge to treat these effects by a unified quantum-statistical approach.

On the other hand, in addition to highly sophisticated approaches to the conductivity accounting for quantum statistical many-particle effects, for practical use interpolation formulas are of interest which are applicable in a large region of plasma parameter values. Such interpolation formulas were developed by several authors [2, 3, 4, 5] in order to evaluate complex physical situations, e.g., in hydrodynamical simulations for the generation and expansion of plasmas produced by high-power lasers, energetic heavy ion beams or magnetic compression (pinches). Based on rigorous results for special limiting cases and possibly numerical simulations in the intermediate regions, Padé-type interpolation formulas have been proven to be highly effective to describe thermodynamic as well as transport properties.

In this paper we consider a fully ionized plasma consisting of electrons (mass m_e) and singly charged ions (mass M), interacting via the Coulomb potential, at density $n_e = n_i = n$ and temperature T (hydrogen plasma). The dimensionless parameters

$$\Gamma = \frac{e^2}{4\pi\epsilon_0 k_B T} \left(\frac{4\pi n}{3} \right)^{1/3}, \quad \Theta = \frac{2m_e k_B T}{\hbar^2} (3\pi^2 n)^{-2/3}, \quad (1)$$

describe the ratio between the mean potential energy and the kinetic energy (Γ) and denote the degree of degeneracy of the electron gas (Θ). Usually, plasmas are classified into ideal ($\Gamma \ll 1$) and nonideal ($\Gamma \geq 1$) as well as degenerate ($\Theta \ll 1$) and nondegenerate ($\Theta \gg 1$) systems.

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Using these dimensionless plasma parameters, the construction of interpolation formulas for the dc conductivity has been performed in different works. Ichimaru and Tanaka [2] considered a two-component plasma at finite temperatures within a generalized Ziman formula by taking into account dynamic local field effects in the dielectric function and the dynamic ion-ion structure factor. The collision integrals were evaluated in Born approximation to study a strongly coupled and degenerate plasma with $\Gamma \geq 1$ and $\Theta \leq 1$. The correct nondegenerate limit was incorporated in a semiempirical way by adopting a prefactor in correspondence to the well-known Spitzer formula.

Ebeling *et al.* [3] and Lee and More [4] used the relaxation time approximation for the evaluation of the collision integrals both in the low-density (nondegenerate) and high-density (degenerate) regime. Electron-electron interactions are neglected in that approximation which is only justified in the degenerate case because of Pauli blocking. The consideration of electron-electron scattering is, however, decisive to obtain the right low-density result, the prefactor of the Spitzer formula. This has been modeled using a semiempirical ansatz. Furthermore, Rinker [5] has derived an interpolation formula for the electrical conductivity from an improved Ziman formula which are applicable in the strongly coupled, degenerate domain.

Within a quantum statistical approach, the transport properties within the generalized linear response theory of Zubarev have been evaluated [7] and rigorous analytical results for the electrical conductivity have been derived which are valid in the low-density (nondegenerate) and high-density (degenerate) limit [7, 8, 9]. The influence of non-equilibrium two-particle correlations in lowest order (Debye-Onsager effect) has been reconsidered recently [10]. Based on these results and taking into account other approaches, we will construct an improved interpolation formula for the electrical conductivity to cover a wide range of temperatures and densities.

2 Electrical conductivity

Using the plasma parameters (1), we can express the electrical conductivity as

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

with a universal function $\sigma^*(\Gamma, \Theta)$ depending on the characteristic plasma parameters exclusively.

Our quantum-statistical approach to the electrical conductivity is based on a generalized Boltzmann equation which is derived from linear response theory [7]. A finite-moment approximation of single and two-particle distribution functions defines the set of relevant observables B_n , and the electrical conductivity is obtained from the ratio

$$\sigma = -\frac{\beta}{\Omega} \frac{1}{|D[B_{n'}; B_n]|} \begin{vmatrix} 0 & N[B_n] \\ Q[B_n] & D[B_{n'}; B_n] \end{vmatrix}. \quad (3)$$

The determinants contain equilibrium correlation functions defined by

$$\begin{aligned} N[B_n] &= (\dot{R}; B_n), \\ Q[B_n] &= (\dot{R}; B_n) + \langle \dot{R}; \dot{B}_n \rangle, \\ D[B_{n'}; B_n] &= (B_{n'}; \dot{B}_n) + \langle \dot{B}_{n'}; \dot{B}_n \rangle, \end{aligned} \quad (4)$$

which are given by Kubo's scalar product between two operators:

$$\begin{aligned} (A; B) &= \frac{1}{\beta} \int_0^\beta d\tau \operatorname{Tr}[\rho_0 A(-i\hbar\tau) B], \\ \langle A(\epsilon); B \rangle &= \lim_{\epsilon \rightarrow 0} \int_{-\infty}^0 dt e^{\epsilon t} (A(t); B). \end{aligned} \quad (5)$$

The two-particle center of mass momentum is defined via $P = -em_e M / (m_e + M) \dot{R}$. Ω is the system volume and $\beta = 1/k_B T$. Furthermore, the time-dependence of the relevant observables B_n and of the equilibrium statistical operator ρ_0 is given by the standard system Hamiltonian of a fully ionized plasma, see Ref. [7]. The

correlation functions $D[B_{n'}; B_n]$ are related to thermodynamic Green functions. Thus, efficient diagram techniques provide a systematic treatment of many-particle effects in a strongly coupled plasma which has been demonstrated for the single and two-particle level, see Refs. [7, 10].

As the relevant observables on the single-particle level are treated the moments of the electron distribution (adiabatic approximation)

$$P_m = \sum_k \hbar k_z \left(\frac{\beta \hbar^2 k^2}{2m_e} \right)^m a_e^\dagger(k) a_e(k), \quad (6)$$

including the total electron momentum (P_0) and the ideal energy current (P_1). A systematic increase in the number of moments results in a converging expression of the conductivity as it is known from the Kohler variational principle or the Grad and Chapman-Enskog method of kinetic theory.

The correlation functions $D[P_n, P_m]$ are given by a sum of ladder diagrams in the low-density limit. Both the electron-electron and the electron-ion scattering processes are included, see Ref. [8]. The scattering integrals have been evaluated in various approximations which are appropriate for a given density and temperature range.

(i) The correlation functions in the classical limit ($\Gamma^2\Theta \gg 1$) are related to Boltzmann collision integrals which are given by transport cross sections. These quantities are treated in the quasi-classical approximation as relevant for low-energy particles. Additional quantum corrections are found from a WKB expansion of the collision integrals. Using a three-moment approximation for the one-particle distribution function [11] we find for $\Gamma^2\Theta \gg 1$

$$\sigma^*(\Gamma^2\Theta \gg 1) = 2a \left(\ln \Gamma^{-3} + 0.2943 - \frac{0.523}{\Gamma^2\Theta} - \frac{0.259}{\Gamma^4\Theta^2} \right)^{-1}. \quad (7)$$

The prefactor $a = 0.591$ is the limiting value of the moment expansion and coincides with the Spitzer result [12].

(ii) Born limit ($\Gamma^2\Theta \ll 1$): The correlation functions are equivalent to the Lenard-Balescu collision integral if the random phase approximation (RPA) is considered for the dielectric function $\epsilon_{\text{RPA}}(q, \omega)$. The following low-density limit is obtained for $\Gamma^2\Theta \ll 1$ [13]:

$$\sigma^*(\Gamma^2\Theta \ll 1) = 2a \left(\ln \frac{\Theta}{\Gamma} + 0.4807 \right)^{-1}. \quad (8)$$

(iii) The correlation functions in the high-density (liquid-like) limit are given by Landau collision integrals which treats the electron-ion scattering in Born approximation. Thus, the corresponding electron-ion contribution is

$$D[P_n; P_m] = \frac{\Omega^2 m_e^2 N_i^2}{12\pi^3 \hbar^3} \int_0^\infty dk \left(-\frac{df_e(k)}{dk} \right) \left(\frac{\beta \hbar^2 k^2}{2m_e} \right)^{m+n} \int_0^{2k} dq q^3 S_{ii}(q) \left| \frac{V_{ei}(q)}{\epsilon(q)} \right|^2. \quad (9)$$

The number of required moments P_m reduces with increasing density; the Ziman-Faber formula is already obtained from Eq. (9) with the lowest moment P_0 . It includes the static ionic structure factor $S_{ii}(q)$, the electron-ion pseudopotential $V_{ei}(q)$, and the static dielectric function of the electrons $\epsilon(q)$.

The consideration of two-particle correlations described by respective moments

$$\delta n_{cd}^{m,m'}(q) = \sum_{k,p} f_{c,d}^{m,m'}(\mathbf{k}, \mathbf{p}, \mathbf{q}) a_c^\dagger(k - \frac{q}{2}) a_d^\dagger(p + \frac{q}{2}) a_d(p - \frac{q}{2}) a_c(k + \frac{q}{2}) \quad (10)$$

leads to a decreased plasma conductivity. Spatial symmetry properties of the two-particle distribution function in the case of an applied electric field restricts the moments to the electron-ion contribution $\delta n_{ei}^{m,m'}(q)$ [10]. The evaluation of the first moment $f_{ei}^{0,0} = 1$ in the low-density regime gives the original Onsager result of the Debye-Onsager relaxation effect [7, 10]. This effect decreases the conductivity due to an incomplete formation of the screening cloud and was first considered in the theory of electrolytes [14]. An equivalent formulation is the hydrodynamic approximation in kinetic theory and assumes a local equilibrium for the distribution functions [15]. As this assumption already fails to describe the single-particle properties (Spitzer formula) properly also higher two-particle moments have been considered in Ref. [10]. Corrections to the Onsager result were indeed

found for a fully ionized plasma from the second moments $\delta n_{ei}^{2,0}(q)$ with $f_{ei}^{2,0} = k^2$ and a virial expansion of the conductivity

$$\sigma^* \approx a(\ln \Gamma^{-3/2} + b + c \Gamma^{3/2} \ln \Gamma^{-3/2})^{-1} \quad (11)$$

could be derived in the classical low-density and nondegenerate limit. We find for hydrogen plasmas

$$\begin{aligned} \sigma &= 0.591 \frac{(4\pi\epsilon_0)^2 (k_B T)^{3/2}}{e^2 m^{1/2}} \left[\ln \Gamma^{-3/2} + 1.124 + \frac{1.078}{\sqrt{6} + \sqrt{3}} \Gamma^{3/2} \ln \Gamma^{-3/2} \right]^{-1} \\ &= 1.530 \times 10^{-2} T^{3/2} \left[\ln \Gamma^{-3/2} + 1.124 + 0.258 \Gamma^{3/2} \ln \Gamma^{-3/2} \right]^{-1} (\Omega \text{mK}^{3/2})^{-1}. \end{aligned} \quad (12)$$

The inclusion of the two-particle nonequilibrium correlations determines the coefficient c of the term $\Gamma^{3/2} \ln \Gamma^{-3/2}$ in Eq. (11).

3 Interpolation formula and results

An interpolation formula can be constructed on the basis of the explicit analytical results given above so that reliable results for the electrical conductivity are obtained easily for a wide range of density and temperature without the necessity to evaluate the underlying complicated many-particle methods in full detail. The original interpolation formula given in Ref. [9] included the low-density ($\Gamma \ll 1$) and Born limit ($\Gamma^2 \Theta \ll 1$). We improve the validity region and the accuracy of that formula in the present paper by (i) taking into account the corrections due to the Debye-Onsager relaxation effect and (ii) by a better analytical structure of the interpolation formula, avoiding unphysical behavior such as, e.g., poles in the entire (Γ, Θ) -plane. (iii) Furthermore we incorporate the results of Ichimaru and Tanaka in the strongly coupled and degenerate limit ($\Theta \leq 1, \Gamma \geq 1$) by analyzing their parameterized numerical results. Thus the validity range of our interpolation formula is extended to a parameter range where the influence of the ion-ion structure factor becomes relevant.

We propose the following interpolation formula [T in K, σ in $(\Omega \text{m})^{-1}$]:

$$\sigma = a_0 T^{3/2} \left(1 + \frac{b_1}{\Theta^{3/2}} \right) \left[\ln(1 + A + B) D - C - \frac{b_2}{b_2 + \Gamma \Theta} \right]^{-1} \quad (13)$$

with the functions

$$\begin{aligned} A &= \Gamma^{-3} \frac{1 + a_4/\Gamma^2 \Theta}{1 + a_2/\Gamma^2 \Theta + a_3/\Gamma^4 \Theta^2} \left[a_1 + c_1 \ln(c_2 \Gamma^{3/2} + 1) \right]^2, \\ B &= \frac{b_3(1 + c_3 \Theta)}{\Gamma \Theta(1 + c_3 \Theta^{4/5})}, \\ C &= \frac{c_4}{\ln(1 + \Gamma^{-1}) + c_5 \Gamma^2 \Theta}, \\ D &= \frac{\Gamma^3 + a_5(1 + a_6 \Gamma^{3/2})}{\Gamma^3 + a_5}. \end{aligned} \quad (14)$$

The parameters a_i are fixed by the low-density virial expansion. In particular, the corrections from the Debye-Onsager relaxation effect are included in the function D . The coefficients b_i are used to adjust the Ichimaru and Tanaka results in the strong degenerate limit, and the parameters c_i were fitted to numerical data of the correlation functions. The explicit set of parameters is given by $a_0 = 0.03064$, $a_1 = 1.1590$, $a_2 = 0.698$, $a_3 = 0.4876$, $a_4 = 0.1748$, $a_5 = 0.1$, $a_6 = 0.258$, $b_1 = 1.95$, $b_2 = 2.88$, $b_3 = 3.6$, $c_1 = 1.5$, $c_2 = 6.2$, $c_3 = 0.3$, $c_4 = 0.35$, $c_5 = 0.1$.

We compare the results of the new interpolation formula (13) with the former one given in [9], the Ichimaru-Tanaka fit formula [2], and experimental data for strongly coupled plasmas [16, 17, 18] in Table 1. In the given parameter range, neutral bound states are present. It is possible to extract the Coulombic part of the electrical conductivity by considering the degree of ionization and the transport cross sections of electron-atom scattering,

Table 1 Electrical conductivity according to the new interpolation formula (13) compared with the former one given in [9], the Ichimaru-Tanaka fit formula [2], and available experimental data for strongly coupled plasmas [16, 17, 18].

	T	n_e	Γ	Θ	$\sigma(10^2 \Omega^{-1} \text{m}^{-1})$			
	(10^3K)	($10^{25}/\text{m}^3$)			exp.	[2]	[9]	(13)
Ar[16]	22.2	2.8	0.368	56.9	190	200	225	220
	20.3	5.5	0.505	33.2	155	203	231	224
	19.3	8.1	0.604	24.4	170	209	239	232
	19.0	14	0.736	16.7	255	234	269	261
	17.8	17	0.838	13.7	245	232	270	262
Xe[16]	30.1	25	0.564	17.9	450	442	458	453
	27.0	79	0.922	7.47	740	546	594	590
	25.1	160	1.26	4.34	780	660	813	797
	22.7	200	1.50	3.38	930	694	933	900
Ne[16]	19.8	1.1	0.303	94.6	130	148	173	169
	19.6	1.9	0.367	65.0	165	160	187	181
Air[16]	11.0	0.13	0.267	218	60	53	67	65
Ar[17]	16.4	0.06	0.128	551	83	78	93	93
		0.1	0.165	385	79	83	102	102
		0.13	0.18	324	76	86	105	105
		0.15	0.19	291	64	88	108	107
Xe[17]	12.4	0.06	0.185	403	46	55	70	69
		0.12	0.234	252	41	60	76	75
	12.6	0.07	0.192	371	48	57	73	72
		0.14	0.239	238	44	65	79	77
H[18]	15.4	0.1	0.175	364	62	77	95	94
	18.7	0.15	0.165	337	91	103	125	124
	21.5	0.25	0.170	276	114	131	156	155

see [19]. Both the experimental and the theoretical data in Table 1 represent the electrical conductivity of the free electron subsystem (fully ionized plasma). Taking into account an experimental error of about 30% we find a good agreement between theory and experiment. However, complete correspondence with the experiments can not be anticipated because of deviations from the Coulomb potential for the electron-ion interaction in rare gases and the occurrence of neutral particles (partial ionization) as mentioned above. The Debye-Onsager relaxation effect leads to a reduction of the electrical conductivity in the order of 5% at $\Gamma \approx 1$. A direct comparison with simulation results would be highly desirable. However, the standard approach through the current-current autocorrelation function is still limited by the small number of simulated particles and the corresponding statistical uncertainties.

The validity range of the new interpolation formula (13) is restricted to a parameter range where the formation of bound states ($\Theta \geq 1$) can be neglected. Partial ionization plays a crucial role in low-temperature plasmas and

can lead to a minimum in the isotherms of the electrical conductivity, see Ref. [19] for the case of hydrogen. Bound states (atoms) are also important when evaluating the hopping conductivity for fluid hydrogen near to the nonmetal-to-metal transition at megabar pressures [20]. At present, the treatment of the dc conductivity for plasmas where bound states may occur is performed within the model of the partially ionized plasma, where the composition is determined within a thermodynamic approach, and the contribution of the interactions between the different components is considered separately. Within such an approach, the interpolation formula given here may be of use to describe the contribution of the interaction between electrons and ions to the conductivity.

The generalization of the present approach to plasmas with higher charged ions $Z \geq 1$ is also possible but not intended here. Then, comparison with new experimental data for strongly coupled metal plasmas with $\Gamma \gg 1$ [21, 22] can be performed, see [23]. The inclusion of bound state formation and the extension to higher charged ions should be considered as possible goals of future work on interpolation formula for the electrical conductivity of nonideal plasmas.

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