Virial Expansion of the Electrical Conductivity of Hydrogen Plasmas

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The low-density limit of the electrical conductivity $\sigma(n,T)$ of hydrogen as the simplest ionic plasma is presented as function of temperature $T$ and mass density $n$ in a form of a virial expansion of the resistivity. Quantum statistical methods yield exact values for the lowest virial coefficients which serve as benchmark for analytical approaches to the electrical conductivity as well as for numerical results obtained from density functional theory based molecular dynamics simulations (DFT-MD) or path-integral Monte Carlo (PIMC) simulations. While these simulations are well suited to calculate $\sigma(n,T)$ in a wide range of density and temperature, in particular for the warm dense matter region, they become computationally expensive in the low-density limit, and virial expansions can be utilized to balance this drawback. We present new results of DFT-MD simulations in that regime and discuss the account of electron-electron collisions by comparing with the virial expansion.

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I. INTRODUCTION.

Besides the equation of state and the optical properties, the direct-current electrical conductivity $\sigma$ is a fundamental characteristic of plasmas which is relevant in various fields. Examples for technical applications reach from the quenching gas in high-power circuit breakers [1] which acts as an efficient dielectric medium up to fusion plasmas produced via magnetic [2] or inertial confinement [3]. The electrical conductivity is indispensable for the verification of the insulator-to-metal transition in warm dense hydrogen [4]. In geophysics, the electrical conductivity determines the properties of the outer liquid core and of the ionosphere, i.e., the entire magnetic field of Earth from the dynamo region [5] up to the magnetosphere [6]. Similarly, the electrical conductivity in the convection zone of giant planets [7], brown dwarfs [8], and stars [9] determines the action of the dynamo that produces their magnetic field. The investigation of the electrical conductivity of charged particle systems is, therefore, an emerging field of quantum statistics. In this work we provide exact benchmarks for this fundamental transport property.

Theoretical approaches to calculate the electrical conductivity of plasmas have been performed first within kinetic theory [10]. In a seminal paper [11], Spitzer and Härm determined $\sigma$ of the fully ionized plasma solving a Fokker-Planck equation. However, to calculate $\sigma(n,T)$ in a wide region of temperature $T$ and mass density $n$, a quantum statistical many-particle theory is needed which describes screening, correlations, and degeneracy effects in a systematic approach. In a very general way, according to the fluctuation-dissipation theorem, the conductivity is expressed in terms of equilibrium correlation functions. Kubo’s fundamental approach [12] relates the electrical conductivity to the current-current correlation function. For the relation between generalized linear response theory [13] and kinetic theory, see [16] and references therein. The evaluation of the corresponding equilibrium correlation functions can be performed by using different methods:

(i) Analytical expressions are derived, e.g., by using thermodynamic Green’s functions. Perturbation theory allows partial summations using diagram techniques which leads to sound results in a wide range of $T$ and $n$. However, as characteristic for perturbative approaches, exact results can be found only in some limiting cases.

(ii) This drawback is removed by numerical $ab\ initio$ simulations of the correlation functions applicable for arbitrary interaction strength and degeneracy. Using density functional theory (DFT) for the electron system and molecular dynamics (MD) for the ion system, see [12]–[20], single electron states are calculated solving the Kohn-Sham equations for a given configuration of ions. The total energy is given by the kinetic energy of a non-interacting reference system, the classical electron-electron interaction, and an exchange-correlation energy which contains all unknown contributions in certain approximation. One of the shortcomings of this approach is that the many-particle interaction is replaced by this mean-field potential.

(iii) In principle, an exact evaluation of the equilibrium correlation functions is possible by using path-integral Monte Carlo (PIMC) simulations, see [21]–[23] and references therein. The shortcomings of this approach are the rather small number of particles (few tens), the sign

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problem for fermions, and the computational challenges to calculate path integrals accurately.

These approaches and other closely related methods have been used to calculate $\sigma(n, T)$ in a wide parameter range, and numerous results have been published, for a recent review see Ref. [24]. Also recently, a comparative study [25] considering different approaches has been published which revealed large differences of calculated conductivities.

In the present study, we demonstrate that the virial expansion of the inverse conductivity serves as an exact benchmark for theoretical approaches so that the accuracy and consistency of results for the conductivity [25] can be checked. In particular, we apply this framework to analytical approaches, DFT-MD results, and experimental data for hydrogen, which was chosen for simplicity. In the course of this discussion, we present new DFT-MD data to extend the previously available conductivity data [27] in the density-temperature region of interest. The virial expansion of $\rho = 1/\sigma$ suggested in this work is a prerequisite to work out interpolation formulas for the conductivity. It can be used in a wide range of $T$ and $n$; analogous to the Gell-Mann–Brueckner result for the virial expansion of the plasma equation of state, see [26]. Finally, the benchmark capability of the virial expansion as discussed in this work may serve as a criterion to check the accuracy of numerical approaches like DFT-MD simulations to evaluate the conductivity.

II. VIRIAL EXPANSION OF THE INVERSE CONDUCTIVITY.

Charge-neutral hydrogen plasma (ion charge $Z = 1$) in thermodynamic equilibrium is characterized by temperature $T$ and the mass density $n$, or the total particle number densities of electrons $\hat{n}_e$ which equals that of the ions $\hat{n}_{\text{ion}}$. Instead, dimensionless parameters can be introduced: the plasma parameter

$$\Theta = \frac{2m_e k_B T}{\hbar^2} (3\pi^2 \hat{n}_e)^{-2/3}. \quad (1)$$

which characterizes the ratio of potential to kinetic energy in the non-degenerate case, and the electron degeneracy parameter

$$\Gamma = \frac{e^2}{4\pi\epsilon_0 k_B T} \left( \frac{4\pi}{3} \hat{n}_e \right)^{1/3} \quad (2)$$

The dc conductivity $\sigma(n, T)$ is usually related to a dimensionless function $\sigma^*(n, T)$ according to

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

where

$$\sigma^*(n, T) = \left( \frac{k_B T}{eV} \right)^{3/2} \frac{32405.4}{12m_e} \left( \frac{k_B T}{eV} \right)^{3/2} \left( \frac{3\pi^2}{2} \right)^{1/3} \frac{1}{3\pi^2} \frac{\Theta}{\Gamma}. \quad (3)$$

In this work, we consider both $\sigma$ and $\sigma^*$ as function of density $n$ at fixed temperature $T$. In the low-density limit, the following virial expansion for the inverse conductivity $\rho^*(n, T) = 1/\sigma^*(n, T)$ was obtained from kinetic theory and generalized linear response theory [13–15]:

$$\rho^*(n, T) = \rho_1(T) n + \rho_2(T) n^{1/2} + \frac{1}{n} + \ldots \quad (4)$$

In contrast to a simple expansion in powers of $n$, the occurrence of terms with $\ln n$ and $n^{1/2} \ln n$ is due to the long-range character of the Coulomb interaction. To describe the collisions between the charged particles, an integral over the Coulomb interaction occurs which gives the so-called Coulomb logarithm, where screening of the Coulomb interaction is taken into account. Typically, such a Coulomb logarithm arises in the correlation functions within the generalized linear response theory [13] [15].

By convention, virial expansions consider the dependence of physical quantities on the density $n$, for instance a power series expansion. However the density $n$ has a dimension, and for $\rho^*$ to be not depending on units, the virial coefficients $\rho_i$ have also in general a dimension. In particular, the term $\rho_1 \ln(1/n)$ needs a compensating term $\rho_1 \ln(A)$, where $A$ has the dimension of density, as a contribution to $\rho_2$ so that $\rho^*$ remains dimensionless. Usually relations like [3] are given after fixing the units in which the physical quantities are measured, but it is also convenient to introduce dimensionless variables. For motivation, we consider the Born approximation for the Coulomb logarithm.

Within static (Debye) screening of the Coulomb interaction to avoid the divergence owing to distant collisions, the Born approximation of the Coulomb logarithm leads to the result, see [13] [15],

$$\int_0^\infty \frac{x}{(x + \kappa_{\text{Debye}}^2)^2} e^{-\kappa_{\text{Debye}}^2 x/(8m_e k_B T)} dx = \ln \left( \frac{\Theta}{\Gamma} \right) - 0.962203 + O \left[ \frac{\Theta}{\Gamma} \ln \left( \frac{\Theta}{\Gamma} \right) \right]. \quad (5)$$

The Debye screening parameter in the low-density (non-degenerate) limit reads

$$\kappa_{\text{Debye}}^2 = 2\hat{n}_e \frac{e^2}{\epsilon_0 k_B T} \quad (6)$$

so that the integral depends only on the parameter

$$\frac{\hbar^2 \kappa_{\text{Debye}}^2}{8m_e k_B T} = \left( \frac{2}{3\pi^2} \right)^{1/3} \frac{\Theta}{\Gamma}. \quad (7)$$

We focus on the first and second term on the right hand side of Eq. [5] which is sufficient in order to derive the first $[\rho_1(T)]$ and second virial coefficient $[\rho_2(T)]$ of the virial expansion [4]. Further contributions are of higher order in density: for $\Gamma/\Theta \leq 0.01$ they contribute to the integral in Eq. [5] by less than 1 %.
In the virial expansion [1], the logarithm can be transformed by introducing the dimensionless parameter
\[ \frac{\Theta}{\Gamma} = \frac{2m}{\hbar^2} \frac{(k_B T)^2}{n_e e^2} \frac{4\pi e^2}{c^2} (36\pi^5)^{-1/3} , \] (8)
see Eq. [5], and we find a modified expression [note that \( T \sim 1/(1-\Theta) \)];
\[ \rho^*(n,T) = \tilde{\rho}_1(T) \ln \left( \frac{\Theta}{\Gamma} \right) + \tilde{\rho}_2(T) + \ldots \enspace (9) \]
To find the relation between \( \tilde{\rho}_i \) and \( \rho_i \) we replace in Eq. [9] the variables \( \Theta, \Gamma \) by \( n, T \) according to Eq. [8] so that
\[ \rho^* = \tilde{\rho}_1(T) \ln \left( \frac{1}{n} \right) + \tilde{\rho}_1(T) \ln \left( \frac{2m}{\hbar^2} (k_B T)^2 \frac{4\pi e^2}{c^2} (36\pi^5)^{-1/3} \right) + \tilde{\rho}_2(T) + \ldots \enspace (10) \]
Comparing with Eq. [4] we find \( \tilde{\rho}_1 = \rho_1 \) and
\[ \tilde{\rho}_2 = \rho_2 + \rho_1 \ln [2(\pi e^2)^{3/2} a_B^3/k_B T^2] \enspace (11) \]
where \( a_B \) is the Bohr radius and \( T_{Ryd} = k_B T/13.6 \) eV is the temperature measured in Rydberg units.

A highlight of plasma transport theory is that the exact value of the first virial coefficient is known for Coulomb systems from the seminal paper of Spitzer and Härn [11],
\[ \rho_1 = \tilde{\rho}_1 = \rho_1^{\text{Spitzer}} = 0.846 \enspace (12) \]
which does not depend on \( T \). Note that Eq. [12] takes into account the contribution of the electron-electron \((e-e)\) interaction. In contrast, for the Lorentz plasma model where the \( e-e \) collisions are neglected so that only the electron-ion interaction is considered, the first virial coefficient amounts to
\[ \rho_1^{\text{Lorenz}} = \frac{1}{16} (2\pi^3)^{1/2} = 0.492126 \enspace (13) \]
Although \( e-e \) collisions do not contribute to a change of the total momentum of the electrons because of momentum conservation, the distribution in momentum space is changed ("reshaping") so that higher moments of the electron momentum distribution are not conserved. The indirect influence of \( e-e \) collisions on the dc conductivity is clearly seen in generalized linear response theory where these higher moments are considered; see [13].

For the second virial coefficient \( \rho_2(T) \) or \( \tilde{\rho}_2(T) \), no exact value is known. It depends on the treatment of many-particle effects, in particular screening of the Coulomb potential. Within a quantum statistical approach, the static (Debye) screening by electrons and ions, see Eq. [5], should be replaced by a dynamical one. For hydrogen plasma as considered here, the Born approximation for the collision integral is justified at high temperatures \( T_{Ryd} \gg 1 \). Considering screening in the random-phase approximation leads to the quantum Lenard-Balescu (QLB) expression. Thus, at very high temperatures where the dynamically screened Born approximation becomes valid, we obtain the QLB result, see [27, 29],
\[ \lim_{T \to \infty} \tilde{\rho}_2(T) = \rho_2^{\text{QLB}} = 0.4917 \enspace (14) \]
With decreasing \( T \), strong binary collisions (represented by ladder diagrams) become important which have to be treated beyond the Born approximation when calculating the second virial coefficient \( \rho_2(T) \). According to Spitzer and Härn [11], the classical treatment of strong collisions with a statically screened potential gives for \( \rho^* = 1/\sigma^* \) the result
\[ \rho_2^{\text{Sp}} = 0.846 \ln \left[ \frac{3}{2} \Gamma^{-3} \right] \enspace (15) \]
Interpolation formulas have been proposed connecting the high-temperature limit \( \rho_2^{\text{QLB}} \) with the low-temperature Spitzer limit. Instead, performing the sum of ladder diagrams with the dynamically screened Coulomb potential, Gould and DeWitt [30] and Williams and DeWitt [31] proposed approximations where the lowest order of a ladder sum with respect to a statically screened potential, the Born approximation, is replaced by the Lenard-Balescu result which accounts for dynamic screening. An improved version was proposed in Refs. [14, 32] by introducing an effective screening parameter \( \kappa_{\text{eff}} \) such that the Born approximation coincides with the Lenard-Balescu result, see also [13–15, 34]. Based on a T-matrix calculation in quasiclassical ( Wentzel-Kramers-Brillouin, WKB) approximation [33, 36], the expression (temperature is given in eV: \( T_{eV} = k_B T/eV \))
\[ \tilde{\rho}_2(T_{eV}) \approx 0.4917 + 0.846 \ln \left[ \frac{1 + 8.492/T_{eV}}{1 + 25.83/T_{eV} + 167.2/T_{eV}^2} \right] \enspace (16) \]
can be considered as simple interpolation which connects the QLB result with the Spitzer limit in WKB approximation. However, the exact analytical form of the temperature dependence of the second virial coefficient \( \rho_2(T) \) remains an open problem.

Thus, the available exact results for the virial expansion [1] of the resistivity of hydrogen plasma are:
(i) the value of the first virial coefficient is \( \tilde{\rho}_1 = 0.846 \);
(ii) the second virial coefficient has the high-temperature limit \( \lim_{T \to \infty} \tilde{\rho}_2(T) = 0.4917 \);
(iii) the second virial coefficient is temperature dependent, a promising functional form is given by Eq. (16).

III. VIRIAL COEFFICIENTS FROM ANALYTICAL APPROACHES.

To extract the first and second virial coefficient from calculated or measured dc conductivities, we plot the ex-
The first virial coefficient is the basis of the Lenard-Balescu approximation, which is shown as a black broken straight line which is expected to be correct in the high-temperature limit.

Two QLB calculations of Desjarlais et al. [27] are shown in Fig. 1, see also [39]. The line including e - e collisions obeys the same asymptote (x → 0) as that of Karakhtanov [28]. With increasing x = 1/ln(Θ/Γ), small deviations from the linear behavior are seen. The line for calculations without e - e collisions (Lorentz plasma) points to the corresponding asymptote given by ρi^Lorentz.

Recently, the transport properties of hydrogen plasma were compiled in Ref. [25]. For a grid of lattice points in the n-T plane (considering n = 0.1, 1.0, 10, 100 g/cm³ and T_eV = 0.2, 2, 20, 200, 2000) the results of different approaches were given. Large deviations were obtained which indicate not only unavoidable numerical uncertainties but also deficits in some of the theoretical approaches. Their consistency can be checked via the virial expansion as benchmark. As an example, we show data of Clérouin et al. and of Copeland for the isotherm T_eV = 2000 taken from Ref. [25] in Fig. 1.

Extrapolating to x = 1/ln(Θ/Γ) → 0, these high-temperature isotherms show already significant differences. The data of Clérouin et al. point to the correct Spitzer limit ρ_i^Spitzer, including e - e collisions, but have a more steep slope. This may be caused by the approximations in treating dynamical screening and the ionic structure factor, in contrast to a strict QLB calculation. The data of Copeland clearly point to the limit ρ_i^Lorentz of the Lorentz model, i.e., this approach does not include e - e collisions and fails to describe the conductivity of hydrogen plasma correctly.

Also shown in Fig. 1 are analytical results for the dc conductivity of hydrogen plasma presented in Lambert et al. [38] at the lowest density n = 10 g/cm³. The data denoted by Hubbard [10] are close to the data of Clérouin et al. discussed above. The asymptote is the correct benchmark ρ_i^Spitzer, but the slope is rather large. The data of Lee and More [41] are closer to the QLB calculations. In contrast to Copeland who also claims to use the Lee-More approach, possibly the e - e collisions are added so that the extrapolation to x → 0 is near to the correct benchmark ρ_i^Spitzer. Because of the approximations in evaluating the Coulomb logarithm, deviations from the QLB result are seen. The kink in the Lee-More and Hubbard data seen in Fig. 1 is due to switching the minimum impact parameter in the Coulomb logarithm from the classical distance of closest approach to the quantum thermal wave length, cf. Ref. [24].

Ichimaru and Tanaka [42] derived an analytical expression for the conductivity which has been improved in [43] by adding a tail-term to the Coulomb logarithm. The latter expression has been used also in Ref. [38], the isochore n = 10 g/cm³ is shown in Fig. 1. The approach is based on a single Sonine polynomial approximation where the effect of e - e collisions is not taken into account. The empirical fit of Kitamura and Ichimaru [43] approximates the conductivity for degenerate plasmas.
see also Fig. 9 of Ref. 38. However, in the low-density limit this approach fails to describe the conductivity approaching \( \rho_1 \) at \( x = 0 \).

IV. VIRIAL REPRESENTATION OF DFT-MD SIMULATIONS.

DFT-MD simulations are of great interest, since they do not suffer from the restrictions of perturbation theory as typical for analytical results and can directly be confronted with the virial expansion. In addition, with the virial expansion the results can be extrapolated to the low-density region were DFT-MD simulations become infeasible.

In this work, we present new DFT-MD results for the electrical conductivity of hydrogen obtained from an evaluation of the Kubo-Greenwood formula 12 17 15 16. The 125-atom simulations are performed with the Vienna \textit{ab initio} simulation package (VASP) 19 51 using the exchange-correlation functional of Perdew, Burke, and Ernzerhof (PBE) 52 and the provided Coulomb potential for hydrogen. The time steps were chosen between 0.2 and 0.1 fs and the simulations ran for at least 4000 time steps. The ion temperature is controlled with a Nosé-Hoover thermostat 53. For all simulations, the reciprocal space was sampled at the Baldescheri mean value point 54. Special attention has been paid to convergence with respect to the particle number. Additional details of the simulations are given in the supplemental material and the results are given in Tab. I.

| \( n \) | \( k_B T \) \([\text{eV}]\) | \( \Gamma \) | \( \Theta \) | \( 1/\ln(\Theta/\Gamma) \) | \( \sigma \) \(\text{[MS/m]}\) | \( \tilde{\rho}(x,T) \) |
|---|---|---|---|---|---|---|
| 2 | 50 | 0.49275 | 1.2172 | 1.2500 | 7.105 | 1.767 |
| 2 | 75 | 0.3285 | 1.8257 | 0.58302 | 11.44 | 1.073 |
| 2 | 100 | 0.24637 | 2.4343 | 0.43657 | 15.26 | 0.9269 |
| 3 | 100 | 0.28203 | 1.8577 | 0.53047 | 16.85 | 1.020 |
| 4 | 150 | 0.18802 | 2.7866 | 0.37092 | 25.67 | 0.8603 |
| 4 | 150 | 0.20694 | 2.3003 | 0.41522 | 27.39 | 0.9026 |

Our DFT-MD results are plotted in Fig. 2 and show a general increase with an increasing \( x = 1/\ln(\Theta/\Gamma) \). In comparison, the virial plot contains previous DFT-MD conductivity data 27 38, which were translated into our \( \tilde{\rho} \) framework. The first set of previous DFT-MD calculations has been published by Lambert et al. 38 which were also used by Starrett 37. Results for \( \tilde{\rho} \) for the lowest values of \( x > 0 \) at three different densities are given in Fig. 3. Inspecting Fig. 3 values for 10 g/cm\(^3\) at 200 eV and for 160 g/cm\(^3\) at 800 eV are close together, i.e., we see a dominant dependence on \( x \), no additional density or temperature effect is seen. They are also close to the Lee-More approach including \( e - e \) collisions so that they are not in conflict with the correct benchmark (KT, Spitzer). Calculations are based on a formulation of the Kubo-Greenwood method for average atom models neglecting the ion structure factor 48 so that these QMD values are possibly also influenced by approximations and, therefore, deviate slightly from other calculations. However, the parameter values \( x \) are too large to estimate the virial expansion.

The second set of previous DFT-MD simulations for hydrogen plasma in the low-\( x \) region were given by Desjarlais et al. 27, see Fig. 2. For a density of 40 g/cm\(^3\), three temperatures \( T_N = 500, 700 \), and 900 were considered. The reduced resistivity \( \tilde{\rho}(x,T) \) approaches the benchmark obtained from the QLB calculations. However, the linear extrapolation to \( \tilde{\rho}_1^{\text{Spitzer}} \) at \( x = 0 \) is not seen by these data.

Interestingly, the results for \( \tilde{\rho} \) of the different DFT-MD simulations do not follow approximately a single curve as expected from the high-temperature limit of the virial expansion. The values of Lambert et al. are significantly higher than ours but the slope is almost the same. While we employ the generalized gradient approximated exchange-correlation energy of PBE 52, Lambert et al. use the local density approximation. They used orbital-free molecular dynamics in order to simulate the system.
and obtain various snapshots for each density-pressure point. Subsequently, these snapshots were evaluated via the Kubo-Greenwood formula using the Kohn-Sham code Abinit, which is equivalent to our used VASP implementation. The DFT-MD simulations of Desjarlais et al. [27] are close to our results, but the slope of the virial plot is quite different. DFT-MD simulations are usually performed at high densities where the electrons are degenerate so that e – e collisions can be neglected. In the low-density region (x < 1) as considered here, we could improve the accuracy by studying the convergence of the DFT-MD results, in particular with respect to particle number and cut-off energy, using high-performance computing facilities.

A long-discussed problem in this context is the question whether or not e – e collisions are taken into account within the DFT-MD formalism. For example, in Ref. [37] it was pointed out that a mean-field approach is not able to describe two-particle correlations, in particular e – e collisions. However, e – e interaction is taken into account by the exchange-correlation energy as shown in Ref. [27] by comparing DFT-MD data for the electrical conductivity to QLB results. The calculations of Desjarlais et al. [27] for n = 40 g/cm³ and our present ones for n = 2 g/cm³ were computationally demanding, but are still not very close to x = 0 so that extrapolation to the limit x = 0 is not very precise. However, the corresponding slopes are quite different: While the present DFT-MD data favor ρ Lorentz as asymptote at x = 0, those of Ref. [27] seem to point to the Spitzer value, Eq. (12). Thus, our results do not solve the lively debate on whether or not DFT-MD simulations include the effect of e – e collisions on the conductivity or not. We conclude that further DFT-MD simulations have to be performed for still higher temperatures and/or lower densities in order to approach the limit x → 0 so that the value for ρ1 can be derived more accurately. Such simulations, e.g., for densities below 1 g/cm³, are computationally very challenging using the Kohn-Sham DFT-MD method so that alternative schemas like stochastic DFT [57] or the spectral quadrature method [58] have to be applied for this purpose.

We would like to mention that in the case of thermal conductivity it has been shown that the contribution of e – e collisions is not taken into account in DFT-MD simulations [27] and gives an additional term. A profound discussion on the mechanism of e – e collisions has been given recently by Shaffer and Starrett [24]. They argued that the precise nature of the incomplete interaction for e – e scattering to avoid double counting. Comparing with QMD results, Shaffer and Starrett [24] point out that their findings support the conclusions of Ref. [27] that the Kubo-Greenwood QMD calculations contain the indirect electron-electron reshaping effect relevant to both the electrical and thermal conductivity, but they do not contain the direct scattering effect which further reduces the thermal conductivity.

V. EXPERIMENTS.

Ultimately, the virial expansion (9) has to be checked experimentally but accurate data for the conductivity of hydrogen plasma in the low-density limit and/or at high temperatures are scarce. Accurate conductivity data for dense hydrogen plasma were derived by Günther and Radtke [44] which are shown in the virial plot, Fig. 2. They are close to the benchmark data of the virial expansion. Note that systematic errors are connected with the analysis of such experiments. For instance, the occurrence of bound states requires a realistic treatment of the plasma composition and of the influence of neutrals on the mobility of electrons. Alternatively, conductivity measurements in highly compressed rare gas plasmas have been performed by Ivanov et al. [55] and Popovic et al. [36, 56], but the interaction of the electrons with the ions deviates from the pure Coulomb potential owing to the cloud of bound electrons. The corresponding virial plot is close to the data of hydrogen plasma, see [39], but requires a more detailed discussion with respect to the role of bound electrons.

VI. CONCLUSIONS.

We propose an exact virial expansion (9) for the plasma conductivity to analyze the consistency of theoretical approaches. For instance, several analytical calculations of the dc conductivity σ(T,n) presented in Ref. [27] miss this strict requirement and fail to give accurate results. Results of DFT-MD simulations are presently considered to be most reliable, and future PIMC simulations can be tested by benchmarking with the virial expansion (9) for x → 0. Note that these ab initio simulations become computationally challenging in the low-density region, but the virial expansion allows the extrapolation into this region. The construction of interpolation formulas is possible, see [59], if the limiting behavior for n → 0 and further data in the region of larger densities not accessible for analytical calculations are known.

An outstanding problem that could potentially be addressed by applying the virial expansion of the conductivity is the question whether or not the e – e collisions are rigorously taken into account. Despite the work presented in [24, 27], there is no final proof whether the
Kubo-Greenwood QMD calculations with the standard expressions for the exchange-correlation energy functional give the exact value for the plasma conductivity in the low-density limit. A Green’s function approach may solve this problem but this has not been performed yet. Therefore, we suggest to apply our benchmark criterium on future large data sets of Kubo-Greenwood QMD calculations to investigate the contribution of $e-e$ collisions in the low-density limit.

The approach described here is applicable also to other transport properties such as thermal conductivity, thermopower, viscosity, and diffusion coefficients. Of interest is also the extension of the virial expansion to elements other than hydrogen, where different ions may be formed and the electron-ion interaction is no longer pure Coulombic.

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