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Transport properties of partially ionized hydrogen plasma

T S Ramazanov[1], **K Zh Galiyev**[1], **K N Dzhumagulova**[1], **G Röpke**[2] **and R Redmer**[2]

[1] IETP, Al Farabi Kazakh National University, Tole bi, 96a, 480012, Almaty, Kazakhstan
[2] Fachbereich Physik, Universität Rostock, D-18051 Rostock, Germany

E-mail: ramazan@physics.kz

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Abstract

We have considered partially ionized hydrogen plasma for the density region $n_e = (10^{18}–10^{22})$ cm^{-3}. Charged particles in the system (electrons, protons) interact via an effective potential taking into account three-particle correlations. We use the Buckingham polarization potential to describe electron–atom and proton–atom interactions. The electrical and thermal conductivity is determined using the Chapman–Enskog method. We compare the obtained results with other available data.

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1. Introduction

The transport properties of dense partially ionized hydrogen plasma play a crucial role in the study of non-ideal plasma existing in different astrophysical objects and technical devices. Dense non-ideal plasma is formed by shock compression experiments [1], in pinch discharges [2], magnetohydrodynamics (MHD) generators, and in the realization of inertial confinement fusion [3]. In particular, the electrical conductivity determines an important characteristic such as the efficiency of pulsed power machines in inertial confinement fusion experiments [4]. Knowledge of thermal conductivity for a large domain of densities and temperatures is necessary for the calculation of the energy balance of astrophysical objects [5]. In several papers [6, 7] the transport properties have been investigated for a partially ionized hydrogen plasma. There, the Debye–Hückel (DH) potential valid for the low density plasma within the pair correlation approximation [8] has been used for describing the charged particle interaction. For a dense plasma, many-particle correlation effects should be taken into account. From such a point of view, the main goal of the present work is to investigate the influence of three-particle correlations in a charged subsystem on the transport properties and ionization degree of non-ideal hydrogen plasma containing charges and neutrals.

In the following, we present the calculations of transport properties performed within the framework of the Chapman–Enskog method. Due to the long-range character of the Coulomb interaction leading to well-known divergences of the collision integrals, it is difficult to apply this method for the calculation of transport properties in plasmas. This problem can be solved by considering the screening between charged particles through the dielectric function of the medium leading to effective, density- and temperature-dependent potentials. Both dynamic [10, 11] and static screening effects [12, 13] have been studied for non-ideal plasmas.

In [14], the scattering cross sections and the electrical conductivity of fully ionized hydrogen plasma have been determined. In this paper, we generalize this approach to the case of a partially ionized hydrogen plasma where neutral atoms may occur. We consider the temperature range $T = (15\text{–}100) \times 10^3$ K and the number densities $n_e = (10^{18}\text{–}10^{22})$ cm^{-3}. The scattering cross sections have been calculated to be fully quantum mechanical using methods with the scattering phase shifts δ_l obtained from the numerical solution of the Schrödinger equation with corresponding interaction potential. The plasma composition (degree of ionization) is determined from a simple Saha equation that takes into account the lowering of the ionization energy of hydrogen atoms. The electrical and thermal conductivities of partially ionized hydrogen plasma have been calculated within the Chapman–Enskog method using the results for the plasma composition and transport cross sections. The results have been compared with the experiments and theoretical approaches of other authors.

2. Interaction models

It is known that charged particles in plasma interact by long-range Coulomb potential, and that the configurational integrals for the average of physical quantities are diverging. We have to take into account collective effects such as screening of charge fields. Within the simplest approximation, i.e. treating the polarization function in random phase approximation (RPA) and performing the static as well as long-wavelength limit, the DH potential can be derived [10]. The DH potential applies for low-density plasmas where the pair correlations are dominant [8]. With increasing plasma density, also higher many-particle correlations have to be taken into account. For instance, the concept of local-field corrections is utilized, which becomes important at very high, metallic densities, see [15].

Another approach to treat screening effects beyond the DH theory has been developed in [9, 12, 13]. There, an integro-differential equation for effective potential $\tilde{\Phi}_{qk}$ of the particle interaction (generalized Poisson–Boltzmann equation) taking into account the simultaneous N particle correlations was obtained on the basis of sequential solution of the Bogolyubov chain equations for the equilibrium particle distribution function of a classical non-ideal plasma:

$$\begin{aligned}\Delta_i \sum_{j=1}^{s} \tilde{\Phi}_{qk}\left({}^q\vec{r}_i, {}^k\vec{r}_j\right) &= -4\pi \sum_{j=1}^{s} \delta\left({}^k\vec{r}_j - {}^q\vec{r}_i\right) e_k e_q \\ &\quad + \sum_{j=s+1}^{N} A_k \int (\nabla_i \Phi_{ij}) \exp\left(-\tilde{\Phi}_{qk}\left({}^q\vec{r}_i, {}^k\vec{r}_j\right)/\theta\right) \nabla_j \\ &\quad \times \exp\left(-\sum_{l=1}^{s} \tilde{\Phi}_{qk}\left({}^q\vec{r}_i, {}^k\vec{r}_l\right)/\theta\right) \mathrm{d}^k\vec{r}_j. \qquad (1)\end{aligned}$$

Here $\tilde{\Phi}_{qk}\left({}^q\vec{r}_i, {}^k\vec{r}_j\right)$ is two-body effective potential taking into account N particle correlation effects; $\Phi_{ij} = ae_ie_j/|r_i - r_j|$; $a = 1$ in the CGS system; $\theta = k_BT$, e_k, e_q are charges of the interacting particles; Δ_i is the Laplace operator; ∇ is the gradient operator; $A_k = (N_k - \nu_k)/V$

is a normalization coefficient; and ν_k and N_k are the number of particles in s and total systems, respectively. V is the volume of system, $\delta(r)$ is the Dirac delta function, and summation excludes $i = j$. The three-particle approximation equation for the effective potential can be obtained from equation (1)

$$\Delta\Psi - \Psi = \pm\Psi^2 \tag{2}$$

where $\Psi(R)$ is the effective potential expressed in units $k_B T$. Minus and plus signs in equation (2) correspond to the interaction of particles with equal or opposite charge, respectively.

Equation (2) with boundary conditions $\Psi|_{R\to 0} = \gamma/R$; $\Psi|_{R\to\infty} = 0$ has no analytical solution. In this paper, we use the analytical interpolation formula for the numerical solution of equation (2), obtained in [12] by application of the spline approximation. The final expression for the pseudopotential of particle interaction in non-ideal plasma is

$$\Psi(R) = \frac{\gamma}{R}\,\mathrm{e}^{-R}\,\frac{1+\gamma f(R)}{1+c(\gamma)} \qquad f(R) = \frac{1}{10}(\mathrm{e}^{-\sqrt{\gamma}R} - 1)(1 - \mathrm{e}^{-2R}). \tag{3}$$

The interparticle distance r is scaled by the Debye screening length r_D, $R = r/r_D$. The parameter $\gamma = \mathrm{e}^2/(r_D k_B T)$ characterizes the non-ideality of plasma. The potential is expressed in terms of thermal energy, $\Psi(R) = \tilde{\Phi}(R)/k_B T$. $c(\gamma)$ is a correction function for different values of γ: $c(\gamma) = -0.008\,617 + 0.455\,861\gamma - 0.108\,389\gamma^2 + 0.009\,377\gamma^3$. Notice that the effective potential (3) rapidly decreases with increasing distance due to screening effects. In fact, due to the consideration of three-particle correlations, the effective potential shows stronger screening than the DH potential where only two-particle correlations are included [12].

The interaction between charged particles ($\beta = e, p$) and neutral atoms (a) is described by a screened polarization potential of the Buckingham form [16]

$$\Phi_{\beta a}(r) = -\frac{\mathrm{e}^2\alpha_D}{2\left(r^2 + r_0^2\right)^2}\exp(-2r/r_D)(1 + r/r_D)^2 \tag{4}$$

where α_D is the polarizability of atoms and r_0 is a cut-off radius. For hydrogen plasma we use $\alpha_D = 4.5a_B^3$ and $r_0 = 1.45a_B$, where a_B is the Bohr radius.

3. The scattering cross sections

The transport cross sections Q^T for plasma particles $\alpha, \beta = e, p, a$ are related to the scattering phase shifts (SPS) in first- and second-order approximations [17, 18] as

$$\begin{aligned} Q^{T(1)}_{\alpha\beta}(k) &= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(l+1)\sin^2\left(\delta^{\alpha\beta}_{l+1}(k) - \delta^{\alpha\beta}_{l}(k)\right) \\ Q^{T(2)}_{ee}(k) &= \frac{2\pi}{k^2}\sum_{l=0}^{\infty}\frac{(l+1)(l+2)}{l+3/2}[1 - (-1)^l/2]\sin^2\left[\delta^{ee}_l(k) - \delta^{ee}_{l+2}(k)\right]. \end{aligned} \tag{5}$$

In this paper, we use two methods to calculate the SPS: the partial wave expansion [20] and the semiclassical (WKB) approximation [17].

For the lowest orbital quantum numbers in the range $0 \leqslant l \leqslant 20$ the SPS are obtained from the radial Schrödinger equation

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}u_l(r) + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2\mu_{\alpha\beta}}{\hbar^2}\Phi_{\alpha\beta}(r)\right]u_l(r) = 0 \tag{6}$$

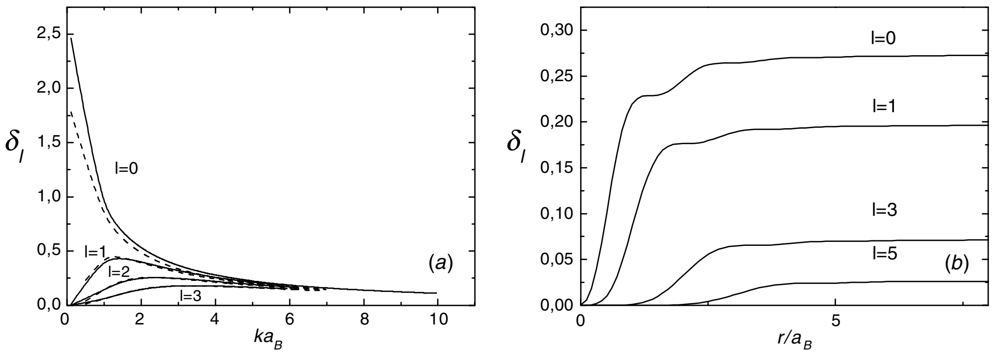

Figure 1. (*a*) Phase shifts for the first four angular momenta calculated by the WKB approximation (- - - -) and by the numerical solution of the Calogero equation (——). (*b*) Curves of the phase function for different partial waves.

where $\Phi_{\alpha\beta}(r)$ is the particle interaction potential. The wavenumber k is related to the kinetic energy E of relative motion as $k^2 = 2\mu_{\alpha\beta}E/\hbar^2$; $\mu_{\alpha\beta}$ is the reduced mass of the particles. To solve equation (6) we have used the amplitude-phase method. The wavefunction $u_l(r)$ may be written as

$$u_l(r) = A_l(r)\left[\cos\delta_l^{\alpha\beta}(r)\hat{j}_l(kr) - \sin\delta_l^{\alpha\beta}(r)\hat{n}_l(kr)\right] \tag{7}$$

where $A_l(r)$ is the amplitude function, and $\hat{j}_l(kr)$ and $\hat{n}_l(kr)$ are Riccati–Bessel functions. In this paper, the recurrence relations for these functions are used which are associated with the Bessel and Neumann functions [19]. After inserting expression (7) into equation (6), the Calogero equation for the SPS $\delta_l^{\alpha\beta}(r)$ is obtained [20]:

$$\frac{\mathrm{d}}{\mathrm{d}r}\delta_l^{\alpha\beta}(r) = -\frac{1}{k}V_{\alpha\beta}(r)\left[\cos\delta_l^{\alpha\beta}(r)\hat{j}_l(kr) - \sin\delta_l^{\alpha\beta}(r)\hat{n}_l(kr)\right]^2. \tag{8}$$

Here $V_{\alpha\beta}(r) = 2\mu_{\alpha\beta}\Phi_{\alpha\beta}(r)/\hbar^2$. The SPS $\delta_l^{\alpha\beta}(k)$ is determined by the asymptotic values of phase functions $\delta_l^{\alpha\beta}(r)$ at $r \to \infty$. Consequently, for the calculation of SPS $\delta_l^{\alpha\beta}(k)$ it is necessary to solve the nonlinear differential equation (8) with the initial condition $\delta_l^{\alpha\beta}(0) = 0$. The numerical evaluation of $\hat{j}_l(kr), \hat{n}_l(kr)$ functions by recurrence relations is difficult for higher orbital quantum numbers. Fortunately, the semiclassical WKB approximation becomes increasingly accurate for higher orbital quantum numbers so that we have used this method for $l > 20$; for more details, see [17]. Figure 1(*a*) shows the phase shifts which were calculated with both methods for the first four angular momenta as a functions of the wavenumber value. It is shown that the WKB results become more applicable with the increase in energy. The asymptotic behaviour of the phase shifts is shown in figure 1(*b*).

4. Transport properties

The transport properties of non-ideal, non-degenerate hydrogen plasma are calculated by the standard Chapman–Enskog method within a two-momentum approximation. The collision integrals $I_{nm} = I_{nm}^{ee} + I_{nm}^{ep} + I_{nm}^{ea}$ can be separated with respect to the scattering processes of free electrons at other electrons, protons and atoms. These contributions are given by the transport cross sections $Q_{\alpha\beta}^T(k)$, see equation (5). The electrical conductivity can be evaluated from the

Table 1. The 1s ground-state energy $\tilde{E}_{10}$ of hydrogen atoms for different screening lengths r_D and non-ideality parameters γ calculated from the Schrödinger equation for the DH potential and effective potential (3).

r_D/a_B	γ	$\tilde{E}_{10}$ (eV) Debye potential	$\tilde{E}_{10}$ (eV) equation (3)
315.000	0.01	−13.398	−13.132
31.500	0.10	−12.018	−11.258
15.750	0.20	−10.745	−9.261
10.500	0.30	−9.682	−7.780
2.864	1.10	−5.022	−2.681
1.750	1.80	−3.285	−1.408

following expression [21, 22]:

$$\sigma = \frac{3e^2}{2\sqrt{2m_e k_B T}} \frac{I_{11}}{I_{00}I_{11} - I_{10}I_{01}}$$
$$I_{nm}^{ec} = \frac{2n_c}{\sqrt{\pi}} \int_0^\infty \mathrm{d}x\, Q_{ec}^T(x) S_n^{3/2}(x) S_m^{3/2}(x) x^2\, \mathrm{e}^{-x} \tag{9}$$
$$I_{nm}^{ee} = 2n_e \sqrt{\frac{2}{\pi}} \int_0^\infty \mathrm{d}y\, Q_{ee}^T(y) R_{nm}(y) y^3\, \mathrm{e}^{-y}.$$

We define $x = \hbar^2 k^2/(2m_e k_B T)$, $y = 2x$, and $c = i, a$. $S_n^{3/2}$ are Sonine polynomials of the order $3/2$ (for details, see [7, 23]) and n_e, n_i and n_a are the density numbers of electrons, ions and atoms, respectively.

The plasma composition, i.e. the ionization degree, is obtained from a simple Saha equation. We consider only hydrogen atoms and neglect other bound states, in particular molecules H_2. These are important at low temperatures which we will not treat here. The Saha equation reads

$$\frac{1-\alpha}{\alpha^2} = n_e^{\mathrm{tot}} \Lambda^3 \exp(-\beta \tilde{E}_{10}(r_D)). \tag{10}$$

The degree of ionization is defined by $\alpha = n_e/n$ where $n = n_e + n_a$ is the total electron density in the plasma. $\Lambda = h/\sqrt{2\pi m_e k_B T}$ is the electron thermal wavelength. The energy of the hydrogen 1s ground state $\tilde{E}_{10}$ is determined by solving the eigenvalue problem of the radial Schrödinger equation with respect to the effective electron–proton potential (3). Correlation effects become important with increasing plasma density. Especially, three-particle correlations have been shown to be important for the transport and thermodynamics properties of fully ionized, non-ideal plasmas [12–14, 24, 25] which were treated using the effective potential (3). Therefore, we study the influence of such three-particle correlations on ionization equilibrium (10) by calculating the ground-state energies with respect to the effective potential (3).

The results for both interaction models, the effective potential (3) and the DH potential are shown for various Debye screening lengths r_D and non-ideality parameters γ in table 1. It can be seen that the ground-state energies derived from the effective potential (3) show pronounced deviations from the DH results, especially for larger values of non-ideality parameters. The results for the degree of ionization are shown in figure 2 for various temperatures as a function of density.

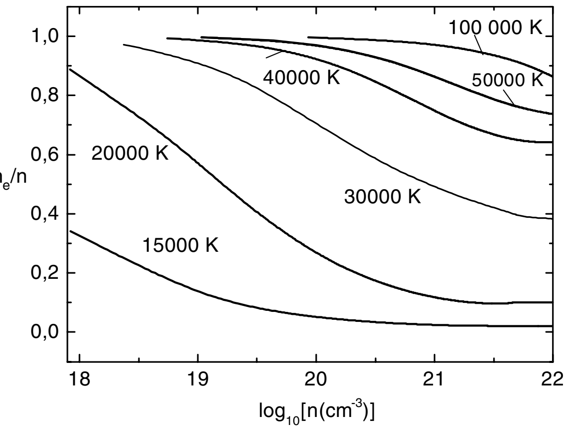

Figure 2. Degree of ionization for hydrogen plasma for various temperatures as a function of the total electron density n.

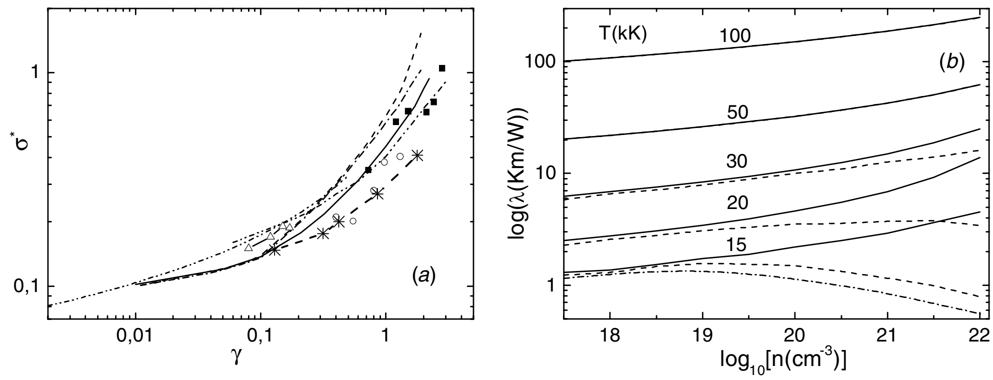

Figure 3. (*a*) Reduced electrical conductivity σ^* as a function of the non-ideality parameter γ: (——), present results using equation (9); (· · · ·), Spitzer theory; ∗- - -∗, results of Ichimaru and Tanaka [29] based on a generalized Ziman formula; (- - - -) and (—·—·—), previous data for fully ionized hydrogen plasma [14, 24]; (··—··): T matrix results [6, 7]; (△), (■) experimental data from [30, 31]; (○) and (■), experimental data from [32]. (*b*) Thermal conductivity λ of partially ionized hydrogen plasma (- - - -) at the various temperatures compared with results for the fully ionized case (——) as a function of the total electron density n. The dash-dotted line (— · —) presents the results of [6] at $T = 15$ kK.

The dimensionless electrical conductivity

$$\sigma^* = \frac{e^2 m_e^{1/2}}{(4\pi\varepsilon_0)^2 (kT)^{3/2}}\sigma \qquad (11)$$

is shown in figure 3(*a*) as a function of the non-ideality parameter γ.

We compare our results for the electrical conductivity with the Spitzer theory [27], with results based on T matrix calculations [6, 7, 23, 28], with the previous results by Nurekenov *et al* [14] using the partial wave method and of Ramazanov *et al* [24] using a Coulomb logarithm for non-ideal plasma [25], as well as with the results of Ichimaru and Tanaka [29] using a generalized Ziman formula. The available experimental data of Radtke *et al* [30, 31] and Ivanov *et al* [32] are also shown.

For ideal plasmas $\gamma \ll 1$, we have good agreement with Spitzer theory. The previous results for the fully ionized case agree well with the present data for the partially ionized plasma if $\gamma \leqslant 0.1$. The divergence between these results can be treated by the difference in plasma composition in the considered region of non-ideality. For higher non-ideality parameters, the electrical conductivity of the partially ionized plasma is substantially lower. Up to $\gamma \approx 0.3$ we have a reasonable coincidence with the experimental data [30–32]. In the weak coupling regime $\gamma \approx (0.4–0.7)$ we have good agreement with the values obtained in T matrix calculations [6, 7]. Such behaviour is a result of the small difference in this region between model (3) and the DH potential. At $\gamma \geqslant 1$ we have good agreement with the experimental data of Ivanov *et al* [32].

The thermal conductivity was calculated within the second expansion by Sonine polynomials and reads

$$\lambda = 4\frac{\begin{vmatrix} L_{ej}^{00} & L_{ej}^{01} & 0 \\ L_{ej}^{10} & L_{ej}^{11} & x_i \\ 0 & x_j & 0 \end{vmatrix}}{\begin{vmatrix} L_{ej}^{00} & L_{ej}^{01} \\ L_{ej}^{10} & L_{ej}^{11} \end{vmatrix}}. \tag{12}$$

Here L_{ej}^{00} are the matrix elements corresponding to the respective transport cross sections of the plasma's components, $(j = e, i, a)$. $x_i = n_i/n$, where n_i is the plasma component density $(i = e, i, a)$, and n is the total density of plasma particles. For instance, see [34] where expression (12) is described in detail. The results of the calculation of the thermal conductivity for various temperatures are shown in figure 3(b). It is shown that taking into account the neutral particles is more important at low temperatures and high densities. In our approach the neutral particles are negligible at temperatures higher than 50 kK at all density regions. In the low-density region our results have good agreement with the calculations of [6] in the framework of linear response theory on the basis of the DH potential, but are essentially different in the high-density region.

5. Conclusions

In this paper, we have investigated the component composition and the transport properties (electrical and thermal conductivity) of partially ionized hydrogen plasma using effective potentials for the interaction between the particles (electrons, protons, atoms). It is shown that the present results for electrical conductivity using the effective potential, which takes into account three-particle correlations for the dense charged subsystem, have good agreement with Spitzer theory at low densities ($\gamma \ll 1$) as well as with available experimental data in the high coupling regime ($\gamma > 1$). Also, the results show that it is important to take into account neutral particles for the calculation of the electrical and thermal conductivities for non-ideal plasmas at lower temperatures, i.e. for plasmas with $\gamma > 0.1$ and $T < 300\,00$ K. This can be seen from the comparison of the present results with the theoretical results of the approach of full ionization with the same model of interaction (for instance, see results of [14, 24] for fully ionized plasma in figure 3(a)). The results for the ionization equilibrium clearly indicate that taking into account the three-particle correlations in charged particle interaction leads to increasing of the ionization degree relatively to the results, on the basis of the DH potential (see table 1). The consideration of further effects, such as the formation of molecules H_2 at low temperatures, is possible; see [33].

Acknowledgments

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