

Comment on “Thermodynamic and transport properties of dense hydrogen plasmas”

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(Received 3 April 1996; revised manuscript received 10 June 1996)

In a recent paper H. Reinholz, R. Redmer, and S. Nagel [Phys. Rev. E. **52**, 5368 (1995)] developed a model of thermodynamic and transport properties of dense hydrogen plasmas, based on the Debye screening potential with the characteristic length interpolating between Debye and Thomas-Fermi radii. It is shown that under the thermodynamic conditions considered this model potential is inapplicable, and the electrical conductivity values predicted are inconsistent with available experimental data. I conclude that the results of Reinholz, Redmer, and Nagel on the plasma composition and the transport coefficient values are thus dubious. [S1063-651X(98)15702-1]

PACS number(s): 52.25.Kn, 52.25.Fi

The keystone of the paper by Reinholz, Redmer, and Nagel [1] is the Debye interaction potential [Eq. (11) of [1]] with the screening length determined by the free electrons only, and constructed (see, e.g., [2]) as an interpolation between the Debye length and the Thomas-Fermi length. Notice that Eq. (12) of [1], which determines the effective screening radius used in [1], contains a small numerical error: to get a correct expression for the screening length one has to multiply the right-hand side of Eq. (12) by 4π . (The Debye model can be more effective if the screening length is determined in a self-consistent way [3].)

To be important, the screening effect has to take place on distances longer than the average distance between charges, or the number N_D of free particles in the Debye sphere, $N_D = (4\pi/3)R_D^3 n_f$, must be at least greater than 1. Nevertheless, a simple calculation shows that under thermodynamic conditions considered in Fig. 1 of [1] (temperature T of 15×10^3 K, and the number density of protons $n = 10^{18} - 10^{25}$ cm $^{-3}$) the average distance between charged particles $d = (3/4\pi n)^{1/3}$ equals the screening length R_D of [1] at $n = 6.4 \times 10^{18}$ cm $^{-3}$, and $N_D = 0.8 - 0.07$ for $n = 10^{19} - 10^{24}$ cm $^{-3}$. For this evaluations I considered all electrons to be delocalized, i.e., since N_D (for $n > 10^{25}$ cm $^{-3}$) is approximately proportional to $n_f^{1/2}$, n_f was substituted by n , otherwise N_D would be even smaller.

In addition, at $n_f = 2.5 \times 10^{25}$ cm $^{-3}$ R_D equals the electronic de Broglie wavelength (about 2 Å) and for $n_f = 1.7 \times 10^{25}$ cm $^{-3}$ the Coulomb corrections ($-e^2/R_D$) to the ionization potential reaches (-13.6 eV). The point is that under the thermodynamic conditions considered the hydrogen plasma is a dense liquidlike Coulomb system with collectivized electrons, and no place for well-defined bound states. The classical Debye potential used in [1] fails at distances of the order of the electronic de Broglie wavelength (see, e.g., [4]), and at least, the exchange interaction contribution to the system Hamiltonian is not taken into account.

The employment of the Debye potential is equivalent, within the dielectric function $[\varepsilon(k)]$ formalism, to the substitution of the polarization operator

$$\Pi(k) = k^2[\varepsilon(k) - 1]/(4\pi e^2)$$

by its long-wavelength asymptotic value. It is well known that the system stability can be guaranteed by the inclusion of the short-wavelength asymptotic form of $\Pi(k)$, and, I believe, the best approach can be achieved by going beyond the (static) random-phase approximation (RPA), as the authors of [1] try to do on p. 5379, calculating the effective ion-ion potential. Notice that already the RPA polarization operator has a sufficiently good short-wavelength behavior, so that one can use a semiclassical local-field correction $G_e(k)$, e.g., of Ref. 77 of [1], without limiting oneself [1] to the parametric form of $G_e(k)$ valid at $T=0$ only.

Perhaps these contradictions and inconsistencies resulted in the overestimation of the bound states' population as described in Fig. 1 of [1] (p. 5373).

The analysis of the conductivity values presented in [1] (Fig. 7, p. 5380) might serve to verify the validity of these results on the plasma ionization degree. In Fig. 7, and especially in the $n = 10^{20} - 10^{22}$ cm $^{-3}$ interval, one observes strong discrepancies between the predictions of the models of fully (FIP) and partially ionized (PIP) plasma. The FIP results are within the error corridor of existing experimental data, and are close to the results of Ref. 77 of [1] and Refs. [5], obtained on the basis of the self-consistent field model of strongly coupled plasmas [6]. [I would like to stress that the basic formulas of this model can hardly be considered “fit” ones. I am afraid the authors of [1] referred to Eq. (7) of Ref. [77], which is not a fit, but an expression describing an approximation to the Spitzer formula, it was never used in our computations.]

Notice that these latter results are in good agreement with the data of the experiments on capillary discharges [7,8], etc.

Particularly, the discharge plasma obtained in [7] was presumed to be the FIP with $n_f = 6 \times 10^{22}$ cm $^{-3}$ and $T = 7 - 13$ eV, and $\sigma^{\text{expt}} = (0.17 - 1.33) \times 10^5$ ($\Omega \text{ m}$) $^{-1}$; the results of our computations for hydrogen plasmas with these conditions varied (Ref. 77 of [1]) between 1.58 and 3.14×10^5 ($\Omega \text{ m}$) $^{-1}$; in the case of Ref. [8] $\sigma^{\text{expt}} = (0.29 - 0.40) \times 10^6$ ($\Omega \text{ m}$) $^{-1}$, and our result for $n_f = 4 \times 10^{21}$ cm $^{-3}$ and $T = 17 - 18$ eV, also reported in Ref. 77 of [1], was $(0.28 - 0.30) \times 10^6$ ($\Omega \text{ m}$) $^{-1}$. More data can be found in [5].

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Our results (see Ref. 77 of [1]) for $T=15\times 10^3$ K vary for $n_f=10^{20}-10^{22}$ cm⁻³ between 10^4 and 2×10^5 (Ωm)⁻¹ (see also [9]), and are higher than the range given in Fig. 7 of [1] for FIP. On the other hand, the PIP results provided in Fig. 7 of [1] achieve these values of conductivity at $n=10^{24}$ cm⁻³, when, according to Fig. 7 of [1], the ionization rate is still about 0.5. This level of matter density, two orders of magni-

tude higher than that of solid state, can be achieved only in inertial-confinement experiments, and has nothing to do with experimental conditions of Refs. [7-9].

I conclude that the results of [1] on composition and transport coefficients of dense hydrogen plasmas are dubious.

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