Thermodynamics and transport of high-density hydrogen plasma

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The development of new technologies and experimental techniques has triggered intensive theoretical studies on modeling spatially confined quantum systems [1, 2] and also extreme-high-pressure plasmas [3] like in stellar envelopes [4]. The thermodynamics of high-density hydrogen plasmas has been deeply investigated [5, 6, 7, 8, 9], due to the necessity of properly accounting for the effects of the multi-body interaction and in principle requiring the reformulation of the statistical mechanics in terms of a global Hamiltonian for the whole gas, instead of the usual separable form of non-interacting chemical species characterized through internal and translational partition functions. The complexity of the rigorous approach led to the development of simplified models, able to include the neighbor-effects on the isolated system though remaining consistent with the traditional thermodynamic approach. The non-ideality affects also the transport properties and in the case of dense, non-ideal, weakly-ionized Debye hydrogen plasma, the electrical conductivity in the non-metal-to-metal transition region at 150 GPa has been measured [10]. The thermodynamic properties and the electrical conductivity of non-ideal, high-density hydrogen plasma have been investigated, accounting for quantum effects due to the change in the energy spectrum of atomic hydrogen when the electron-proton interaction is considered embedded in the surrounding particles. High-density conditions have been simulated assuming a simple confined-atom model, with the atom fixed in the centre of a spherical box, or atomic hydrogen subject to a screened Coulomb potential.

The spectrum of electronic levels characterizing the hydrogen atom in different confining configurations has been derived, implementing finite difference algorithm in the solution of the eigenvalue problem. Decreasing the radius of the spherical domain, i.e. in very high-pressure regimes, quantum effects act moving the bound (negative) levels to the continuum edge (*Mott effect*) [7], reducing the number of terms in the internal partition function of the atomic hydrogen, and decreasing the ionization potential. Considering the electron-proton interaction embedded in a plasma the effect of the surrounding particles have to be taken into account and the Coulomb potential replaced by an effective screened potential characterized by the Debye length λ_D. In this case the influence of the plasma, accounted including the Debye-Hückel correction, produces a lowering of the ionization energy, that for the hydrogen atom corresponds to the

so-called *self-energy shift*, $\Delta = -e^2/\lambda_D$, thus leading to an *effective* value [7, 11] $I_{eff} = I_0 + \Delta$, where I_0 is the ionization potential of the isolated, unperturbed hydrogen atom. Actually an additional lowering is due to the effect of the presence of a screened Debye potential on the eigenvalues for electronic levels, obtained solving the Schrödinger equation. In fact, as in the case of box confinement, the negative eigenvalues progressively move towards the continuum edge and then fall into the pseudo-continuum as the Debye length decreases.

In the frame of the statistical mechanics and adopting a self-consistent cutoff, including all the bound (negative) levels compatible with λ_D value [11], the equilibrium constant for the ionization process has been estimated with the Saha equation.

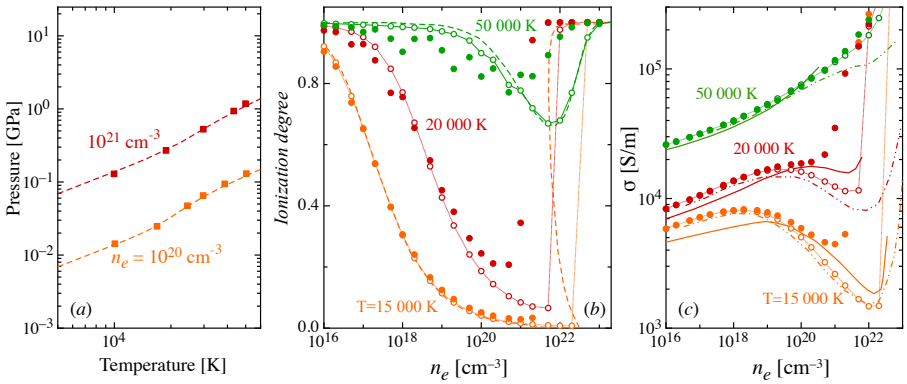

Figure 1: *Debye hydrogen plasma: (a) pressure isochors (close squares) as a function of temperature (dashed lines) Ref. [12], (b) ionization degree as a function of total (bound+free) electron density, for different temperatures, (full circles) including or neglecting (open circles) the effect on atomic electronic levels, (dashed lines) results from Ref. [7], (c) electrical conductivity as a function of the total (bound+free) electron density, for different temperatures, including (full circles) or neglecting (open circles) the effect on atomic electronic levels in the equilibrium calculation, (solid lines) Ref. [17], (dashed-dotted lines) Ref. [18].*

Non-ideality is accounted by including the Debye-Hückel correction for the lowering of ionization potential and the actual ensemble of levels consistent with the Debye length value, affecting the internal partition function of H atom and the effective ionization potential. The pressure isochors (Fig. 1(*a*)) compare rather satisfactorily with the results obtained in Ref. [12] performing a direct path integral Monte Carlo simulation, i.e. estimating the internal partition function from configurational integrals that includes simultaneously the different interactions. The ionization degree $\alpha = N_e/(N_e + N_H)$ has been calculated at constant total electron density $n_e = N_e + N_H$, i.e. electrons bound in atomic system plus free electrons formed in ionization, over the explored temperature. The isotherms (Fig. 1(*b*)) exhibit the phenomenon of *pressure ionization* [7, 11], i.e. the rapid increase of α attaining the high-density regime, where non-ideal effects dominate. The results obtained including or neglecting the effect on atomic electronic

levels due to the screened Coulomb potential, has been compared for different temperatures to results in Ref. [7]. In the high-density region the change, usually neglected, in the spectrum of levels is effective in emphasizing the pressure ionization.

The effects of non-ideality on transport properties have been investigated in the frame of the Chapman-Enskog theory [13], assuming the collision integrals for *e*-H interaction unaffected, while charged-particle interactions modelled with accurate Debye-length-dependent collision integrals by Mason [14, 15], recently fitted in a wide temperature range in Ref. [16]. The electrical conductivity of Debye plasma (Fig. 1(*c*)), exhibits a dependence on the total electron density that is affected by the pressure ionization, i.e. the minimum behaviour of the conductivity and the Mott transition, merging to the fully ionized regime. The present results have been compared with results in literature, obtained in the frame of different theories. In particular, in Ref. [17] the two-term Boltzmann equation is solved including in the collisional terms accurate elastic transport cross sections for *e*-*e* and *e*-H interactions, re-evaluated so as to account for the additional screened Coulomb potential in the first Born approximation, while in Ref. [18] the linear response theory is used for transport. Both Refs. [17, 18] neglect the contribution of excited levels in the atomic internal partition function, one dealing with the ground-state approximation and the second using the Planck-Larkin approach to avoid divergence. Significant differences are observed when the effect of the Debye screening on atomic electronic levels, and in turn on the internal partition function, is considered, while a satisfactory agreement is found neglecting the change in the level ensemble.

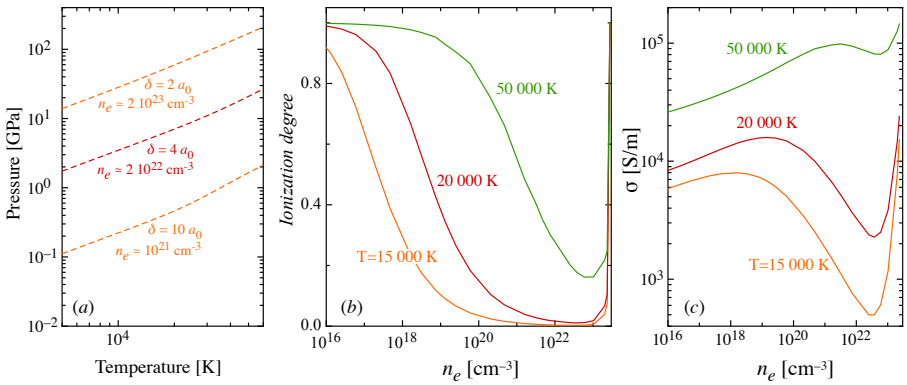

Figure 2: *Confined hydrogen: (a) pressure isochors as a function of temperature, (b) ionization degree and (c) electrical conductivity as a function of the total (bound+free) electron density, for different temperatures.*

The ionization equilibrium for a H atom confined in a spherical domain has been calculated, for each confining configuration, adopting a *natural cutoff* [8], i.e. including only bound eigenvalues in the internal partition function of H atom, the lowering of ionization potential due, in this case, only to the level shift to the pseudo-continuum in decreasing the box radius. The ion-

ization degree isotherms (Fig. 1(*b*)) show the minimum due to the pressure ionization, though the phenomenon is less effective, in fact a sharp increase of α to unitary value, following the rapid transition to the non-ideal behaviour, is observed only for confining radii that are of the order of few bohrs, when almost all levels fall in the pseudo-continuum and only the 1*s* level does exist. The electrical conductivity (Fig. 1(*c*)) is largely determined by the electron density, thus displaying a dependence on n_e that mimics the one of the ionization degree.

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