Realization of electron degeneracy effects as virtual upshifting in the ionization energies in the classical Saha equation

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We explain that the effects of electron degeneracy on the calculation of ionization equilibrium can be implemented and simply realized as virtual upshifting in the ionization energies in the classical Saha equation. Previous quantitative findings indicating depressed quantum statistical ionization compared to classical ionization are derived and abstracted in an analytical form. A simple ready-to-use approximate formula for the upshifting in ionization energies due to partial degeneracy is presented and used to work a sample problem.

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I. INTRODUCTION

Accurate description of strongly coupled plasma systems with completely or partially degenerate electrons is a subject of great interest to both fundamental and applied sciences. These plasmas do exist naturally in the compressed high-density interiors of the evolved stars and are being generated in the laboratory by virtue of different techniques and applications such as (a) irradiating solid targets by short laser pulses or ion beams, (b) shock compression of metals, and (c) discharges of high current densities in inertial confinement experiments such as Z pinches, etc. The understanding and interpretation of the observations and experimental results from the above-mentioned plasma systems necessitate rigorous approaches for modeling the equation of state and thermodynamic and radiative properties, taking into account both of the coupling and degeneracy effects. The importance of taking degeneracy and quantum effects into consideration is well recognized in previous studies by Rogers *et al.* in the "physical picture" (see, for example, [1]).

The routine approach to the calculation of ionization equilibrium, within the chemical picture, for *classical* plasma systems involves the construction and minimization of the Helmholtz free-energy function. Electrostatic interactions among charged particles and other possible couplings and corrections are usually condensed in a correction term—*excess free energy* ΔF^{int}—to be added to the classical ideal free-energy function where

$$F^{\text{cls}} = F^{\text{cls}}_{\text{ion,id}} + F^{\text{cls}}_{e,\text{id}} + \Delta F^{\text{int}}. \tag{1}$$

The term ΔF^{int} can be generally expressed as the sum of a Coulombic or electrical part plus a non-Coulombic part $\Delta F^{\text{int}} = \Delta F^{\text{Coul}} + \Delta F^{\text{non-Coul}}$.

Heavy particles remain classical, even when the plasma density is very high, and their free energy from Maxwell-Boltzmann statistics can be written as

$$F^{\text{cls}}_{\text{ion,id}} = K_B T\left[- N_{\text{ion}} + \sum_{j=1}^{J} \sum_{\zeta=0}^{\zeta_{\max}} N_{j,\zeta} \ln(N_{j,\zeta}\Lambda^3_{j,\zeta}/VU_{j,\zeta})\right], \tag{2}$$

where K_B is the Boltzmann constant, T is the absolute temperature, V is the volume of the system, $N_{j,\zeta}$, $\Lambda_{j,\zeta} = \frac{h}{\sqrt{2\pi m_{j,\zeta} K_B T}}$ and $U_{j,\zeta}$ are the number, thermal wavelength, and internal partition function of the ion ζ of the chemical element j, respectively. The corresponding expression for the classical ideal free energy of electrons is therefore

$$F^{\text{cls}}_{e,\text{id}} = K_B T N_e[-1 + \ln(N_e \Lambda^3_e/2V)], \tag{3}$$

where N_e is the number of free electrons in the system.

This approach leads to the eminent advantage that the free-energy minimization technique automatically engenders thermodynamically consistent properties. Free-energy minimization can also lead to a system of minimization equations having the form of the well-known Saha equations with shifting in the ionization energies for the ζ-fold ion in the system given by [2,3]

$$\Delta I_\zeta = (\partial/\partial N_e - \partial/\partial N_\zeta + \partial/\partial N_{\zeta+1})\Delta F^{\text{int}}. \tag{4}$$

Supplemented by the constraints of electroneutrality and conservation of nuclei, one can determine the detailed plasma composition either by optimization algorithms of the free energy function or by solving the set of coupled nonideal and classical Saha equations.

The aforementioned classical statistical approach falls short at sufficiently high densities suffering major thermodynamic instabilities. For example, the classical plasma pressure would collapse at high densities due to the negative electron-ion interaction energy; whereas in reality the pressure remains positive. These instabilities are generally inhibited in a plasma system by quantum effects due to the Fermi pressure (exclusion principle) of the electrons. As a consequence, the Fermi statistics has to be used for electrons in order to take the degeneracy into consideration.

Recently, Molinari *et al.* [4] considered the case of weak degeneracy and cast the Fermi distribution function into an *approximate* form of a Maxwellian distribution with a correction term linear in the Sommerfield parameter and they derived an *approximately* corrected Saha equation. The nonlinear correction term in Molinari *et al.* corrected Saha equation vanishes as the Sommerfield parameter goes to zero. However, their quantitative results showed the absolute relative error resulting from ignoring the degeneracy and calculating the ionization equilibrium from the classical Saha equation for hydrogenic plasma. It was not clear whether the degeneracy of free electrons will enhance or depress ionization, although it was shown to be important for high-density and low-temperature region.

In an earlier and more complete work, Wilhelm and Hong [5] considered the partial degeneracy of free electrons to any degree of degeneracy and derived a quantum statistical Saha equation as given in Eq. 9 in Ref. [5]. The form of Wilhelm and Hong equation—though correct—did not allow direct analytical conclusion about the effects of degeneracy on the calculation of ionization equilibrium. Conclusions were obtained only from quantitative results for the studied cases (Cs and H plasmas), where a comparison of the quantum statistical and classical Saha ionization equations indicated that degeneracy effects in the electron gas suppress somewhat the ionization at high densities and that the classical Saha equation can be satisfactorily used at low to moderate densities.

In this Brief Report, we present the simple realization of quantum statistical (degeneracy) effects on the ionization equilibrium as a virtual shifting in the ionization energies. The condensation of the corrections in such a simple well-understood term allows a direct analytical abstraction of the effect of degeneracy on the ionization equilibrium as shown below.

II. DEGENERACY AND IONIZATION EQUILIBRIUM

For partially degenerate electrons, the free energy of an ideal Fermi gas is used for quantum electrons to replace the corresponding classical term in Eq. (3), where

$$\begin{aligned} F_{e,\mathrm{id}}^{\mathrm{deg}} &= -P_e V + N_e \mu_{e,\mathrm{id}} \\ &= -(2K_B T V/\Lambda_e^3) I_{3/2}(\mu_{e,\mathrm{id}}/K_B T) + N_e \mu_{e,\mathrm{id}}. \end{aligned} \tag{5}$$

In which P_e and $\mu_{e,\mathrm{id}}$ represent the pressure and chemical potential of the ideal Fermi electron gas, respectively, and I_ν is the complete Fermi-Dirac integral,

$$I_\nu(x) = \frac{1}{\Gamma(\nu+1)} \int_0^\infty \frac{y^\nu}{\exp(y-x)+1} dy. \tag{6}$$

The electron chemical potential $\mu_{e,\mathrm{id}}$ is related to the number of free electrons in the system by

$$N_e = (2V/\Lambda_e^3) I_{1/2}(\mu_{e,\mathrm{id}}/K_B T), \tag{7}$$

where $\Lambda_e = \frac{h}{\sqrt{2\pi m_e K_B T}}$ is the average thermal wavelength of the electrons.

A simple way to consider and to implement electron degeneracy in the Saha equation and the corresponding thermodynamic functions is to add to the free-energy function, which contains Eq. (5) instead of the classical expression for the electron [Eq. (3)], the classical expression $F_{e,\mathrm{id}}^{\mathrm{cls}}$, and subtract it again. The final expression for the free-energy function will be the same as that for the classical plasma plus a correction term $(F_{e,\mathrm{id}}^{\mathrm{deg}} - F_{e,\mathrm{id}}^{\mathrm{cls}})$. This correction term can be used to find the virtual change in the ionization energies as explained above. Noting that the degeneracy correcting term $(F_{e,\mathrm{id}}^{\mathrm{deg}} - F_{e,\mathrm{id}}^{\mathrm{cls}})$ does not depend on the heavy particle densities indicates that the shifting in the ionization energies resulting from considering the electron degeneracy will be the same for all ions and can be found as follows

$$\begin{aligned} \frac{\Delta I_{\mathrm{deg}}}{K_B T} &= \frac{\partial}{\partial N_e}\left(\frac{F_{e,\mathrm{id}}^{\mathrm{deg}}}{K_B T} - \frac{F_{e,\mathrm{id}}^{\mathrm{cls}}}{K_B T} \right) \\ &= \frac{\mu_{e,\mathrm{id}}^{\mathrm{deg}}}{K_B T} - \frac{\mu_{e,\mathrm{id}}^{\mathrm{cls}}}{K_B T} = I_{1/2}^{-1}\left(\frac{n_e \Lambda_e^3}{2} \right) - \ln\left(\frac{n_e \Lambda_e^3}{2} \right), \end{aligned} \tag{8}$$

where $I_{1/2}^{-1}(x)$ is the inverse Fermi-Dirac integral. One can investigate the sign of the term $\frac{\Delta I_{\mathrm{deg}}}{K_B T}$ in Eq. (8) by considering the two integrals

$$K_1 = \frac{1}{\Gamma(3/2)} \int_0^\infty \frac{y^{1/2}}{\exp(y-x')+1} dy = I_{1/2}(x'), \tag{9}$$

and

$$K_2 = \frac{1}{\Gamma(3/2)} \int_0^\infty \frac{y^{1/2}}{\exp(y-x)} dy = e^x. \tag{10}$$

The integrands of both K_1 and K_2 are positive, finite, and continuous. For $x=x'$ the integrand of K_2 shows higher values than that of K_1 over the whole domain of integration, which implies that

$$K_2(x) > K_1(x'=x). \tag{11}$$

Inspection of the integrand of K_1 shows that the integrand and consequently K_1 increases with the increase of x' (for both positive and negative values of x'). Now, in order to make K_1 and K_2 equal (i.e., $K_1=K_2=\beta$), the argument of K_1 (i.e., x') must be undoubtedly greater than the argument of K_2 (i.e., x); that is,

$$[x' = K_1^{-1}(\beta)] > [x = K_2^{-1}(\beta)]$$

or

$$I_{1/2}^{-1}(\beta) > \ln(\beta). \tag{12}$$

The superscript (-1) used with K_1, K_2, and $I_{1/2}$ above refers to the inverse of the function. Equation (12) directly implies that the term $\frac{\Delta I_{\mathrm{deg}}}{K_B T}$ in Eq. (8) is always positive with the implication that *considering electron degeneracy virtually elevates the ionization energies in the classical Saha equation*. It has to be noted that one can arrive at the same analytical result from Wilhelm and Hong's equation by simple algebraic manipulation of their equation.

For practical use of Eq. (8), we provide herein a ready-to-use approximate expression for the shifting in the ionization energies resulting from degeneracy effects. The expression is derived using Zimmermann's [6] approximation of the inverse Fermi-Dirac integral, where one can write

$$\begin{aligned} \frac{\Delta I_{\mathrm{deg}}}{K_B T} &= [-1 + 0.176\,8y - 0.001\,65y^2 + 0.000\,031y^3] \\ &\quad + y\left[\frac{1}{y} + 0.176\,8 - 0.003\,3y + 0.000\,093y^2 \right] \\ &\quad \text{for } \boldsymbol{y} = \frac{N_e \Lambda_e^3}{2V} < 5.5, \end{aligned} \tag{13}$$

$$\frac{\Delta I_{\mathrm{dgc}}}{K_B T} = [-\ln y + 0.725\,4y^{2/3} - 2.040\,9y^{-2/3} + 0.85y^{-2}] + y[0.483\,6y^{-1/3} + 1.360\,6y^{-5/3} - 1.7y^{-3}] \quad \text{for } \boldsymbol{y} \geq 5.5. \tag{13}$$

III. SAMPLE PROBLEM

The above approximate expression [Eq. (13)] is used to study the electron degeneracy effects on the composition of dense helium plasma. The customary lowering of ionization energy for the dense plasma resulting from the electric or Coulombic correction to the free energy is taken from Zimmerman and More [7]. Details about the calculation of the partition functions and the algorithm used to solve the set of governing equations can be found elsewhere [8].

Figure 1 shows the values of the average ionization state, ζ_{av}, versus the number density of heavy particles, n_H, for 2 eV He plasma calculated considering the electron degeneracy in comparison to the results from the classical noncorrected Saha equation. As can be noted from the figure, the general effect of electron degeneracy is to depress ionization as analytically predicted above. The degeneracy effects become significant and cannot be overlooked at high densities, while the classical Saha equation can still be satisfactorily used for low to intermediate densities which agrees with Wilhelm and Hong's quantitative findings.

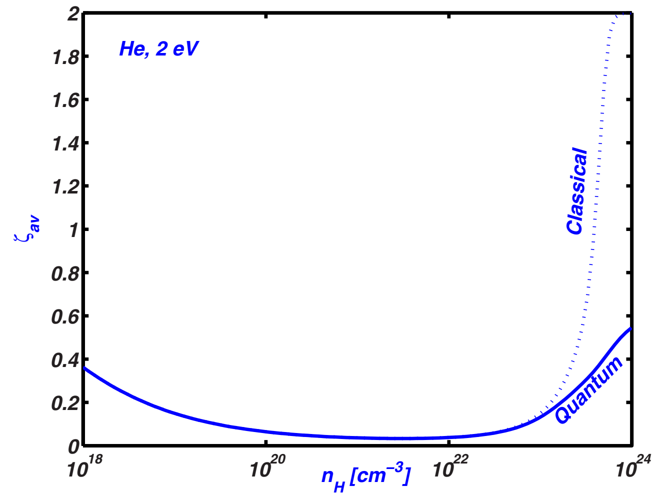

FIG. 1. (Color online) Values of the average ionization state ζ_{av} for 2 eV He plasma calculated considering the electron degeneracy (solid line) in comparison to the results from the classical noncorrected Saha equation (dotted line).

IV. CONCLUSIONS

The effects of electron degeneracy on the calculation of ionization equilibrium are simply realized as virtual upshifting in the ionization energies in the classical Saha equation. A simple ready-to-use approximate formula for the upshifting in ionization energies due to partial degeneracy is presented and used to work a sample problem.

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