Parametrized equation of state for dense hydrogenic plasmas

Shigenori Tanaka and Setsuo Ichimaru
Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan
(Received 2 July 1985)

We derive analytic formulas for the interaction and excess-free energies of dense hydrogenic plasmas, which accurately parametrize the numerical data calculated earlier in the hypernetted chain approximation at various degrees of intermediate Fermi degeneracy of the electrons and which exactly satisfy the known boundary conditions at complete degeneracy as well as in the weak- and strong-coupling regimes. The resulting equation of state is valid over a wide range of densities and temperatures, as long as the system is in a liquid-metallic state.

In a recent series of publications,[1] Mitake, Yan, and the present authors developed a general theory of interparticle correlations in dense plasmas within the framework of the hypernetted chain (HNC) approximation,[2] and thereby calculated various physical quantities for the special cases of the hydrogenic plasmas where the ionic charge number $Z=1$. The interaction energy $E_{\rm int}$ was computed, in particular, for 32 parametric combinations at various degrees of intermediate Fermi degeneracy of the electrons in III; the numerical results were then parametrized in analytic interpolation formulas.

For hydrogenic plasmas we define a set of dimensionless parameters as

$$\Gamma=\frac{e^2}{k_BT}\left[\frac{4\pi n}{3}\right]^{1/3}, \tag{1}$$

$$\theta=\frac{2mk_BT}{\hbar^2}(3\pi^2n)^{-2/3}, \tag{2}$$

$$r_s=\left[\frac{3}{4\pi n}\right]^{1/3}\frac{me^2}{\hbar^2}=\frac{1}{2}\left[\frac{9\pi}{4}\right]^{2/3}\Gamma\theta, \tag{3}$$

where m is the rest mass of an electron and n refers to the number density of the electrons (or the protons). Γ, θ, and r_s, respectively, are the Coulomb-coupling constant of the ions, the Fermi degeneracy parameter, and the density parameter of the electrons.

The interpolation formula for $E_{\rm int}$ derived in III had a simple structure and was capable of reproducing all the 32 cases of the computed values for $\theta=0.1$, 1, 10, and $\Gamma\le 2$ with disgressions of less than 2%. Although successful in reproducing those computed results, the formula did not take a proper account of the existing knowledge on $E_{\rm int}$ in the limit of $\theta\to 0$ or $\Gamma\to 0$, nor did it describe appropriately the behavior of $E_{\rm int}$ in the strong coupling regime, $\Gamma\gg 1$.

The purpose of the present paper is therefore to revise and improve on the interpolation formulas obtained in III, so that those limiting properties are correctly taken into account as well. Such formulas have been derived for the electron one-component plasma (OCP) in the Singwi-Tosi-Land-Sjölander approximation[2,3] elsewhere.[4]

We begin with consideration of various limiting behaviors in $E_{\rm int}$.

(a) $\theta\to 0$. When Γ is kept at a finite value, r_s approaches zero in this limit as Eq. (3) indicates. The electrons thus form an unpolarizable negative-charge background to the ions. The system may be looked upon as an independent superposition of an ionic OCP and a collection of free electrons. The contribution E_{11} of the electrons to the interaction energy is given by the Hartree-Fock value,

$$-\frac{1}{\Gamma}\frac{E_{11}}{Nk_BT}=\frac{3}{4\pi}\left[\frac{9\pi}{4}\right]^{1/3}\simeq 0.458\,17, \tag{4}$$

where N is the total number of the electrons in the system. For the ionic OCP contribution, $-(1/\Gamma)(E_{22}/Nk_BT)$, we take note of the Debye-Hückel values $(\sqrt{3}/2)\Gamma^{1/2}$ for $\Gamma\le 0.003$, the HNC values[5] and parametrization[6] for $0.003<\Gamma<1$, and the Monte Carlo (MC) simulation values and fitting formula[7] for $\Gamma\ge 1$. Consequently, in the limit of $\theta\to 0$, we have

$$-\frac{1}{\Gamma}\frac{E_{\rm int}}{Nk_BT}=-\frac{1}{\Gamma}\frac{E_{11}}{Nk_BT}-\frac{1}{\Gamma}\frac{E_{22}}{Nk_BT}=\begin{cases}0.458\,17+0.866\,03\Gamma^{1/2}, & \Gamma\ll 1\\ 0.458\,17+\alpha, & \Gamma\gg 1\end{cases} \tag{5}$$

where α represents the coefficient of the Madelung-like strong coupling contribution in $-E_{22}/Nk_BT$.

(b) $\Gamma\to 0$. In the weak coupling limit, the lowest-order exchange energy of the electrons is the dominant contribution to $E_{\rm int}$, so that we may express

$$-\frac{1}{\Gamma}\frac{E_{\rm int}}{Nk_BT}=a(\theta)+O(\Gamma^{1/2}). \tag{6}$$

An accurate fitting formula for $a(\theta)$ has been obtained by Perrot and Dharma-wardana[8] as

$$a(\theta)=\frac{1}{\pi}\left[\frac{9\pi}{4}\right]^{1/3}\frac{0.75+3.043\,63\theta^2-0.092\,270\theta^3+1.703\,50\theta^4}{1+8.310\,51\theta^2+5.1105\theta^4}\tanh\left[\frac{1}{\theta}\right], \tag{7}$$

which we adopt. In the classical limit ($\theta\to\infty$), $a(\theta)$ naturally vanishes and the second term in Eq. (6) proportional to $\Gamma^{1/2}$ becomes the leading contribution in the weak coupling regime; this term can be evaluated in the two-component Debye-Hückel calculation as

$$O(\Gamma^{1/2})=\sqrt{6}\Gamma^{1/2} \ . \tag{8}$$

(c) $\Gamma\gg 1$. In the strong coupling regime, both E_{11}/Nk_BT and E_{22}/Nk_BT behave proportionally to Γ, as one can confirm in the numerical values listed in Tables I–III as well as in the local-field correction curves in Figs. 1 and 2 of III. We note also in Tables I–III and in Fig. 3 of III that the electron-ion interaction energy, E_{12}/Nk_BT, tends to be proportional to $\Gamma^{3/2}$ in the large Γ domain. As a comparison between the local-field correction and random-phase approximation curves in Fig. 3 indicates, this new feature appears to be a consequence of the strong coupling effects described by the local-field corrections. In the expression for $E_{\rm int}/Nk_BT$ we must therefore retain a term proportional to $\Gamma^{3/2}$.

Taking account of those boundary conditions mentioned above, we propose an analytic formula parametrizing the 32 values of $E_{\rm int}$ in III as

$$-\frac{1}{\Gamma}\frac{E_{\rm int}}{Nk_BT}=\frac{a(\theta)+b(\theta)\Gamma^{1/2}+c(\theta)\Gamma+d(\theta)\Gamma^{3/2}}{1+e(\theta)\Gamma^{1/2}+\Gamma} \ , \tag{9}$$

where $a(\theta)$ has been given in Eq. (7), and

$$b(\theta)=\frac{1.3617+0.339\,54\theta+10.100\theta^2}{1+0.286\,38\theta+4.1234\theta^2} \ , \tag{10}$$

$$c(\theta)=\frac{1.3472+3.5283\theta+0.877\,46\theta^2}{1+4.3074\theta+\theta^2} \ , \tag{11}$$

$$d(\theta)=\frac{0.252\,96\theta^{1/2}+1.3094\theta}{1+0.083\,147\theta^{1/2}+\theta} \ , \tag{12}$$

$$e(\theta)=\frac{1.0819+3.8306\theta^{1/2}+0.163\,75\theta}{1+5.9994\theta^{1/2}+\theta} \ . \tag{13}$$

It is clear that the boundary conditions, Eqs. (5)–(8), are exactly satisfied with the coefficient $\alpha=0.889\,03$ in Eq. (5). The formula (9) reproduces the 32 computed values for $0.1\le\theta\le 10$ in III with disgressions of less than 0.4%. It also fits the HNC[5,6] or MC[7] results for $0.003\le\Gamma\le 160$ at the boundary $\theta\to 0$ with relative errors less than 0.8%.

As we observe in Fig. 1 of I, the strong coupling regime $\Gamma>10$ corresponds to $\theta<0.1$ and $\Gamma\theta<0.6$. It thus follows that $c(\theta)\Gamma>d(\theta)\Gamma^{3/2}$ even in the strong coupling regime, so that the former term remains the leading contribution in the numerator on the right-hand side of Eq. (9).

The excess free energy is then given by the coupling-constant integration[9] of Eq. (9) as

$$\begin{aligned}-\frac{F_{\rm ex}}{Nk_BT}&=-\int_0^\Gamma\frac{d\Gamma}{\Gamma}\left[\frac{E_{\rm int}}{Nk_BT}\right]_\theta \\ &=\frac{2}{3}d\Gamma^{3/2}+(c-de)\Gamma+2[b-d-e(c-de)]\Gamma^{1/2}+\{a-c+de-e[b-d-e(c-de)]\}\ln|\Gamma+e\Gamma^{1/2}+1| \\ &\quad-\frac{2}{(4-e^2)^{1/2}}\{e(a-c+de)+(2-e^2)[b-d-e(c-de)]\}\left[\tan^{-1}\frac{2\Gamma^{1/2}+e}{(4-e^2)^{1/2}}-\tan^{-1}\frac{e}{(4-e^2)^{1/2}}\right] \ . \end{aligned} \tag{14}$$

We confirm that the condition, $4-e(\theta)^2>0$, is satisfied at all the possible values of θ.

In conclusion we have derived the analytic expressions, Eqs. (9) and (14), for the interaction and excess-free energies of hydrogenic plasmas, which are valid as long as the system is in a liquid-metallic state.

This research was supported in part through Grant-in-Aid for Scientific Research No. 59380001, provided by the Japanese Ministry of Education, Science, and Culture.

[1]S. Ichimaru, S. Mitake, S. Tanaka, and X.-Z. Yan, Phys. Rev. A **32**, 1768 (1985), referred to as I; S. Mitake, S. Tanaka, X.-Z. Yan, and S. Ichimaru, *ibid.* **32**, 1775 (1985); S. Tanaka, S. Mitake, X.-Z. Yan, and S. Ichimaru, *ibid.* **32**, 1779 (1985), referred to as III; X.-Z. Yan, S. Tanaka, S. Mitake, and S. Ichimaru, *ibid.* **32**, 1785 (1985); S. Ichimaru and S. Tanaka, *ibid.* **32**, 1790 (1985). We closely follow the notation in those papers unless otherwise specified.

[2]See, e.g., S. Ichimaru, Rev. Mod. Phys. **54**, 1017 (1982).

[3]K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).

[4]S. Tanaka, S. Mitake, and S. Ichimaru, Phys. Rev. A **32**, 1896 (1985).

[5]J. F. Springer, M. A. Pokrant, and F. A. Stevens, J. Chem. Phys. **58**, 4863 (1973).

[6]B. Brami, J. P. Hansen, and F. Joly, Physica A **95**, 505 (1979).

[7]W. L. Slattery, G. D. Doolen, and H. E. DeWitt, Phys. Rev. A **21**, 2087 (1980); **26**, 2255 (1982).

[8]F. Perrot and M. W. C. Dharma-wardana, Phys. Rev. A **30**, 2619 (1984).

[9]See, e.g., A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971), Chap. 7.