

Free energies of electron-screened ion plasmas in the hypernetted-chain approximation

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(Received 25 October 1985)

Free-energy formulas applicable to the electron-screened ion plasmas are derived in the hypernetted-chain approximation. The formulas are expressed in terms of the correlation functions and do not involve cumbersome thermodynamic integrations. Accuracy and thermodynamic consistency of the proposed formulas are examined and ascertained through explicit numerical comparison with the results of other independent calculations taking account of electronic screening in the interionic potentials.

I. INTRODUCTION

The hypernetted-chain (HNC) approximation,¹ developed in the study of simple liquids,^{2,3} has been used quite extensively in the theoretical analyses of static correlations in those dense plasmas which may be found in stellar interiors. It has been well demonstrated^{4,5} that the HNC scheme offers an accurate way of describing interparticle correlations in such plasmas. The reason for the accuracy of the HNC scheme in the Coulombic system has been elucidated theoretically through the analyses of the multiparticle correlation functions.⁶

As has been noted by earlier investigators,^{4,7,8} the HNC scheme has a unique feature in that the chemical potential and hence the Helmholtz free energy can be calculated directly through integration involving the correlation functions [see Eq. (3) following]. The calculation of the free energy in the HNC scheme can thus be performed with an accuracy comparable to those of the internal energy and the pressure; the latter quantities involve analogous integrations. In contrast, a general prescription for the calculation of the free energy in an interacting many-particle system⁹ is to carry out an integration of the internal or interaction energy with respect to the inverse temperature or the coupling constant. The numerical errors in the internal or interaction energy are accumulated in the process of such an integration, and the resulting evaluation of the free energy may thus contain a substantial degree of inaccuracy. The aforementioned feature of the HNC scheme has been used advantageously in the analysis of delicate thermodynamic properties of dense-plasma-like matter such as phase separation in multi-ionic plasmas.^{8,10,11}

When the laws of interaction between two particles in the system are specified, the HNC scheme provides a closed set of equations; through a solution to those equations one determines various interparticle correlation functions. In many practical cases of application one encounters a situation in which the "effective" interparticle potential may be regarded as dependent on the thermodynamic variables such as the number density and temperature. For example, the electrons in a dense matter may be assumed to provide a dielectric background which

acts to screen the interaction between the ions;^{4,5} the dielectric screening function may then depend on the number density and temperature of the electrons.¹² The existing derivation of the HNC free-energy formula^{4,7,8} has not, however, anticipated such dependence of the interparticle potential on the thermodynamic variables.

The purpose of the present paper is to provide a theoretical foundation to the HNC free-energy formulas applicable to those cases in which the effective interparticle potentials may depend on the density and temperature. The validity and utility of the resulting formulas are then examined and confirmed through numerical comparisons with the existing calculations in the screened, one-component-plasma (OCP) systems.

In Sec. II, we formulate the problem in physical terms; in Sec. III we define the screened OCP model for the two-component electron-ion plasma. The HNC free-energy formulas are derived in Sec. IV and their accuracy and consistency are examined in Sec. V. Concluding remarks are given in Sec. VI. Some of the calculational details are described in the Appendix.

II. FORMULATION OF THE PROBLEM

For a classical many-particle system with a single species of particles, the radial distribution function $g(r)$ is expressed in the HNC approximation as

$$g(r) = \exp[-\beta\phi(r) + h(r) - c(r)]. \quad (1)$$

Here β is the inverse temperature in energy units, $\phi(r)$ represents the potential of binary interaction, and $h(r) = g(r) - 1$ refers to the pair-correlation function. The direct correlation function $c(r)$ is related to $h(r)$ via the Ornstein-Zernike relation

$$h(r) = c(r) + n \int d\mathbf{r}' c(|\mathbf{r} - \mathbf{r}'|) h(r'), \quad (2)$$

where n is the number density of the particles. Assuming that $\phi(r)$ is independent of the thermodynamic variables, one proves⁷ that the excess chemical potential, i.e., the chemical potential arising from the interaction potential, is given by

$$\beta\mu^{\text{ex}} = \frac{n}{2} \int d\mathbf{r} h(r)[h(r) - c(r)] - n\tilde{c}(q=0), \quad (3)$$

where

$$\tilde{c}(q=0) \equiv \int d\mathbf{r} c(r) \quad (4)$$

is the long-wavelength ($q=0$) value of the Fourier transform to the direct correlation function. For an OCP with ionic charge Ze , $\tilde{c}(q=0)$ in Eq. (3) is replaced^{4,8} by $\tilde{c}_R(q=0)$ with

$$\tilde{c}_R(q) \equiv \tilde{c}(q) + 4\pi(Ze)^2\beta/q^2. \quad (5)$$

This replacement takes account of the presence of the neutralizing background of negative charges in the OCP.

In this paper we wish to extend the derivation described above to those cases in which the potential $\phi(r)$ may depend on the thermodynamic variables; we thereby aim at finding the formulas corresponding to Eq. (3). In particular, we consider the cases of a two-component plasma consisting of N ions with the electric charge Ze and ZN electrons, contained in a box of volume V ; the ions are assumed to obey the classical dynamics and statistics. The Coulomb coupling constant of the ions may be defined as^{4,5}

$$\Gamma = \beta(Ze)^2/a, \quad (6)$$

where $a = (3V/4\pi N)^{1/3}$ is the ion-sphere radius. We may likewise set the Fermi-degeneracy parameter of the electrons as⁵

$$\theta = \frac{2m}{\beta\hbar^2} \left[\frac{V}{3\pi^2 ZN} \right]^{2/3}, \quad (7)$$

where m is the rest mass of an electron. The usual density parameter for the electrons is then given by⁵

$$r_s = \left[\frac{3V}{4\pi ZN} \right]^{1/3} \frac{me^2}{\hbar^2} = \frac{1}{2} \left[\frac{9\pi}{4} \right]^{2/3} Z^{-5/3} \Gamma \theta. \quad (8)$$

In the treatment of two-component plasmas we adopt the adiabatic approximation in the response of the electrons to the ionic field, so that the system under consideration turns into one of an electron-screened ionic plasma, or a screened OCP.¹³ The Fourier transformation of the effective potential $\phi_e(r)$ between ions is then expressed as

$$\tilde{\phi}_e(q) = \frac{4\pi(Ze)^2}{q^2\epsilon(q,0)}, \quad (9)$$

where $\epsilon(q,0)$ is the static dielectric function of the electrons.⁵ The effective potential thus carries dependence on the number density $n_e = ZN/V$ and temperature of the electrons through $\epsilon(q,0)$. The problem at hand then is the derivation of the chemical potential formula, analogous to Eq. (3), when the number density- and temperature-dependent $\phi_e(r)$ is substituted in place of $\phi(r)$ in the HNC equation (1).

The complexities in the derivation of the HNC free-energy formula lie in the treatment of density dependence in the potential; temperature dependence, on the other hand, introduces no such complications.¹⁴ The reason

may be understood by recalling the definition of the chemical potential: It is the change in the Helmholtz free energy induced when a particle is added to the system by keeping the temperature and volume constant. An addition of an ion brings about an addition of electrons, to keep the charge neutrality of the system, which in turn introduces a change in the effective potential through the density dependence of $\epsilon(q,0)$.

In this paper we limit ourselves to the consideration of plasmas with single ionic species only. It is straightforward, however, to extend the results obtained here to the cases of multi-ionic plasmas with electronic screening. In a subsequent paper¹⁵ we shall analyze miscibility problems in hydrogen-iron mixtures which simulate certain features in the dense solar-interior plasma.

III. THE SCREENED OCP MODEL

The Hamiltonian for the screened OCP is expressed as^{4,5}

$$H = F_e + K + \frac{Z^2}{2V} \sum_{q \neq 0} v(q)(\rho_q \rho_{-q} - N) + \frac{Z^2}{2V} \sum_{q \neq 0} v(q) \left[\frac{1}{\epsilon(q,0)} - 1 \right] \rho_q \rho_{-q}. \quad (10)$$

Here K represents the kinetic energy of the ions, $v(q) = 4\pi e^2/q^2$ is the Fourier transform of the bare Coulomb potential, ρ_q is the Fourier component of the ion-density fluctuations, F_e represents the Helmholtz free energy of the uniform electron background. In Eq. (10) we have assumed the electron-ion interaction to be weak, and thereby retained the linear-response contributions only. The terms F_e and K , being simply additive in Eq. (10), will be omitted hereafter.

The screening function $\epsilon(q,0)$ of the uniform electron system may generally be expressed as⁵

$$\epsilon(q,0) = 1 - \frac{v(q)\chi_0(q,0)}{1 + G(q)v(q)\chi_0(q,0)}, \quad (11)$$

where $\chi_0(q,0)$ and $G(q)$ refer to the static values of the free-particle polarizability and the local-field correction for the electrons. As we have remarked earlier, it is important in the ensuing theory that the density and temperature dependence of the screening function be appropriately taken into consideration. We shall write Eq. (11) as $\epsilon(Q,0)$ or more explicitly $\epsilon(Q,0; r_s, \theta)$ when it is re-expressed as a function of the dimensionless variables: $Q \equiv q/q_F$, r_s , and θ , where $q_F = (3\pi^2 n_e)^{1/3}$ is the Fermi wave number.

The product of $v(q)$ and $\chi_0(q,0)$ takes the form

$$v(q)\chi_0(q,0) = - \frac{4\lambda r_s}{\pi Q^2} \left[\sqrt{2\theta} \int_0^\infty dy \frac{y^2}{[\cosh(y^2 - \beta\mu_0/2)]^2} \times J_0 \left[\frac{Q}{2\sqrt{2\theta}y} \right] \right], \quad (12)$$

where $\lambda \equiv (4/9\pi)^{1/3}$, $J_0(x)$ is the usual Kohn function at $\theta=0$,

$$J_0(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|, \quad (13)$$

and μ_0 is the chemical potential in the corresponding noninteracting system. In the limit of $\theta \rightarrow 0$, the factor in the large square brackets of Eq. (12) approaches $J_0(Q/2)$ since $\lim_{\theta \rightarrow 0} (\theta \beta \mu_0) = 1$. If one sets $G(q) = 0$ in Eq. (11), the Lindhard screening function in the random-phase approximation^{5,16} (RPA) is recovered; the function $G(q)$ thus measures the extent of strong-coupling effects beyond the RPA.

The excess Helmholtz free energy in the screened OCP is related with the Hamiltonian (10) in accordance with the basic formula of statistical mechanics,

$$\beta F_{sc} = -\ln(\text{Tr} e^{-\beta H}), \quad (14)$$

where Tr means taking the trace with respect to the ionic coordinates. The excess internal energy U_{sc} is then calculated from Eq. (14) as

$$U_{sc} = \left[\frac{\partial}{\partial \beta} (\beta F_{sc}) \right]_{V,N}, \quad (15)$$

$$\begin{aligned} \frac{P_{sc}}{n} &= \frac{Z^2}{6V} \sum_{q(\neq 0)} v(q) [S(q) - 1] + \frac{Z^2}{6V} \sum_{q(\neq 0)} v(q) \left[\frac{1}{\epsilon(Q,0)} - 1 \right] S(q) \\ &\quad - \frac{Z^2}{6V} \sum_{q(\neq 0)} v(q) \left[r_s \frac{\partial}{\partial r_s} \frac{1}{\epsilon(Q,0)} \right]_{\theta} S(q) - \frac{Z^2}{3V} \sum_{q(\neq 0)} v(q) \left[\theta \frac{\partial}{\partial \theta} \frac{1}{\epsilon(Q,0)} \right]_{r_s} S(q). \end{aligned} \quad (17)$$

IV. HNC FREE-ENERGY FORMULAS

We now wish to derive a free-energy formula in the HNC approximation which is applicable to the system as described by the Hamiltonian (10). For this purpose we find it instructive to rewrite Eq. (10) (with omission of F_e and K) in the real-space form

$$H = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \phi_e(|\mathbf{r}_i - \mathbf{r}_j|) + \frac{N}{2} \phi^{(0)} - \frac{N^2}{2V} \tilde{\phi}_e(q=0), \quad (18)$$

where

$$\phi^{(0)} = \frac{Z^2}{V} \sum_{q(\neq 0)} v(q) \left[\frac{1}{\epsilon(q,0)} - 1 \right]. \quad (19)$$

For the calculation of the free energy, the HNC formula (3) is not directly applicable to the screened OCP system because of the density- and temperature-dependent interparticle potential and the structure-independent terms in the Hamiltonian (18).

The derivation of the free-energy formula may be facilitated by introduction of a fictitious screening function $\epsilon(\bar{Q} \equiv q/\bar{q}_F, 0; \bar{r}_s, \bar{\theta})$ and through comparison between two reference systems which are constructed in relation to the fictitious screening function. The screening function $\epsilon(\bar{Q}, 0; \bar{r}_s, \bar{\theta})$ is defined to take on the same value as $\epsilon(Q, 0;$

where V and N are kept constant in the differentiation. Substitution of Eq. (14) into Eq. (15) yields

$$\begin{aligned} \frac{U_{sc}}{N} &= \frac{Z^2}{2V} \sum_{q(\neq 0)} v(q) [S(q) - 1] \\ &\quad + \frac{Z^2}{2V} \sum_{q(\neq 0)} v(q) \left[\frac{1}{\epsilon(Q,0)} - 1 \right] S(q) \\ &\quad - \frac{Z^2}{2V} \sum_{q(\neq 0)} v(q) \left[\theta \frac{\partial}{\partial \theta} \frac{1}{\epsilon(Q,0)} \right]_{r_s} S(q), \end{aligned} \quad (16)$$

where $S(q)$ refers to the static structure factor of the screened OCP system. We note here that the excess internal energy of the screened OCP is not simply given by the statistical average of H ; it contains an additional term [the third term on the right-hand side of Eq. (16)] which stems from the temperature dependence of $\epsilon(q, 0)$. One can likewise obtain the expression for the excess pressure P_{sc} through partial differentiation of Eq. (14) with respect to V ,

r_s, θ) at the given combination of the density and temperature under consideration, but the state (i.e., the density and temperature) dependence in the latter function is not to be taken into account; in $\epsilon(\bar{Q}, 0; \bar{r}_s, \bar{\theta})$, we regard q_F , r_s , and θ as constants. The reference system (I) then corresponds to the screened ion plasma with $\epsilon(\bar{Q}, 0; \bar{r}_s, \bar{\theta})$, whose Hamiltonian is given by

$$H_I = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \phi_I(|\mathbf{r}_i - \mathbf{r}_j|) + \frac{N}{2} \phi_I^{(0)} - \frac{N^2}{2V} \tilde{\phi}_I(q=0). \quad (20)$$

Here $\phi_I(r)$ is the inverse Fourier transform of

$$\tilde{\phi}_I(q) = Z^2 v(q) / \epsilon(\bar{Q}, 0; \bar{r}_s, \bar{\theta}), \quad (21)$$

and

$$\phi_I^{(0)} = \frac{Z^2}{V} \sum_{q(\neq 0)} v(q) \left[\frac{1}{\epsilon(\bar{Q}, 0; \bar{r}_s, \bar{\theta})} - 1 \right]. \quad (22)$$

The reference system (II) is defined as that which is described by the Hamiltonian

$$H_{II} = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \phi_{II}(|\mathbf{r}_i - \mathbf{r}_j|). \quad (23)$$

This Hamiltonian is thus obtained by setting the last two structure-independent terms of Eq. (20) equal to zero. We may call this system "normal" in the sense that the interparticle potential is short ranged and independent of the thermodynamic variables and that the structure-

independent terms are not retained in the Hamiltonian.

We first observe that the excess Helmholtz free-energy F_{sc} in the original screened OCP should amount to that in reference system I, F_I at the given combination of q_F , r_s , and θ ,

$$F_{sc} = F_I. \quad (24)$$

The excess free energy F_I is in turn related with that in reference system II, F_{II} via

$$F_I = F_{II} + \frac{N}{2} \phi_I^{(0)} - \frac{N^2}{2V} \tilde{\phi}_I(q=0). \quad (25)$$

In contrast with Eq. (24), this relation now holds true even if we change the density and temperature. Thus differentiating both hands of Eq. (25) with respect to N , we obtain the relation between the excess chemical potentials, μ_I and μ_{II} , as

$$\mu_I = \mu_{II} + \frac{1}{2} \phi_I^{(0)} - \frac{N}{V} \tilde{\phi}_I(q=0). \quad (26)$$

For the correlation functions, we need not distinguish between the original screened OCP and the reference systems because the Hamiltonians have the same structure dependence at the given specification of q_F , r_s , and θ .

We have thus established the inter-relationship among the three systems. On the basis of this inter-relationship we now derive the desired HNC free-energy formula for the screened OCP system in the following way.

We first evaluate the excess chemical potential for reference system II in the HNC approximation. Since this system is normal, the usual HNC formula (3) for the excess chemical potential applies, and we find

$$\beta\mu_{II} = \frac{n}{2} \int d\mathbf{r} h(r)[h(r) - c(r)] - n\tilde{c}(q=0). \quad (27)$$

Substitution of Eq. (27) in (26) then yields μ_I .

The excess Helmholtz free-energy F_I is calculated in accord with the standard thermodynamic procedure

$$\frac{F_I}{N} = \mu_I - \frac{P_I}{n}, \quad (28)$$

where the excess pressure P_I of the reference system I is calculated in the same way as in the screened OCP,

$$\begin{aligned} \frac{P_I}{n} &= \frac{Z^2}{6V} \sum_{q(\neq 0)} v(q)[S(q) - 1] \\ &+ \frac{Z^2}{6V} \sum_{q(\neq 0)} v(q) \left[\frac{1}{\epsilon(Q,0)} - 1 \right] S(q) \\ &+ \frac{Z^2}{6V} \sum_{q(\neq 0)} v(q) Q \frac{\partial}{\partial Q} \left[\frac{1}{\epsilon(Q,0)} \right] S(q). \end{aligned} \quad (29)$$

The last term of Eq. (29) accounts for the volume derivative of $\epsilon(Q,0)$ arising from the length scaling of q due to the fact that q_F in the definition of Q is fixed at the value \bar{q}_F .

Finally, the equality of F_{sc} and F_I at the given q_F , r_s , and θ yields the desired HNC formula

$$\begin{aligned} \frac{\beta F_{sc}}{N} &= \frac{n}{2} \int d\mathbf{r} h(r)[h(r) - c(r)] - n\tilde{c}(q=0) \\ &- n\beta\tilde{\phi}_e(q=0) + \frac{\beta}{2} \phi^{(0)} - \frac{\beta P_I}{n}. \end{aligned} \quad (30)$$

The excess chemical potential μ_{sc} of the screened OCP is also derived from Eq. (30) combined with Eq. (17) as

$$\begin{aligned} \beta\mu_{sc} &= \frac{n}{2} \int d\mathbf{r} h(r)[h(r) - c(r)] - n\tilde{c}(q=0) - n\beta\tilde{\phi}_e(q=0) + \frac{\beta}{2} \phi^{(0)} - \frac{Z^2}{6V} \sum_{q(\neq 0)} \beta v(q) \left[r_s \frac{\partial}{\partial r_s} \frac{1}{\epsilon(Q,0)} \right]_{\theta} S(q) \\ &- \frac{Z^2}{3V} \sum_{q(\neq 0)} \beta v(q) \left[\theta \frac{\partial}{\partial \theta} \frac{1}{\epsilon(Q,0)} \right]_{r_s} S(q) - \frac{Z^2}{6V} \sum_{q(\neq 0)} \beta v(q) Q \frac{\partial}{\partial Q} \left[\frac{1}{\epsilon(Q,0)} \right] S(q). \end{aligned} \quad (31)$$

The third and fourth terms on the right-hand side of Eq. (31) are the structure-independent contributions; the last three terms stem from the density and temperature dependence of the potential. If one neglects the polarization effect of the electrons by setting $\epsilon(q,0)=1$ in Eq. (31), the formula in the OCP is recovered.

V. NUMERICAL RESULTS AND DISCUSSION

In this section we apply the formulas derived in the previous section to the evaluation of the thermodynamic functions for the screened OCP in the HNC approximation. For simplicity we assume hydrogenic plasmas with $Z=1$ throughout this section. The HNC equations for the screened OCP may be solved quite accurately with the numerical technique described in Ref. 17.

To carry out the calculations, we need to specify the

screening function $\epsilon(q,0)$. As a first example, we shall consider the ionic OCP screened by the completely degenerate electron liquid, a system relevant to the interior of the heavy planets such as Jupiter. For $\epsilon(q,0)$, we adopt the analytic formula due to Ichimaru and Utsumi^{5,18} (IU) as well as the Lindhard screening function.¹⁶

As a second example, we investigate the finite-temperature effects of the electrons on the thermodynamic properties of the plasma, using the RPA expression for $\epsilon(q,0)$. Those effects may be significant in the description of such plasmas as encountered in the inertial confinement fusion experiments and in the interior of the main-sequence stars. The local-field effects in the electrons, on the other hand, are not considered in this case.

The derivatives of $\epsilon(q,0)$ appearing in Eqs. (16), (17), (30), and (31) can be explicitly calculated in terms of the screening functions described above; the results are summarized in the Appendix.

TABLE I. Excess internal energy, $-\beta U_{sc}/N$, calculated with the Lindhard and Ichimaru and Utsumi screening functions at $r_s=1$. VAR refers to those obtained through the OCP variational method (Ref. 19); HNC, through the present HNC method.

Γ	Lindhard		Ichimaru and Utsumi	
	VAR	HNC	VAR	HNC
6	5.101	5.108	5.155	5.173
10	8.745	8.726	8.830	8.813
20	17.95	17.89	18.08	18.02
40	36.51	36.40	36.71	36.61
60	55.17	55.00	55.41	55.27
80	73.86	73.65	74.15	73.98
100	92.57	92.34	92.90	92.70
130	120.65	120.36	121.05	120.83
160	148.75	148.43	149.21	148.97

A. The degenerate electron liquid

Since the electrons are assumed to be in the ground state, we set $\theta=0$ in $\epsilon(Q,0)$. The plasma state is described in terms of Γ and r_s ; the derivatives of $\epsilon(Q,0)$ with respect to θ vanish in Eqs. (16), (17), and (31).

In Tables I and II we list the excess contributions to the thermodynamic functions at $r_s=1$, obtained with the Lindhard and IU screening functions. For comparison, we also list the corresponding OCP variational results¹⁹ in those tables. Considering the substantial difference between the variational method and the present HNC computations, we find the close agreement between those two sets of calculations to be remarkable.

The excess Helmholtz free energy is usually evaluated by integrating the excess internal energy with respect to the temperature [see Eq. (15)] as

$$\frac{\beta F_{sc}}{N}(\Gamma, r_s) - \frac{\beta F_{sc}}{N}(\Gamma_0, r_s) = \int_{\Gamma_0}^{\Gamma} \frac{d\Gamma}{\Gamma} \frac{\beta U_{sc}}{N}(\Gamma, r_s), \quad (32)$$

TABLE II. Excess Helmholtz free energy, $-\beta F_{sc}/N$. Designation is the same as in Table I.

Γ	Lindhard		Ichimaru and Utsumi	
	VAR	HNC	VAR	HNC
6	4.726	4.772	4.825	4.868
10	8.182	8.225	8.317	8.360
20	17.06	17.08	17.27	17.29
40	35.19	35.15	35.51	35.48
60	53.52	53.42	53.93	53.84
80	71.95	71.79	72.44	72.30
100	90.44	90.23	91.00	90.82
130	118.25	117.96	118.90	118.65
160	146.12	145.75	146.86	146.55

where it is assumed that the value of $\beta F_{sc}/N$ has already been known at the initial point (Γ_0, r_s) of the integration. Inversely, we can apply the thermodynamic relation (32) to examine the self-consistency of the present scheme: The left-hand side of Eq. (32) is calculated directly from the HNC free-energy formula (30), while the right-hand side of Eq. (32) is calculated by performing the integration numerically; comparison between the two values thus indicates the degree of consistency achieved. The numerical results in Tables I and II show that the thermodynamic consistency is satisfied with a high degree of confidence in the present scheme. If one takes, for example, $\Gamma_0=6$ and $\Gamma=160$ in Eq. (32), then the two values agree with each other within the accuracy of 0.05%.

B. The finite-temperature electron gas

In Fig. 1 we show the screening corrections to the excess Helmholtz free energy for three values of θ , calculated with the RPA screening function of the electrons at finite temperatures. The screening corrections are defined as the differences between the screened OCP values and the corresponding OCP values, i.e., $\Delta F \equiv F_{sc} - F_{OCP}$. As one would expect, the electron-screening effects play an important part in determining the correlational properties of the plasma in the partially degenerate regime ($\theta \gtrsim 1$) of the electrons; even at $\theta=1$, the screening corrections are of the same order of magnitude as the original OCP values.

In this connection we may raise a question as to the validity and accuracy of the adiabatic approximation for the electron system in the partially degenerate regime ($\theta \gtrsim 1$). To cope with this question, we compare in Table III the "total" excess Helmholtz free energies with the nonadiabatic calculations by Ichimaru, Mitake, Tanaka, and Yan²⁰ (IMTY), and with the RPA calculations.^{9,20} In the present scheme the total excess free energy of the plasma

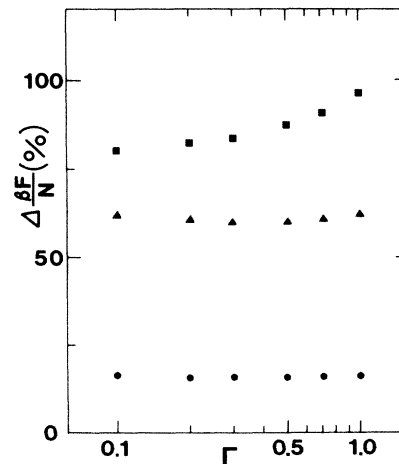


FIG. 1. Relative magnitude of the screening corrections to the excess Helmholtz free energy obtained with the finite-temperature RPA screening function. The points with closed circles represent those for $\theta=0.1$; closed triangles, for $\theta=1.0$; and closed squares, for $\theta=10.0$.

TABLE III. Total excess Helmholtz free energy in various schemes. HNC refers to those obtained through the present HNC method with the finite-temperature random-phase approximation (RPA) screening function; IMTY, by Ichimaru, Mitake, Tanaka, and Yan (Ref. 20); RPA, based upon the RPA scheme.

θ	Γ	$-\beta F_e^{ex}/N$		
		HNC	IMTY	RPA
0.1	0.1	0.0652	0.0648	0.0658
	0.3	0.235	0.234	0.245
	0.5	0.432	0.429	0.461
	1.0	0.984	0.982	1.117
1.0	0.1	0.0574	0.0569	0.0576
	0.3	0.246	0.243	0.253
	0.5	0.483	0.478	0.509
	1.0	1.199	1.182	1.321
10.0	0.1	0.0511	0.0506	0.0515
	0.3	0.250	0.245	0.259
	0.5	0.519	0.508	0.543
	1.0	1.387	1.305	1.486

is given by adding the excess contribution F_e^{ex} of the uniform electron gas to F_{sc} , Eq. (30). Recently, fitting formulas for the RPA (exchange and ring) contributions to F_e^{ex} have been obtained by Perrot and Dharma-wardana,²¹ and analytic formulas parametrizing the free energies in the Singwi-Tosi-Land-Sjölander approximation have been derived by Tanaka, Mitake, and Ichimaru.²² To be consistent with the use of the RPA screening function here, we adopt Perrot and Dharma-wardana's formulas for F_e^{ex} . It is remarkable that magnitudes of F_e^{ex} are almost as large as those of F_{sc} in the parameter region of Table III. From Table III, we see the present results are in better agreement with those of IMTY than with the RPA results. We may thus conclude that the adiabatic approximation for the electrons works fairly well even in the range of $\theta \geq 1$, for the calculations of the thermodynamic quantities; the slight discrepancies observed may in part be ascribed to the local-field effects of the electrons included in the IMTY's scheme.

One can examine the consistency between the thermodynamic functions in this partially degenerate electron case in the same way as in the completely degenerate electron case; the pertinent thermodynamic relation is now

$$\frac{\beta F_{sc}}{N}(r_s, \theta) - \frac{\beta F_{sc}}{N}(r_s, \theta_0) = - \int_{\theta_0}^{\theta} \frac{d\theta}{\theta} \frac{\beta U_{sc}}{N}(r_s, \theta), \quad (33)$$

APPENDIX: DERIVATIVES OF $\epsilon(q, 0)$

According to the expression (11) for $\epsilon(q, 0)$, the derivatives of $\epsilon(q, 0)$ appearing in Eqs. (16), (17), (29), and (31) are calculated explicitly as

TABLE IV. Excess thermodynamic functions calculated with the finite-temperature RPA screening function for $r_s = 1$.

θ	$-\beta U_{sc}/N$	$-\beta F_{sc}/N$
1.0	0.3880	0.3091
2.0	0.1687	0.1255
3.0	0.1000	0.07214
4.0	0.06808	0.04823
5.0	0.05017	0.03514
6.0	0.03893	0.02706
7.0	0.03135	0.02166
8.0	0.02594	0.01784
9.0	0.02193	0.01503
10.0	0.01885	0.01289

where the pair of r_s and θ is chosen as independent variable for convenience of the numerical computations, instead of the pair of Γ and r_s in Eq. (32). As an example, we have tabulated U_{sc} and F_{sc} in Table IV, as a function of θ at a fixed value of $r_s = 1$. These numerical results again ensure the thermodynamic consistency in the present scheme.

VI. CONCLUDING REMARKS

We have derived the free-energy formulas for the electron-screened OCP in the HNC approximation. The formulas, expressed in terms of the correlation functions, enable one to avoid the more cumbersome and less accurate calculations involving the thermodynamic integrations. Accuracy and thermodynamic consistency of the proposed formulas have been examined and ascertained through explicit comparison with the results of other independent calculations which take account of the screening of interionic potentials by electrons at zero temperature with local-field corrections or at a finite temperature without local-field corrections.

Although we have presented the theory in terms of the screened OCP for simplicity, the scheme developed here is equally applicable to the plasmas with multi-ionic species. The simplicity and accuracy achieved in the present scheme may be valuable in the analyses of the phase properties in such multicomponent plasmas; a reliable treatment of such a problem would call for extremely accurate evaluations of the free energies. In a subsequent paper,¹⁵ we shall consider one of such problems.

ACKNOWLEDGMENTS

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

$$\left[r_s \frac{\partial}{\partial r_s} \frac{1}{\epsilon(Q,0)} \right]_{\theta} = \frac{1}{\bar{\epsilon}(q,0)} \left[\frac{1}{\epsilon(q,0)} - 1 \right] - \left[\frac{1}{\epsilon(q,0)} - 1 \right]^2 \left[r_s \frac{\partial}{\partial r_s} G(Q) \right]_{\theta}, \quad (\text{A1})$$

$$\left[\theta \frac{\partial}{\partial \theta} \frac{1}{\epsilon(Q,0)} \right]_{r_s} = \frac{1}{\bar{\epsilon}(q,0)} \left[1 - \frac{1}{\epsilon(q,0)} \right] - \frac{4\lambda r_s}{\pi[\bar{\epsilon}(q,0)]^2 Q^2} \\ \times \left[\sqrt{2\theta} \int_0^{\infty} dy \frac{y^2 \left[2y^2 + \theta \frac{d}{d\theta}(\beta\mu_0) \right] \tanh(y^2 - \beta\mu_0/2)}{[\cosh(y^2 - \beta\mu_0/2)]^2} J_0 \left[\frac{Q}{2\sqrt{2\theta}y} \right] \right] \\ - \left[\frac{1}{\epsilon(q,0)} - 1 \right]^2 \left[\theta \frac{\partial}{\partial \theta} G(Q) \right]_{r_s}, \quad (\text{A2})$$

$$Q \frac{\partial}{\partial Q} \left[\frac{1}{\epsilon(Q,0)} \right] = \frac{2}{\bar{\epsilon}(q,0)} \left[1 - \frac{1}{\epsilon(q,0)} \right] - \frac{4\lambda r_s}{\pi[\bar{\epsilon}(q,0)]^2 Q^2} \\ \times \left[\sqrt{2\theta} \int_0^{\infty} dy \frac{y^2 [3 - 4y^2 \tanh(y^2 - \beta\mu_0/2)]}{[\cosh(y^2 - \beta\mu_0/2)]^2} J_0 \left[\frac{Q}{2\sqrt{2\theta}y} \right] \right] - \left[\frac{1}{\epsilon(q,0)} - 1 \right]^2 Q \frac{\partial}{\partial Q} G(Q), \quad (\text{A3})$$

where the function $\bar{\epsilon}(q,0)$ is defined as

$$\bar{\epsilon}(q,0) = 1 - v(q)\chi_0(q,0)[1 - G(q)]. \quad (\text{A4})$$

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¹²Another example may be found in those treatments of electron-ion plasmas in which the quantum nature (diffraction and symmetry effects) of the electrons is taken into account through the use of effective potentials (Refs. 14, 23–25) those potentials act to prevent the collapse in the electron-ion correlation characteristic of a purely classical treatment. Among them, Deutsch and his collaborators (Ref. 25) proposed simple analytic expressions for the effective potentials, which were sometimes used in the study of the thermodynamic and transport properties of dense plasmas (Refs. 26 and 27). The proposed temperature-dependent potentials, however, do not appear capable of describing the strong-coupling effects typical in dense plasmas. The use of those effective po-

tentials leads to the Coulomb logarithm of transport coefficients slightly different from the correct expression even in the limit of weak coupling (Ref. 26).

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