Theory of interparticle correlations in dense, high-temperature plasmas. II. Correlation functions

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On the basis of the general theoretical framework constructed in the preceding paper (paper I in the present series), we calculate in this paper various correlation functions in dense plasmas, taking account of local-field corrections and varied degrees of electron degeneracy; physical implications of the results are investigated.

I. INTRODUCTION

In the preceding paper,[1] hereafter referred to as paper I, we constructed a theoretical framework in which the interparticle correlations may be formulated and analyzed for dense plasmas. In the present paper we apply the general formalism to explicit calculation of various correlation functions and to investigation of salient features arising from strong Coulomb-coupling effects.

The correlation properties of dense plasmas have been considered by various investigators[2–6] in the past. The present paper aims at elucidating systematically the effects of both varied degrees of the electron degeneracy and local-field corrections (LFC's) describing those Coulomb correlations beyond the random-phase approximation (RPA). Since this work is a continuation of paper I, we closely follow the notation and convention used in paper I unless otherwise specified.

II. STRUCTURE FACTOR

We calculate the structure factors defined by Eq. (I.23),[1] for two-component plasmas (TCP's) with $Z=1$ at 32 combinations of the electron degeneracy parameter $\theta=0.1$, 1, and 10 and the Coulomb-coupling constant $\Gamma\leq 2$, following the scheme described in Sec. IV of paper I. In this paper (except for the numerical data to be cited in Table II), we shall be concerned with investigation of the results only for the cases of $\Gamma=1.0$, $\theta=0.1$ and $\Gamma=0.1$, $\theta=1.0$, both of which assume the same density at $r_s=0.184$. The rest of the computed results will be of use for the calculations of the thermodynamic quantities in the following paper.[7]

For calculation of the ion-ion correlation ($\mu=\nu=2$), we use the classical expression, Eq. (I.25b). For the electron-electron ($\mu=\nu=1$) and the electron-ion ($\mu=1$, $\nu=2$) correlations, we retain the quantum expression and carry out the ω integration of Eq. (I.24a) in Eq. (I.25a) by the summation of contributions arising from the poles of $\coth(\hbar\omega/2k_BT)$ on the imaginary ω axis:[8]

$$S_{\mu\nu}(k)=-\frac{k_BT}{n}\sum_{l=-\infty}^{\infty}\chi_{\mu\nu}(k,iz_l)\ , \tag{1}$$

where

$$z_l=2\pi lk_BT/\hbar\ . \tag{2}$$

In the actual calculation of $S_{11}(k)$, we note the identity

$$\chi_{11}(k,iz_l)=\chi_1^{(0)}(k,iz_l)+F(k,iz_l)+[\chi_{11}(k,iz_l)-\chi_1^{(0)}(k,iz_l)-F(k,iz_l)]\ . \tag{3}$$

Here $\chi_1^{(0)}(k,\omega)$ is the free-electron polarizability as given by Eq. (I.20),

$$F(k,iz)=\left[\frac{2nE_F}{\hbar^2}\right]^2\frac{v(k)(k/k_F)^4[1-G_{11}(k)]}{(z^2+b)(z^2+c)}\ , \tag{4a}$$

$$b=-\frac{2nE_F}{\hbar^2\chi_1^{(0)}(k,0)}\left[\frac{k}{k_F}\right]^2\ , \tag{4b}$$

$$c=\frac{b[1-G_{11}(k)]D(k,0)}{v(k)\chi_2^{(0)}(k,0)+[1-G_{11}(k)]\{1-v(k)\chi_2^{(0)}(k,0)[1-G_{22}(k)]\}}\ . \tag{4c}$$

The infinite summations with respect to l of the first two terms on the right-hand side of Eq. (3) can be carried out analytically. Since the last, square-bracketed term in Eq. (3) decreases at least as fast as $(z_l)^{-6}$ in the large-$|l|$ domain, we find it sufficient in accuracy to sum this term over $|l|\leq 300$. $S_{12}(k)$ can likewise be calculated with analogous prescription.

As mentioned in Sec. V of I, we evaluate the electron-electron LFC from the solution to the hypernetted-chain (HNC) equations for the electron one-component plasma

TABLE I. Structure factors $S_{\mu\nu}(k)$ at $\Gamma=1.0$ and $\theta=0.1$. The numbers in the first column represent the values of ak in units of $(25\pi/256)$.

ak $\left(\frac{25\pi}{256}\right)$	$S_{11}(k)$		$S_{22}(k)$		$S_{12}(k)$	
	LFC	RPA	LFC	RPA	LFC	RPA
0	0.1392	0.1295	0.1392	0.1295	0.1392	0.1295
1	0.1711	0.1618	0.1633	0.1524	0.1358	0.1258
2	0.2501	0.2410	0.2305	0.2144	0.1269	0.1158
3	0.3496	0.3407	0.3262	0.2998	0.1140	0.1021
4	0.4547	0.4457	0.4336	0.3922	0.09921	0.08717
5	0.5579	0.5487	0.5389	0.4804	0.08426	0.07292
6	0.6549	0.6458	0.6337	0.5587	0.07028	0.06021
7	0.7432	0.7344	0.7141	0.6253	0.05782	0.04931
8	0.8207	0.8124	0.7795	0.6809	0.04704	0.04011
9	0.8857	0.8781	0.8314	0.7267	0.03782	0.03237
10	0.9366	0.9299	0.8717	0.7645	0.02991	0.02576
11	0.9720	0.9664	0.9027	0.7957	0.02302	0.01999
12	0.9913	0.9868	0.9262	0.8214	0.01689	0.01481
13	0.9979	0.9944	0.9441	0.8430	0.01177	0.01042
14	0.9991	0.9964	0.9578	0.8611	0.008193	0.007322
15	0.9995	0.9973	0.9682	0.8766	0.005927	0.005342
16	0.9997	0.9980	0.9762	0.8897	0.004441	0.004035

(OCP); purely quantum-mechanical effects such as the Pauli exclusion-principle contributions are thus ignored in this evaluation of $G_e(k)$. In Fig. 1 we plot the classical HNC values of $G_e(k)$ for $\theta=1$ and for $\theta=0.1$, both at the constant density $r_s=0.184$. Those are then compared with $G_e(k)$ derived by Ichimaru and Utsumi[9] for a degenerate electron liquid ($\theta=0$) at the same density, $r_s=0.184$. Naturally the classical evaluation does not exhibit a peak structure around $k=2k_F$, which is essential to account for the exchange effects.[9] Otherwise the two curves for $\theta=0$ and $\theta=0.1$ in Fig. 1 appear quite similar in the small-k domain, where the Coulomb-induced effects are predominant.

In Table I we list the computed values of $S_{\mu\nu}(k)$ at $\Gamma=1.0$ and $\theta=0.1$, both with and without the LFC's. This is one of those among the calculated cases of the parametric combinations where the departure between the LFC and RPA values is fairly significant, sometimes exceeding 10%.

In Fig. 2 we compare the values of $S_{\mu\nu}(k)$ between the cases with $\Gamma=0.1$, $\theta=1.0$ and with $\Gamma=1.0$, $\theta=0.1$, evaluated with the LFC's. When the effect of electron degeneracy increases to $\theta=0.1$, we observe that the relative importance of the electron-ion coupling [manifested in $S_{12}(k)$] decreases.

Contrary to the cases of an OCP, the TCP structure factors do not vanish in the limit of $k\to 0$. Retaining the degeneracy effect of the electrons, we find that those take on the same value,

$$S_{11}(0)=S_{22}(0)=S_{12}(0)=\frac{A}{1+A-3(\gamma_1+\gamma_2)A\Gamma}\ , \tag{5}$$

where

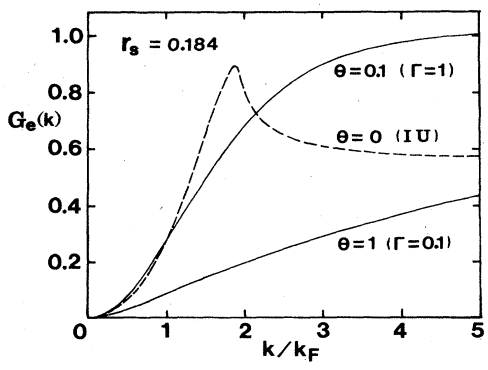

FIG. 1. Electronic local-field correction evaluated in the HNC scheme at $\theta=1$ and $\theta=0.1$ with the density parameter $r_s=0.184$. The dashed curve (IU) represents the local-field correction for a degenerate electron liquid ($\theta=0$) at the same density, obtained in Ref. 9.

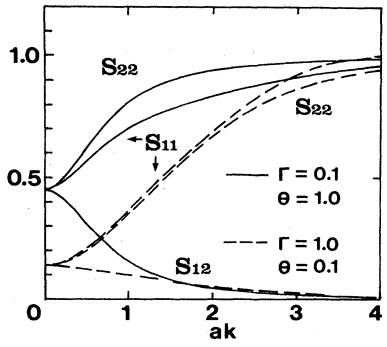

FIG. 2. Structure factors $S_{\mu\nu}(k)$ at $\Gamma=0.1$ and $\theta=1.0$ (solid curves) and at $\Gamma=1.0$ and $\theta=0.1$ (dashed curves).

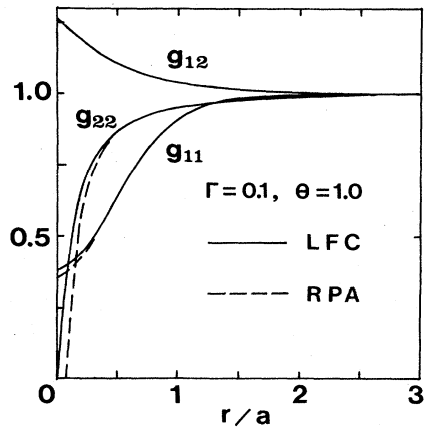

FIG. 3. Radial distribution functions $g_{\mu\nu}(r)$ at $\Gamma=0.1$ and $\theta=1.0$, evaluated with the local-field corrections (the solid curves) and without them (the dashed curves). The two curves for $g_{12}(r)$ almost coincide.

$$A=\frac{3\theta}{2}\int_0^\infty dx\{1+\exp[(E_F x^2-\mu_0)/k_BT]\}^{-1}, \quad (6)$$

$$\gamma_1=\lim_{k\to 0}[G_{11}(k)/(ak)^2],$$

$$\gamma_2=\lim_{k\to 0}[G_{22}(k)/(ak)^2], \quad (7)$$

and μ_0 is the Fermi level of the electrons determined from the normalization condition such as Eq. (I.22). In the classical limit for the electrons, the integral A tends to unity, so that $S_{11}(0)=S_{22}(0)=S_{12}(0)=\frac{1}{2}$ in the RPA, where $\gamma_1=\gamma_2=0$; with LFC's, $S_{\mu\nu}(0)$ deviate from $\frac{1}{2}$. We remark in passing that an accurate evaluation of μ_0 is essential particularly for ensuring the correct limiting behaviors of $S_{\mu\nu}(k)$ in the large-k limit.

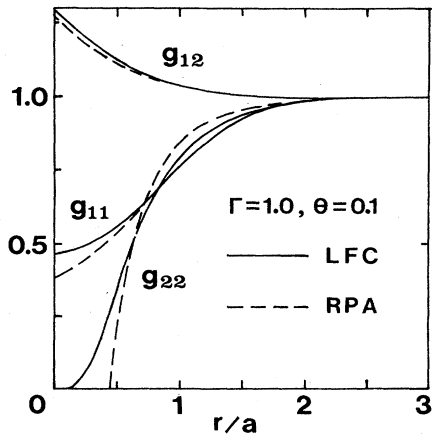

FIG. 4. The same as Fig. 4, but at $\Gamma=1.0$ and $\theta=0.1$.

TABLE II. Values of $g_{12}(0)$ computed at various combinations of Γ and θ with and without the local-field corrections.

	$\theta=0.1$		$\theta=1.0$		$\theta=10$	
Γ	1.0	0.3	0.3	0.1	0.1	0.03
LFC	1.295	1.103	1.704	1.258	1.968	1.299
RPA	1.266	1.100	1.684	1.256	1.962	1.298

III. RADIAL DISTRIBUTION FUNCTIONS

With the knowledge of various structure factors evaluated in Sec. II, we calculate the radial distribution functions $g_{\mu\nu}(r)$ in accord with Eq. (I.26). Figure 3 shows the compared values of $g_{\mu\nu}(r)$ at $\Gamma=0.1$ and $\theta=1.0$ with and without LFC's. As has been often pointed out,[10] RPA calculations tend to overestimate the short-range correlations in $g_{11}(r)$ and $g_{22}(r)$, leading to such an unphysical prediction as $g_{22}(r\simeq 0)<0$. An analogous feature is observed in Fig. 4, where the case with $\Gamma=1.0$ and $\theta=0.1$ is exhibited.

Since the quantum-diffraction effects of electrons are appropriately taken into account through $\chi_1^{(0)}(k,\omega)$, the radial distribution function $g_{12}(r)$ between the electrons and ions remains finite and convergent in the limit of $r\to 0$. In Table II we compare the computed values of $g_{12}(0)$ with and without the LFC's for several parametric combinations of Γ and θ. As we observe in this numerical comparison, the screening action of the electrons around an ion is generally underestimated in RPA. The physical origin of this underestimation has been accounted for in Ref. 4, where the screening effect has been investigated through a thermodynamic variational principle.

IV. CONCLUSION

On the basis of the general theoretical framework constructed in paper I,[1] we have calculated various correlation functions in dense plasmas for various parameteric combinations of Γ and θ. We have presented some typical examples of the calculations where the effects of the LFC's and varied degrees of the electron degeneracy are demonstrated; physical origins of those effects have been investigated.

In the following paper,[7] we shall extend the present results to the calculation of thermodynamic functions for dense plasmas.

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