Long-range correlations in degenerate multicomponent systems of charged fermions

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The partial structure factors and the pair correlation functions in a degenerate multicomponent system of charged fermions are considered. The long-range behavior of the particle density correlations are specifically analyzed by extending to multicomponent fermionic systems the known properties of the degenerate electron gas (jellium), particularly the long-wavelength limit of the first-moment sum (f-sum). By assuming that this limit is dominated by collective modes, namely, plasmons and phonons, explicit expressions for the leader terms in the correlations are obtained. Based on this dominant asymptotic behavior, we propose effective pair potentials that allow us to incorporate the main quantum effects into a pseudoclassical description of the multicomponent plasma.

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I. INTRODUCTION

The Sommerfeld free electron model (jellium) has proved to be very useful in describing many of the electronic properties of metallic solids. In the model, the conduction electrons are represented as a zero temperature ensemble of point charged fermions moving against a rigid uniform neutralizing background, that plays the role of the ionic lattice.

The equilibrium behavior of this system has been widely studied through quantal Monte Carlo simulations [1] and also from a variety of many-body theories [2–6]. Many of them center on the electrons density correlations [7]. In particular, the short-range and the long-range correlations have received special attention [8–14] because in those limits physics becomes more transparent than in the intermediate region, where the sum of equally important effects of very diverse origin can make comprehension difficult.

A simple analytical approach to the electron's density correlations, first considered by Rajagopal, Kimball, and Banerjee [14], consists of writing parametrized correlation functions that interpolate between the asymptotic extremes [15,16]. In this way, very simple formulas that compare rather well with more laborious numerical calculations can be obtained.

In particular, in Ref. [16], the electron-electron correlations in jellium are considered by using an effective pair potential to incorporate quantal effects into a pseudoclassical description of the degenerate electron gas. Effective pair potentials between simultaneous electron density fluctuations and an effective temperature are built from known asymptotic properties of the jellium, namely, first-moment sum the plasmon (f-sum) rule [5], the Kimball-Niklasson relation [8,9], and Yasuahra's value of the electron pair correlation function at contact [10,12]. From these effective potentials and temperature, the structure factors for the electrons can be obtained using classical liquid state theory. In particular, if the Debye-Hückel approximation is used, then a full analytical expression is found [16].

In this work we study, along these lines, the pair correlation function and the partial structure factors for a system composed of several species of point charged fermions moving against a neutralizing background. In the binary case, this model can be used to describe semiconductors as electron-hole mixtures. It also serves to model hypothetical electron-positron mixtures at low temperatures.

Some of the many-body theories used to describe the one-component jellium have been extended to degenerate mixtures of charged fermions, particularly to binary mixtures. The theory of electron correlation of Singwi *et al.* [17] was generalized to binary systems of degenerate electrons and a few positrons by Sjölander and Stott [18] and by Bhattacharyya and Singwi [19]. This extended theory was also applied to describe electron-hole liquids [20]. Also, Lantto, after having applied the Fermi hypernetted-chain (FHNC) method of Fantoni and Rosati [21] to the one-component jellium [22], used it to describe low temperature electron-positron plasmas [23].

The asymptotic behavior of the correlations in degenerate multicomponent systems has been comparatively less studied than it has been in the one-component case. The short-range behavior of correlation functions was analyzed by Pastore, Senatore, and Tosi [24], who generalized to many components the Kimball-Niklasson relation for the logarithmic derivative, at contact, of the pair correlation functions [8,9]. Very recently, we have extended [25] the Yasuhara formula [10–12] to mixtures with arbitrary charge, mass, and relative densities.

Here, we study the long-range behavior of the correlation functions; that is, the long-wavelength limit of the partial structure factors for multicomponent plasmas. We obtain dominant terms of the structure factors in that limit by assuming that the small-q limit of the partial structure factors is dominated by collective modes, whereas single-particle and multiparticle excitations play a less important role. We also mention the construction of effective potentials that, in a classical description, give partial structure factors and pair distribution functions that conserve the asymptotic properties.

II. DEGENERATE MULTICOMPONENT PLASMA

A. Model

We consider an ensemble of N species of charged fermions moving against a neutralizing background. The system is assumed to have a volume V and a temperature $T=0$. The number of particles of the species i ($i=1,2,\ldots,N$) is denoted N_i, so that $n_i=N_i/V$ is the corresponding number density. In our model, the particles of type i are represented as points of mass m_i and charge Z_ie, where e is the electron charge.

Electroneutrality implies that $e\sum_i n_iZ_i=\rho_b$, where ρ_b is the background density. First we will suppose a very general system with arbitrary n_i and Z_i, so that ρ_b can be nonzero. Later we will restrict the model to electroneutral mixtures of fermions with charges of the same magnitude but opposite sign.

The Hamiltonian of the system is written in second quantizations as

$$\hat{H}=\sum_{\mathbf{k}}\sum_{i=1}^{N}\epsilon_{\mathbf{k}}^{i}\hat{a}_{\mathbf{k}}^{i\dagger}\hat{a}_{k}^{i}+\frac{1}{2V}\sum_{\mathbf{q}}\sum_{ij}v_{ij}(\mathbf{q})(\hat{n}_{\mathbf{q}}^{i}\hat{n}_{-\mathbf{q}}^{j}-\hat{N}_i\delta_{ij}) , \quad (1)$$

where $\epsilon_{\mathbf{k}}^{i}$ denotes the kinetic energy for particles of type i with momentum $\mathbf{k}$ and $v_{ij}(\mathbf{q})$ is the Coulomb interaction between particles of type i and j, in momenta space:

$$\epsilon_{\mathbf{k}}^{i}=\frac{\hbar^2k^2}{2m_i} , \quad (2)$$

$$v_{ij}(\mathbf{q})=\frac{4\pi e^2Z_iZ_j}{q^2} . \quad (3)$$

In Eq. (1), $\hat{N}_i=\hat{n}^{i}{}_{\mathbf{q}=0}$ indicates the particle number operator for species i, and $\hat{n}_{\mathbf{q}}^{i}$ the particle density operator for particles of species i and momentum $\mathbf{q}$,

$$\hat{n}_{\mathbf{q}}^{i}=\sum_{\mathbf{k}}\hat{a}_{\mathbf{k}+\mathbf{q}}^{i\dagger}\hat{a}_{\mathbf{k}}^{i} . \quad (4)$$

Here $\hat{a}_{\mathbf{k}}^{i\dagger}$ and $\hat{a}_{\mathbf{k}}^{i}$ are creation and annihilation operators, respectively, for species i.

B. Correlation functions and partial structure factors

Here we introduce the main objects we consider in this work, namely, the pair correlation functions in r space and the partial structure factors in momentum space. These related functions are very appropriate for describing the structural behavior of the system under study.

In order to define the pair correlation function $g_{ij}(r)$ for a particle of species i at a distance $r=|\mathbf{r}_1-\mathbf{r}_2|$ from another particle of species j, we write the system wave function with the coordinates for those particles written in center-of-mass coordinates

$$\Psi=\Psi(\mathbf{r},\mathbf{R},\mathbf{r}_3,\ldots,\mathbf{r}_M) , \quad (5)$$

$$\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2,\quad \mathbf{R}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2) . \quad (6)$$

Here M denotes the total number of particles: $M=\sum_{i=1}^{N}N_i$. A density matrix $\rho_{ij}(\mathbf{r},\mathbf{r}')$ is then defined, for the various pairs of species, as

$$\rho_{ij}(\mathbf{r},\mathbf{r}')=\int\psi^*(\mathbf{r},\mathbf{R},\mathbf{r}_3,\ldots,\mathbf{r}_M)\times\Psi(\mathbf{r}',\mathbf{R},\mathbf{r}_3,\ldots,\mathbf{r}_M)d^3\mathbf{R}\prod_{l=3}^{M}d^3\mathbf{r}_l , \quad (7)$$

whose diagonal elements give the pair correlation functions

$$g_{ij}(r)=\rho_{ij}(\mathbf{r},\mathbf{r}) . \quad (8)$$

The function $g_{ij}(r)$ is the probability density of finding a particle of species i at a distance r from a particle of type j. An equivalent structural information, in q space, is given by the partial structure factors defined as

$$S_{ij}(\mathbf{q})=\frac{1}{(n_in_j)^{1/2}}\frac{\langle\hat{n}_{\mathbf{q}}^{i}\hat{n}_{-\mathbf{q}}^{j}\rangle}{V} . \quad (9)$$

The structure factors $S_{ij}(\mathbf{q})$ are directly related to the scattered intensity in radiation scattering experiments. The functions $g_{ij}(r)$ and $S_{ij}(\mathbf{q})$ are related via three-dimensional Fourier transforms

$$g_{ij}(r)=1+\frac{1}{(n_in_j)^{1/2}}\int\frac{d^3\mathbf{q}}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{r}}[S_{ij}(\mathbf{q})-\delta_{ij}] . \quad (10)$$

III. LONG-RANGE CORRELATIONS

A. Zeroth- and first-moment sum rules

The static partial structure factors can be expressed as the integral over energy transfers of the dynamic structure factors $S_{ij}(\mathbf{q},\omega)$ [26],

$$S_{ij}(\mathbf{q})=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}S_{ij}(\mathbf{q},\omega) . \quad (11)$$

In turn, the fluctuation-dissipation theorem [27] links the dynamic partial structure factors to the imaginary part of the density response functions $\chi_{ij}(\mathbf{q},\omega)$ according to

$$\mathrm{Im}\chi_{ij}(\mathbf{q},\omega)=-\frac{(n_in_j)^{1/2}}{2\hbar\omega}(1-e^{-\hbar\omega/k_BT})S_{ij}(\mathbf{q},\omega) . \quad (12)$$

Here k_B denotes the Boltzmann constant and T is the absolute temperature. At $T=0$, the degenerate plasma is in the ground state and cannot transfer any energy to the scattered particles. Hence,

$$S_{ij}(\mathbf{q},\omega)=-\frac{2\hbar}{(n_in_j)^{1/2}}\Theta(\omega)\mathrm{Im}\chi_{ij}(\mathbf{q},\omega) , \quad (13)$$

where Θ denotes the Heaviside step functions. Thus the zero-moment sum rule, Eq. (11), is written

$$S_{ij}(\mathbf{q})=-\frac{\hbar}{\pi(n_in_j)^{1/2}}\int_{0}^{\infty}d\omega\,\mathrm{Im}\chi_{ij}(\mathbf{q},\omega) . \quad (14)$$

We will also use the first-moment sum rule or f-sum rule [28],

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \, \mathrm{Im} \left[\frac{1}{\epsilon(\mathbf{q},\omega)} \right] = -\omega_P^2 , \tag{15}$$

where the mixture plasma frequency is

$$\omega_P^2 = 4\pi e^2 \sum_{i=1}^{N} \frac{n_i Z_i^2}{m_i} . \tag{16}$$

In terms of the response function, the longitudinal dielectric function is written [7] as

$$\frac{1}{\epsilon(\mathbf{q},\omega)} = 1 + \sum_{ij} \frac{4\pi e^2 Z_i Z_j}{q^2} \chi_{ij}(\mathbf{q},\omega) \tag{17}$$

and hence the f-sum rule for the mixture reads

$$\sum_{ij} Z_i Z_j \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \, \mathrm{Im}\chi_{ij}(\mathbf{q},\omega) = -q^2 \sum_{i=1}^{N} \frac{n_i Z_i^2}{m_i} . \tag{18}$$

Since the exact structure factors verify the above sum rules, they can be used as a guide in constructing approximate theories of multicomponent systems.

B. Plasmon-phonon model

In order to obtain explicit forms for the dominant asymptotic terms of the partial structure factors at very long wavelength, we assume that single-particle and multiparticle excitations are less important that collective modes in that limit. Following the work of Tosi and March on liquid metals [29], we assume the dominant collective modes are plasmonlike and phononlike. Hence, we approximate the partial response function as

$$\mathrm{Im}\chi_{ij}(\mathbf{q},\omega) = -\frac{\pi}{2}(n_i n_j)^{1/2} \{ \alpha_{ij} q^2 [\delta(\omega-\omega_P) - \delta(\omega-\omega_P) + \beta_{ij} q [\delta(\omega - q v_s) - \delta(\omega + q v_s)]] \} , \tag{19}$$

where $\delta(x)$ is the Dirac delta function, ω_P is the plasma frequency [see Eq. (16)] and v_s denotes the sound velocity.

By subsituting the expression (19) for the partial dissipation functions into the zero-moment-sum rule Eq. (14), we obtain the explicit long-wavelength asymptotic form for the partial structure factors

$$S_{ij}(\mathbf{q}) \underset{q \to 0}{\sim} \frac{\hbar}{2} [\beta_{ij} q + \alpha_{ij} q^2] . \tag{20}$$

Also, using Eq. (19) for $\chi_{ij}(\mathbf{q},\omega)$ in the f-sum rule, we obtain a couple of relations that the coefficients α_{ij} and β_{ij} must verify

$$4\pi e^2 \sum_{ij} (n_i n_j)^{1/2} Z_i Z_j \alpha_{ij} = 1 , \tag{21}$$

$$\sum_{ij} (n_i n_j)^{1/2} Z_i Z_j \beta_{ij} = 0 . \tag{22}$$

In what follows, we will consider electroneutral binary mixtures. Thus we restrict the indices i,j to be $+$ or $-$. The electroneutrality condition implies that $\rho_b = 0$, so that $n_+ Z_+ + n_- Z_- = 0$.

A solution of Eqs. (21) and (22) is given by [29]

$$\alpha_{ij} = (-1)^{i+j} \frac{1}{\omega_P M} \frac{n_+ n_-}{(n_i n_j)^{1/2}} \frac{m_+ m_-}{m_i m_j} , \tag{23}$$

where $M = n_+ m_+ + n_- m_-$, and

$$\beta_{ij} = (n_i n_j)^{1/2} \beta \tag{24}$$

with

$$\beta = \frac{3}{4\hbar (n_+ n_-)^{1/2}} \{ [(k_F^+)^2 + (k_F^-)^2]/2 \}^{-1/2} . \tag{25}$$

These values of α_{ij} and β_{ij} give asymptotic partial structure factors which are consistent with those found in the FHNC approximation [25,23].

C. Direct correlation functions

The direct correlation functions in momenta space, $\tilde{c}_{ij}(\mathbf{q})$, are defined by the Ornstein-Zernlike relations [30]

$$S_{ij}(\mathbf{q}) - \delta_{ij} = \tilde{c}_{ij}(\mathbf{q}) + \sum_k [S_{ik}(\mathbf{q}) - \delta_{ik}] \tilde{c}_{kj}(\mathbf{q}) . \tag{26}$$

Explicitly, we have

$$\begin{aligned} 1 - \tilde{c}_{++}(\mathbf{q}) &= \frac{S_{--}(\mathbf{q})}{D(\mathbf{q})} , \\ \tilde{c}_{+-}(\mathbf{q}) &= \frac{S_{+-}(\mathbf{q})}{D(\mathbf{q})} , \\ 1 - \tilde{c}_{--}(\mathbf{q}) &= \frac{S_{++}(\mathbf{q})}{D(\mathbf{q})} , \end{aligned} \tag{27}$$

where the denominator reads

$$D(\mathbf{q}) = S_{++}(\mathbf{q}) S_{--}(\mathbf{q}) - S_{+-}^2(\mathbf{q}) . \tag{28}$$

Accordingly, the long-wavelength limit of the direct correlation functions can be written

$$\begin{aligned} \tilde{c}_{++}(\mathbf{q}) &\sim -\frac{2}{\hbar\gamma} \left[\frac{\beta_{--}}{q^2} + \frac{\alpha_{--}}{q} \right] , \\ \tilde{c}_{+-}(\mathbf{q}) &\sim \frac{2}{\hbar\gamma} \left[\frac{\beta_{+-}}{q^2} + \frac{\alpha_{+-}}{q} \right] , \\ \tilde{c}_{--}(\mathbf{q}) &\sim -\frac{2}{\hbar\gamma} \left[\frac{\beta_{++}}{q^2} + \frac{\alpha_{++}}{q} \right] , \end{aligned} \tag{29}$$

with

$$\gamma = [n_+ \alpha_{--} + n_- \alpha_{++} - 2(n_+ n_-)^{1/2} \alpha_{+-}] \beta . \tag{30}$$

The asymptotic long-range behavior of the direct correlations in r space is obtained from the small-q behavior of $\tilde{c}_{ij}(\mathbf{q})$, taking into account that they are

Fourier transforms of each other,

$$\tilde{c}_{ij}(\mathbf{q})=\frac{4\pi(n_i n_j)^{1/2}}{q}\int_0^\infty \sin(qr) r c_{ij}(r)dr \ . \tag{31}$$

This way, we have for $r\to\infty$:

$$\begin{aligned} c_{++}(r)&\sim \frac{2}{\hbar\gamma}\frac{1}{4\pi n_+}\left[\frac{\beta_{--}}{r}+\frac{2}{\pi}\frac{\alpha_{--}}{r^2}\right] , \\ c_{+-}(r)&\sim \frac{2}{\hbar\gamma}\frac{1}{4\pi(n_+n_-)^{1/2}}\left[\frac{\beta_{+-}}{r}+\frac{2}{\pi}\frac{\alpha_{+-}}{r^2}\right] , \\ c_{--}(r)&\sim -\frac{2}{\hbar\gamma}\frac{1}{4\pi n_-}\left[\frac{\beta_{++}}{r}+\frac{2}{\pi}\frac{\alpha_{++}}{r^2}\right] . \end{aligned} \tag{32}$$

D. Electron-positron-like mixtures

For electroneutral binary mixtures where both species have the same mass $(m_+=m_-=m)$ and charge $(Z_+=-Z_-=1)$, namely, for electron-positron-like mixtures, the above formulas simplify even more. Because of the symmetry between species we have

$$\begin{aligned} S_{++}(\mathbf{q})&\equiv S_{--}(\mathbf{q})\equiv S_0(\mathbf{q}) , \\ S_{+-}(\mathbf{q})&\equiv S_{-+}(\mathbf{q})\equiv S_1(\mathbf{q}) , \end{aligned} \tag{33}$$

and equivalent relations for the pair distribution and direct correlation functions. Thus Eqs. (10) and (27) and (28) now read $(n_+=n_-=n)$

$$\begin{aligned} g_{++}(r)&\equiv g_{--}(r) \\ &\equiv g_0(r) \\ &=1+\frac{1}{n}\int\frac{d^3\mathbf{q}}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{r}}[S_0(\mathbf{q})-1] , \\ g_{+-}(r)&\equiv g_{-+}(r) \\ &\equiv g_1(r) \\ &=1+\frac{1}{n}\int\frac{d^3\mathbf{q}}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{r}}S_1(\mathbf{q}) , \end{aligned} \tag{34}$$

and

$$\begin{aligned} \tilde{c}_{++}(\mathbf{q})&\equiv\tilde{c}_{--}(\mathbf{q})\equiv\tilde{c}_0(\mathbf{q})=1-\frac{S_0(\mathbf{q})}{D(\mathbf{q})} , \\ \tilde{c}_{+-}(\mathbf{q})&\equiv\tilde{c}_1(\mathbf{q})=\frac{S_1(\mathbf{q})}{D(\mathbf{q})} , \end{aligned} \tag{35}$$

where

$$D(\mathbf{q})=S_0^2(\mathbf{q})-S_1^2(\mathbf{q}) \ . \tag{36}$$

The parameters α_{ij} and β_{ij} in the phonon-plasmon model simplify to

$$\alpha_{++}\equiv\alpha_{--}\equiv-\alpha_{+-}\equiv\alpha=\frac{1}{2\omega_p m} , \tag{37}$$

$$\beta_{++}\equiv\beta_{--}\equiv\beta_{+-}\equiv n\beta=\frac{1}{4\hbar k_F} , \tag{38}$$

where the plasma frequency ω_P and the Fermi momentum k_F are

$$\omega_P^2=\frac{8\pi e^2 n}{m} , \tag{39}$$

$$k_F=(3\pi^2 n)^{1/3} \ . \tag{40}$$

The asymptotic limits also simplify. The long-wavelength behavior of the partial structure factors is given by

$$S_0(\mathbf{q})\underset{q\to0}{\sim}\frac{3}{8}\frac{q}{k_F}+\frac{1}{4}\frac{q^2}{k_S^2} , \tag{41}$$

$$S_1(\mathbf{q})\underset{q\to0}{\sim}\frac{3}{8}\frac{q}{k_F}-\frac{1}{4}\frac{q^2}{k_S^2} , \tag{42}$$

with

$$k_S^2=\frac{8\pi e^2 n}{\hbar\omega_P}=2\left[\frac{3}{r_s^3}\right]^{1/3}\frac{1}{a_0^2} \ . \tag{43}$$

Here the dimensionless Wigner-Seitz radius r_s is defined as $r_s a_0=[3/4\pi n]^{1/3}$ and a_0 is the positronium Bohr radius.

From the partial structure factors we can evaluate the particle-particle and charge-charge structure factors defined, for a binary mixture, by [26]

$$\begin{aligned} S_{NN}(\mathbf{q})=&\frac{n_+}{n_++n_-}S_{++}(\mathbf{q})+\frac{n_-}{n_++n_-}S_{--}(\mathbf{q}) \\ &+2\frac{(n_+n_-)^{1/2}}{n_++n_-}S_{+-}(\mathbf{q}) \end{aligned} \tag{44}$$

and

$$\begin{aligned} S_{QQ}(\mathbf{q})=&|Z_+|S_{++}(\mathbf{q})+|Z_-|S_{--}(\mathbf{q}) \\ &-2|Z_+Z_-|^{1/2}S_{+-}(\mathbf{q}) \ . \end{aligned} \tag{45}$$

respectively. For 1:1 mixtures, they reduce to

$$S_{NN}(\mathbf{q})=S_0(\mathbf{q})+S_1(\mathbf{q}) , \tag{46}$$

$$S_{QQ}(\mathbf{q})=2[S_0(\mathbf{q})-S_1(\mathbf{q})] , \tag{47}$$

whose long-wavelength behavior is

$$S_{NN}(\mathbf{q})\underset{q\to0}{\sim}\frac{3}{4}\frac{q}{k_F} , \tag{48}$$

$$S_{QQ}(\mathbf{q})\underset{q\to0}{\sim}\frac{q^2}{k_S^2} \ . \tag{49}$$

We observe that the charge-charge structure factor, like the jellium structure factor, is asymptotically dominated by plasmonic modes. The particle-particle structure factor behaves as an ideal fermionic gas instead.

Using Eqs. (35) and (36), we also obtain the long-wavelength dominant behavior of the direct correlation function in 1:1 mixtures:

$$\tilde{c}_0(\mathbf{q})\underset{q\to0}{\sim}-\frac{k_S^2}{q^2}-\frac{2}{3}\frac{k_F}{q} , \tag{50}$$

$$\tilde{c}_1(\mathbf{q}) \underset{q\to 0}{\sim} \frac{k_S^2}{q^2} - \frac{2}{3}\frac{k_F}{q} \ . \tag{51}$$

The corresponding long-range behavior long-range behavior in r space is

$$c_0(r) \underset{r\to\infty}{\sim} \frac{1}{4\pi n}\left[\frac{k_S^2}{r} + \frac{4}{3\pi}\frac{k_F}{r^2}\right] , \tag{52}$$

$$c_1(r) \underset{r\to\infty}{\sim} \frac{1}{4\pi n}\left[\frac{k_S^2}{r} - \frac{4}{3\pi}\frac{k_F}{r^2}\right] . \tag{53}$$

It is worthwhile to compare the small-q limit of the partial structure factors we have obtained for degenerate electron-positron-like mixtures [Eqs. (41) and (42)] to the corresponding behavior found for liquid metals [29]. In liquid metals a sharp distinction between the two species, ions and electrons, exists. While the former can be taken as classical objects, electrons are essentially quantum objects. The ion-ion structure factor at zero-moment transfer determines the isothermal compressibility, so that the dominant small-q term is a constant, as it is in fully classical systems. From the work of Watanabe and Hasegawa [31] and Chiara [32], we know that because of the system electroneutrality, the ion-ion structure factor constraints the small-q dominant term in electron-ion and electron-electron structure factors to be proportional to the compressibility also.

IV. PSEUDOCLASSICAL DESCRIPTION

A. Effective classical potential

In this section we consider the problem of constructing effective pair potentials that allow the inclusion of the previous long-range behavior into a pseudoclassical description of the multicomponent plasma. It is known that the classical direct correlation functions asymptotically behave as the pair potentials [33]:

$$c_{ij}(r) \sim -\frac{1}{k_B T}\Phi_{ij}(r) \quad (r\to\infty) \ . \tag{54}$$

Therefore, from Eqs. (52) and (53), we see that if an effective temperature is defined as

$$k_B T = \frac{4\pi e^2 n}{k_S^2} = \tfrac{1}{2}\hbar\omega_P \ , \tag{55}$$

then, in order for the classical relation (54) to hold, the pair potential must asymptotically go as

$$\Phi_{++}(r) \equiv \Phi_{++}(r)$$
$$\equiv \Phi_0(r) \sim \frac{e^2}{r} + \frac{3}{4\pi}\frac{e^2 k_F}{k_S^2}\frac{1}{r^2} \quad (r\to\infty) \ , \tag{56}$$

$$\Phi_{+-}(r) \equiv \Phi_{-+}(r)$$
$$\equiv \Phi_1(r) \sim -\frac{e^2}{r} + \frac{3}{4\pi}\frac{e^2 k_F}{k_S^2}\frac{1}{r^2} \quad (r\to\infty) \ . \tag{57}$$

We can write parametrized pair potentials that verify the above asymptotic forms in the long-range limit. Simple expressions for such potentials are

$$\Phi_0(r) = \frac{e^2}{r}[1-e^{-\lambda_0 r}] + \frac{3}{4\pi}\frac{e^2 k_F}{k_S^2}\frac{1}{r^2}[1-e^{-\mu_0^2 r^2}], \quad 0 \le r < \infty \ , \tag{58}$$

$$\Phi_1(r) = -\frac{e^2}{r}[1-e^{-\lambda_1 r}] + \frac{3}{4\pi}\frac{e^2 k_F}{k_S^2}\frac{1}{r^2}[1-e^{-\mu_1^2 r^2}], \quad 0 \le r < \infty \ , \tag{59}$$

where λ_i, μ_i^2 $(i=0,1)$ are positive real numbers.

Besides the long range behavior, it is also interesting to compare the short-range behavior of the effective potentials with those corresponding to the bare Coulomb potentials. At contact, these last potentials diverge (to $+\infty$ for electron-electron and for positron-positron pairs and to $-\infty$ for electron-positron pairs). Consequently, the classical correlations for electron-electron and positron-positron pairs are vanishingly small, whereas the electron-positron correlation function is infinitely large. The effective potentials Φ_0, Φ_1 are finite at $r=0$, giving finite pair correlations as they should be from a quantum point of view. Electrons (positrons) can overcome the infinitely repulsive potential generated by another electron (positron) because of tunneling. In turn, the system stability is guaranteed by an uncertainty principle (kinetic effect) that prevents electron-positron pairs from collapse [34]. These quantum effects are thus incorporated into a classical description of the degenerate plasma through the effective pair potentials.

Since by construction the effective potentials verify the previous long-range asymptotic behavior, it still remains to fit the parameters λ_i, μ_i $(i=0,1)$ so that Φ_0 and Φ_1 behave correctly at contact. If accurate values for the contact values of the correlation functions are known, namely, $g_0(r=0)|_{\text{input}}$ and $g_1(r=0)|_{\text{input}}$, we can adjust the λ's and μ's. To this end we use Kimball-Niklasson relation [8,9]. For electron-positron-like mixtures it reads [24]

$$\lim_{q\to\infty} q^4(S_0(\mathbf{q})-1) = -8\pi n \left.\frac{\partial g_0(r)}{\partial r}\right|_{r=0} = -\frac{8\pi n}{a_0} g_0(r=0) \ , \tag{60}$$

$$\lim_{q\to\infty} q^4 S_1(\mathbf{q}) = -8\pi n \left.\frac{\partial g_1(r)}{\partial r}\right|_{r=0} = -\frac{8\pi n}{a_0} g_1(r=0) \ . \tag{61}$$

Taking into account that [35,24]

$$-\frac{1}{k_B T}\left.\frac{\partial \Phi_{ij}(r)}{\partial r}\right|_{r=0} = \left.\frac{\partial g_{ij}(r)}{\partial r}\right|_{r=0} , \tag{62}$$

the Kimball-Niklasson relation can be written involving the effective pair potentials,

$$-\frac{k_S^2}{4\pi n e^2}\frac{\partial\Phi_0(r)}{\partial r}\bigg|_{r=0}=\frac{g_0(r=0)}{a_0}\,, \tag{63}$$

$$\frac{k_S^2}{4\pi n e^2}\frac{\partial\Phi_1(r)}{\partial r}\bigg|_{r=0}=\frac{g_1(r=0)}{a_0}\,. \tag{64}$$

Thus we find explicit expressions for the parameters λ_0,λ_1 in terms of the input contact correlation functions:

$$\begin{aligned}\lambda_0&=\left[\frac{8\pi n g_0(r=0)|_{\rm input}}{a_0 k_S^2}\right]^{1/2},\\ \lambda_1&=\left[\frac{8\pi n g_1(r=0)|_{\rm input}}{a_0 k_S^2}\right]^{1/2}.\end{aligned} \tag{65}$$

The parameters μ_0 and μ_1, finally, can be adjusted so that the resulting correlation functions coincide with the input values:

$$\begin{aligned}&1+\frac{1}{2\pi^2}\int_0^\infty q^2[S_0(\mathbf{q};\mu_0,\mu_1)-1]dq=g_0(r=0)|_{\rm input}\,,\\ &1+\frac{1}{2\pi^2}\int_0^\infty q^2 S_1(\mathbf{q};\mu_0,\mu_1)dq=g_1(r=0)|_{\rm input}\,,\end{aligned} \tag{66}$$

where $S_0(\mathbf{q};\mu_0,\mu_1)$ and $S_1(\mathbf{q};\mu_0,\mu_1)$ are the partial structure factors for a binary mixture at the effective temperature and whose particles interact via the pair potentials Φ_0,Φ_1 [Eqs. (58) and (59)] with the parameters λ_0,λ_1 given by Eq. (65).

The input contact correlation functions must be obtained from an independent theory. For example, we can generalize to many components [25] Yasuhara's formula for the degenerate electron gas [10–12]. It should be noted that the influence of the spin of the particles on the correlations functions is essentially contained in $g_0(r=0)$.

B. Debye-Hückel approximation

In order to classically evaluate the partial structure factors and the pair correlation functions using the previous effective potentials, some approximated theory is needed. The simplest one we can think of is the Debye-Hückel approximation [30].

In this approximation the relation (54) between the direct correlation function and the pair potentials is assumed to hold not just asymptotically but also for all r:

$$c_i(r)=-\frac{1}{k_BT}\Phi_i(r)\quad(i=0,1),\quad 0\le r<\infty\,. \tag{67}$$

Therefore we have, in q space

$$\tilde{c}_0(\mathbf{q})=-\frac{k_S^2}{q^2}\frac{\lambda_0^2}{q^2+\lambda_0^2}-\frac{2}{3}\frac{k_F}{q}\left[1-\operatorname{erf}\left[\frac{q}{2\mu_0}\right]\right],\quad 0\le q<\infty\,, \tag{68}$$

$$\tilde{c}_1(\mathbf{q})=\frac{k_S^2}{q^2+\lambda_1^2}-\frac{2}{3}\frac{k_F}{q}\left[1-\operatorname{erf}\left[\frac{q}{2\mu_1}\right]\right],\quad 0\le q<\infty\,, \tag{69}$$

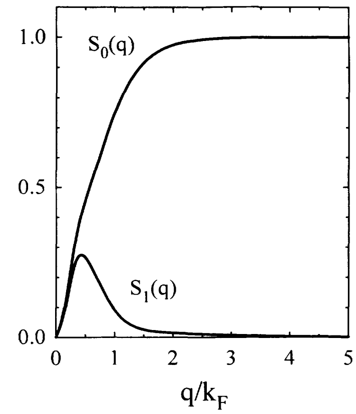

FIG. 1. Partial structure factors $S_0(\mathbf{q})$ $[=S_{++}(\mathbf{q})=S_{--}(\mathbf{q})]$ and $S_1(\mathbf{q})$ $[=S_{+-}(\mathbf{q})=S_{+-}(\mathbf{q})]$ for an electron-positron-like mixture at $r_s=1$.

where $\operatorname{erf}(x)$ denotes the error function.

Using these expressions for the direct correlation functions, we obtain, via the Ornstein-Zernike relations (26), the partial structure factors

$$S_0(\mathbf{q})=\frac{1-\tilde{c}_0(\mathbf{q})}{\Delta(\mathbf{q})}\,, \tag{70}$$

$$S_1(\mathbf{q})=\frac{\tilde{c}_1(\mathbf{q})}{\Delta(\mathbf{q})}\,, \tag{71}$$

with

$$\Delta(\mathbf{q})=[1-\tilde{c}_0(\mathbf{q})]^2-[\tilde{c}_1(\mathbf{q})]^2\,. \tag{72}$$

The correlation functions $g_0(r)$ and $g_1(r)$ can be evalu-

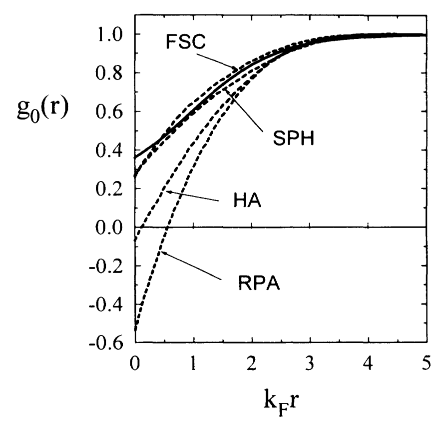

FIG. 2. The pair correlation function $g_0(r)$ $[=g_{++}(r)=g_{--}(r)]$ for an electron-positron-like mixture at $r_s=1$. The solid line shows the result of the present work. The dashed curves represent the result obtained from several theories: RPA (random-phase approximation); HA (Hubbard approximation); FSC (fully self-consistent approximation); and SPH (self-consistent particle-hole approximation) as read from Fig. 2 in Ref. [20(b)].

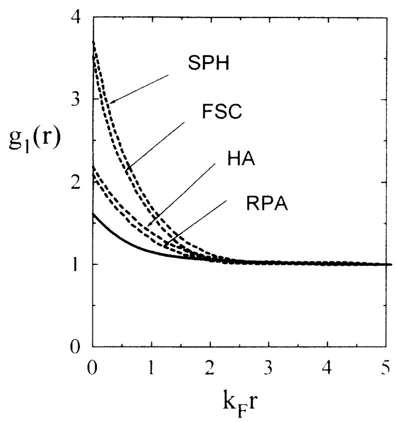

FIG. 3. The pair correlation function $g_1(r)$ $[=g_{+-}(r)=g_{+-}(r)]$ for an electron-positron-like mixture at $r_s=1$. The lines and abbreviations have the same meaning as in Fig. 2.

ated by Fourier transforming the partial structure factors [see Eqs. (34)].

Partial structure factors for an electron-positron mixture as obtained by the previous procedure are shown in Fig. 1. They correspond to a Wigner-Seitz radius $r_s=1$. The input correlation functions at contact were calculated using the generalized Yasuhara's formula, as described in Ref. [25]. Figures 2 and 3 show the corresponding pair correlation functions for like and unlike species, respectively. A series of curves obtained from several full quantal theories are also included, although a comparison of diverse approaches is not the aim of this paper.

V. CONCLUDING REMARKS

We have presented a simple pseudoclassical approach to the description of degenerate multicomponent systems of charged fermions. The basic idea of the method is to interpolate, via a classical theory, between the short- and long-range limits of the correlation functions. These asymptotic behaviors being independently obtained from quantum considerations.

To this end, we construct effective pair potentials that classically describe the same asymptotic behavior as the quantum plasma. In this work we have chosen a very simple form for these effective potentials, but more elaborate analytical forms that also yield the desired asymptotic limits can be found. Also, in our calculations, we have closed the Ornstein-Zernike relations with the simplest approximation available, namely, the Debye-Hückel closure. However, it is well known that better closures (e.g., the hypernetted-chain approximation) [30], which incorporate many of the diagrams that the Debye-Hückel theory ignores, exist.

The small-momentum behavior of the partial structure factors was found from a simple model of plasmons and phonons that satisfies the f-sum rule and gives asymptotic particle-particle and charge-charge mean density fluctuations corresponding to an ideal fermionic gas and the one component jellium, respectively.

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[1] D. Ceperley, Phys. Rev. B **18**, 3126 (1978); D. Ceperley and B. J. Adler, Phys. Rev. Lett. **45**, 566 (1980).
[2] N. H. March, W. H. Young, and S. Sampanthar, *The Many-Body Problem in Quantum Mechanics* (Cambridge University Press, London, 1967).
[3] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw Hill, New York, 1981).
[4] G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
[5] N. M. March and M. P. Tosi, *Coulomb Liquids* (Academic, London, 1984).
[6] W. D. Kraeft, D. Kremp, W. Ebeling, and G. Ropke, *Quantum Statistics of Charged Particle Systems* (Plenum, New York, 1986).
[7] K. S. Singwi and M. P. Tosi, Solid State Phys. **36**, 177 (1981).
[8] J. C. Kimball, Phys. Rev. A **7**, 1648 (1973).
[9] G. Niklasson, Phys. Rev. B **10**, 3052 (1974).
[10] H. Yashuhara, Solid State Commun. **11**, 1481 (1972).
[11] H. Yasuhara, J. Phys. Soc. Jpn. **36**, 361 (1974).
[12] H. Yasuhara, Physica **78**, 420 (1974).
[13] K. Bedell and G. E. Brown, Phys. Rev. B **17**, 4512 (1978).
[14] A. K. Rajagopal, J. C. Kimball, and M. Banerjee, Phys. Rev. B **18**, 2339 (1978).
[15] V. Contini, G. Mazzone, and F. Sacchetti, Phys. Rev. B **33**, 712 (1986).
[16] F. Vericat, G. Pastore, and M. P. Tosi, Nuovo Cimento D **8**, 59 (1986).
[17] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).
[18] A. Sjölander and M. J. Stott, Phys. Rev. B **5**, 2109 (1972).
[19] P. Bhattacharyya and K. S. Singwi, Phys. Rev. Lett. **29**, 22 (1972).
[20] (a) P. Vashista, P. Bhattacharyya, and K. S. Singwi, Nuovo Cimento B **23**, 172 (1974); (b) Phys. Rev. B **10**, 5108 (1974).
[21] S. Fantoni and S. Rosati, Nuovo Cimento Lett. **10**, 545 (1974); Nuovo Cimento A **25**, 593 (1975).
[22] L. J. Lantto, Phys. Rev. B **22**, 1380 (1980).
[23] L. J. Lantto, Phys. Rev. B **36**, 5160 (1987).
[24] G. Pastore, G. Senatore, and M. P. Tosi, Phys. Lett. A **84**, 369 (1981).
[25] F. Vericat and A. A. Melgarejo, Phys. Chem. Liq. **27**, 235 (1994).
[26] N. H. March and M. P. Tosi, *Atomic Dynamics in Liquids* (Academic, London, 1986).
[27] C. G. Callen and E. A. Welton, Phys. Rev. **83**, 34 (1951).
[28] P. C. Martin, Phys. Rev. **161**, 143 (1967).
[29] M. P. Tosi and N. H. March, Nuovo Cimento B **15**, 308 (1973).
[30] J.-P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (Academic, London, 1986).

[31] M. Watanbe and H. Hasegawa, in *The Properties of Liquid Metals,* edited by Sakae Takeuchi (Taylor and Francis, London, 1973), p. 133.
[32] J. Chiara, in *The Properties of Liquid Metals* (Ref. [31]), p. 137.
[33] G. Stell, in *Modern Theoretical Chemistry,* edited by B. J. Berne (Plenum, New York, 1977).
[34] E. H. Lieb, Rev. Mod. Phys. **48**, 553 (1976).
[35] B. Widom, J. Chem. Phys. **39**, 2808 (1963); **42**, 1128 (1965).