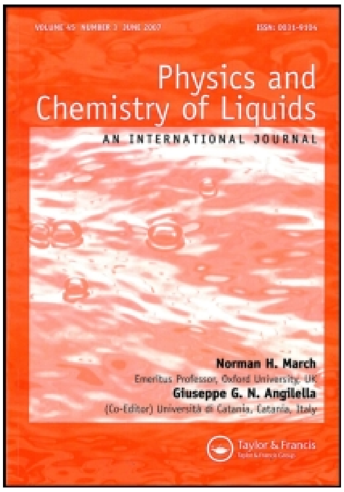

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SHORT-RANGE CORRELATIONS IN DEGENERATE MULTICOMPONENT PLASMAS

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The short-range behavior of correlation functions in a multicomponent plasma of charged fermions at $T = 0$ and metallic densities is considered. A known approximate expression for the contact value of the electron-electron correlation function in jellium, obtained by summing only ladder diagrams in Goldstone formula, is first generalized to many species and then improved by including screening effects. Comparison is made with quantal hypernetted-chain calculations on electron-positron mixture and with experimental data on positron-annihilation in metals.

KEY WORDS: Degenerate plasmas, multicomponent jellium, Yasuhara formula, positron-annihilation rate.

PACS Numbers: 5.30 Fk; 61.20 Gy; 78.70 Bj

I. INTRODUCTION

The knowledge of the short-range correlations is of great help to design approximate theories in order to describe many-body systems. In particular, the short-range correlations in the degenerate electron gas ("jellium")[1] have deserved much study[2–9]. Two important results are the exact Kimball-Niklasson expressions[2,3,6] for the logarithmic derivative of the correlation function and the approximate formula of Yasuhara[4] for the correlation function itself, both evaluated at contact.

Tosi and collaborators[10] extended Kimball-Niklasson expressions to multicomponent plasmas at degenerate regimes as well as at finite temperatures. In this paper, following Yasuhara arguments, we sum ladder interactions between particles of different species in order to find approximate expressions for the corresponding two-particle correlations at contact in the multicomponent "jellium". Our treatment explicitly incorporates the coulombic screening in ladder expressions.

We compare our results with those obtained from the quantal version of the hypernetted-chain approximation (FHNC)[11]. We also use the contact correlation functions so obtained to evaluate the positron-annihilation rate in metals.

II. DEGENERATE MULTICOMPONENT PLASMA

A. Model

We consider a system composed of N species of charged fermions at temperature $T=0$ in a volume V. We indicate with N_i number of particles of species i $(i=1,2,\ldots,N)$ so that $n_i=N_i/V$ denotes the corresponding number density. We represent a particle of type i as a point of mass m_i and charge Z_ie where e is the elemental electronic charge.

The interaction Hamiltonian for this system is written in momentum space as

$$\hat{H}_1(\vec{q})=\frac{1}{2V}\sum_{ij}\frac{4\pi e^2Z_iZ_j}{q^2}(\hat{n}^i_q\hat{n}^j_{-q}-\hat{N}_i\delta_{ij}) \tag{2.1}$$

where $\hat{N}_i=\hat{n}^i_{\vec{q}=0}$ and $\hat{n}^i_q$ is the particle number operator for particles of species i and momentum $\vec{q}$.

B. Correlation functions

Our interest is on the short-range behavior of the pair correlation functions $g_{ij}(r)$ or, equivalently, on the long wave-number limit of the partial structure functions $S_{ij}(\vec{q})$.

The functions $g_{ij}(r)$ and $S_{ij}(\vec{q})$ are Fourier transforms each other:

$$g_{ij}(r)-1=\frac{1}{\sqrt{\hat{n}_i\hat{n}_j}}\int\frac{d^3\vec{q}}{(2\pi)^3}e^{i\vec{q}\cdot\vec{r}}[S_{ij}(\vec{q})-\delta_{ij}] \tag{2.2}$$

From Eq. (2.1), we obtain the energy shift caused by the perturbative interaction:

$$\begin{aligned}\Delta E&\equiv E_1(e^2)-E_1(0)\\&=\int_0^{e^2}\frac{de^2}{e^2}\frac{1}{2}\sum_{ij}\sum_{\vec{q}}v_{ij}(\vec{q})(n_in_j)^{1/2}[S_{ij}(\vec{q})-\delta_{ij}]\end{aligned} \tag{2.3}$$

where $v_{ij}(\vec{q})$ denotes the pair potential in momentum space. This equation says that the partial structure factors are functional derivatives of the energy shift

$$\frac{\delta\Delta E}{\delta v_{ij}(\vec{q})}=\frac{1}{2}(n_in_j)^{1/2}[S_{ij}(\vec{q})-\delta_{ij}] \tag{2.4}$$

Replacing Eq. (2.2) into the multicomponent version of Kimball's expression[10], we also obtain

$$\lim_{r\to0}g_{ij}(r)=\frac{\hbar^2}{16\pi e^2Z_iZ_j(n_in_j)^{1/2}\mu_{ij}}\lim_{q\to\infty}[q^4(S_{ij}(\vec{q})-\delta_{ij})] \tag{2.5}$$

where $\mu_{ij} = m_i m_j/(m_i + m_j)$. Equation (2.5) relates the short-range asymptotic behavior of $g_{ij}(r)$ to the long wavenumber behavior of $S_{ij}(\vec{q})$.

C. Yasuhara formula for multicomponent systems

By summing ladder diagrams in Goldstone formula for the energy shift[12], Yasuhara obtained an approximate expression for the large-q limit of the electron-electron structure factor in the electron gas. Yasuhara's expression yields, via the one component version of Eq. (2.5), the short range behavior of the jellium correlation function. Here we extend his arguments to multicomponent plasmas.

The class of diagrams we consider in Goldstone formula, are those shown in Figure 1. As usual, the upward line denotes a particle and the downward a hole, while a wavy line denotes a coulomb interaction.

The contribution of ladder diagrams to the energy shift can be written

$$\Delta E = \frac{1}{2}\sum_{\vec{q}}\sum_{\vec{k}_1\vec{k}}\sum_{ij} v_{ij}(\vec{q})\frac{f_i(\vec{k}_1)[1-f_i(\vec{k}_1+\vec{q})]f_j(\vec{k}_2)[1-f_j(\vec{k}_2-\vec{q})]}{\varepsilon^i_{\vec{k}_1}-\varepsilon^i_{\vec{k}_1+\vec{q}}+\varepsilon^j_{\vec{k}_2}-\varepsilon^j_{\vec{k}_2-\vec{q}}} I_{ij}(\vec{k}_1\vec{k}_2;\vec{q}) \tag{2.6}$$

where

$$I_{ij}(\vec{k}_1\vec{k}_2;\vec{q}) = v_{ij}(\vec{q}) + \sum_{\vec{q}'}\frac{v_{ij}(\vec{q}-\vec{q}')[1-f_i(\vec{k}_1+\vec{q})][1-f_j(\vec{k}_2-\vec{q})]}{\varepsilon^i_{\vec{k}_1}-\varepsilon^i_{\vec{k}_1+\vec{q}}+\varepsilon^j_{\vec{k}_2}-\varepsilon^j_{\vec{k}_2-q}} I_{ij}(\vec{k}_1\vec{k}_2;\vec{q}') \tag{2.7}$$

Here $\varepsilon^i_{\vec{q}} = \hbar^2 q^2/2m_i$ denotes the kinetic energy for particles of kind i and $f_i(\vec{k})$ the corresponding Fermi distribution function: $f_i(\vec{k}) = 1 - \Theta(k - k^i_F)$ with $\Theta(x)$ the Heaviside step function and $k^i_F = (3\pi^2 n_i)^{1/3}$ the Fermi momentum.

From Eqs. (2.5), (2.4) and (2.6) we obtain, following the work of Yasuhara[4-6], an approximate expression for the short-range limit of the ladder correlation functions

$$g_{ij}(r=0) = \left[1 - \frac{\mu_{ij}}{\hbar^2\pi^2}\int_0^\infty I_{ij}(q)\Theta(q-k^i_F)\Theta(q-k^j_F)\,dq\right]^2 \tag{2.8}$$

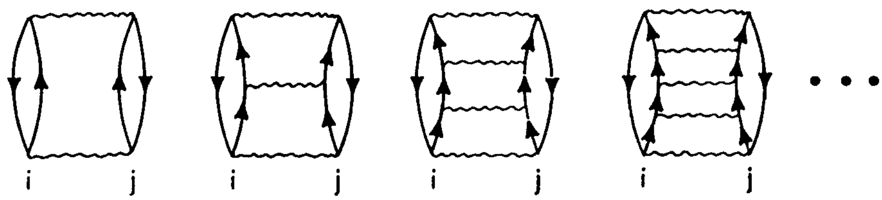

Figure 1 A series of ladder diagrams for a particle of species i and other of species j.

where

$$I_{ij}(q) \equiv I_{ij}(\vec{k}_1 = \vec{0}, \vec{k}_2 = \vec{0}; \vec{q})$$

$$= v_{ij}(q) - \frac{2\mu_{ij}}{\hbar^2} \int \frac{d^3\vec{k}}{(2\pi)^3} v_{ij}(|\vec{k} - \vec{q}|) I_{ij}(k) k^{-2} \Theta(k - k_F^i) \Theta(k - k_F^j) \tag{2.9}$$

and we have transformed the sums into integrals as it is usually done.

We further replace the product of Heaviside step functions in the integrands of Eqs. (2.8) and (2.9): $\Theta(k - k_F^i)\Theta(k - k_F^j) \rightarrow \Theta(k - k_F^{ij})$. Mathematically, the common momentum cut-off is $k_F^{ij} = \mathrm{Max}(k_F^i, k_F^j)$. We choose for $k_F^{ij}(i \neq j)$ the form

$$k_F^{ij} = \left[(k_F^i)^2 + (k_F^j)^2 \right]^{1/2}$$

$$= k_F^e r_{ij} \tag{2.10}$$

where $k_F^e = \mathrm{Max}(k_F^1, k_F^2, \ldots, k_F^N)$ and

$$r_{ij} = [x_i^{2/3} + x_j^{2/3}]^{1/2} \quad (i \neq j) \tag{2.11}$$

Here $x_i = n_i/n_e$ (n_e being defined by $k_F^e = (3\pi^2 n_e)^{1/3}$).

In choosing the form (2.10) for k_F^{ij} $(i \neq j)$ we have taken into account that the main approximations involved into Eqs. (2.8) and (2.9) are: i) we neglect all but the ladder diagrams and ii) we consider that the two root particles are created with zero moment ($\vec{k}_1 = \vec{k}_2 = \vec{0}$). Thus, although mathematically the common momentum cut-off should be $k_F^{ij} = \mathrm{Max}(k_F^i, k_F^j)$, we can obtain, under different basis, a new value for k_F^{ij} that compensates in part for the approximation i). To this end, we analyze the long wavelength limit ($k \rightarrow 0$) of the structure factors. Assuming a model of collective excitations (phonons and plasmons) we can obtain the dominant asymptotic behavior in the form

$$\frac{1}{S_{ij}(k)} \approx \frac{4 k_F^{ij}}{3\, k} = \frac{1}{S_F^i} + \frac{1}{S_F^j} \quad (i \neq j) \tag{2.12}$$

where $S_F^i(k)$ is the long wavelength limit of the structure factor for ideal fermions of type i: $S_F^i(k) \approx \dfrac{3\,k}{4 k_F^i}$. Then we arrive to $k_F^{ij} = k_F^i + k_F^j$ $(i \neq j)$. This result is consistent with the full HNC calculations of Lantto (reference 11).

Since the approximation $k_1 = k_2 = 0$ overestimates the value of the parameter k_F^{ij}, we finally use an intermediate value $\sqrt{(k_F^i)^2 + (k_F^j)^2}$ $(i \neq j)$ that verifies $\mathrm{Max}\,(k_F^i, k_F^j) \leqslant \sqrt{(k_F^i)^2 + (k_F^j)^2} \leqslant k_F^i + k_F^j$ $(i \neq j)$. This value for the momentum cut-off does fit the available theoretical and experimental data better than the other values.

We reduce q and k with the unit k_F^{ij} and $I_{ij}(q)$ and $v_{ij}(q)$ with the unit $v_{ij}(k_F^{ij})$. Thus Eq. (2.9) yields

$$I_{ij}(q) = \frac{1}{q^2} - \frac{\lambda_{ij}}{2\pi}\int \frac{\Theta(k-1)}{|\vec{k}-\vec{q}|^2}\frac{I_{ij}(k)}{k^2} d^3\vec{k} \tag{2.13}$$

where

$$\lambda_{ij} = \frac{2Z_iZ_j}{r_{ij}}\frac{\mu_{ij}}{m_e}\lambda \tag{2.14}$$

with $\lambda = \alpha r_s/\pi$. The dimensionless parameter r_s is defined: $r_s = (k_F^e a_0 \alpha)^{-1}$; $\alpha = (4/9\pi)^{1/3}$ and a_0 is the Bohr radius for particles of species e.

The integral equation (2.13) is the same one Yasuhara obtained[5] for the one component jellium (electron gas). By reducing its kernel into a tractable form, he was able to obtain an approximate solution for $I_{ij}(q)$ that, introduced into the one component version of Eq. (2.8), gives a closed analytical expression for the contact electron–electron pair correlation function in the electron gas. The generalization to multicomponent degenerate plasmas is just considered by the coupling parameters λ_{ij}.

D. Screening

As it is evident from the previous calculations, the ladder approximation essentially takes into account coulombic interactions between independent pairs of particles. The interactions with all other particles are, in principle, neglected, although they do revel their presence through the existence of the Fermi spheres.

When charges of opposite sign coexist, screening effects become very important and the interaction between any two particles will only be effective for momenta transfer larger than some momentum cut-off k_c.

From the observation of formulas (2.8) and (2.9) (or (2.13)), we conclude that, within the ladder approximation, and since we are interested in very large values of q, it is enough to include the screening condition only in Eq. (2.13). The improved integral equation now reads

$$I_{ij}(q) = \frac{1}{q^2} - \frac{\lambda_{ij}}{2\pi}\int_{|\vec{k}-\vec{q}|>k_c^{ij}} \frac{\Theta(k-1)I_{ij}(k)}{|\vec{k}-\vec{q}|^2\, k^2} d^3\vec{k}. \tag{2.15}$$

As cut-off momentum k_c we choose the Thomas-Fermi screening momentum. In reduced form we have

$$k_c^{ij} \equiv \frac{k_c}{k_F^{ij}} = \sqrt{\frac{4\alpha}{\pi}}\left[\sum_{k=1}^{N}\frac{m_k}{m_e}Z_k^2 x_k^{1/3}\right]\frac{r_s^{1/2}}{r_{ij}}. \tag{2.16}$$

Next, we divide the integration domain in Eq. (2.15):

$$\int_{|\vec{k}-\vec{q}|>k_c^{ij}} \cdot d^3\vec{k} = \int_{|\vec{k}-\vec{q}|<\infty} \cdot d^3\vec{k} - \int_{|\vec{k}-\vec{q}|<k_c^{ij}} \cdot d^3\vec{k} \tag{2.17}$$

and note that, for $q > k_F + k_c$, the last integral can be approximated in the form[13]

$$\int_{|\vec{k}-\vec{q}|<k_c^{ij}} \frac{\Theta(k-1)}{|\vec{k}-\vec{q}|^2} I_{ij}(k) d^3\vec{k} \approx 4\pi k_c^{ij} s I_{ij}(q) \tag{2.18}$$

where s is a number included in order to account for the various errors introduced in our approximations. It can be utilized to minimize these errors, but, in principle, we presume it takes values between 0.1 and 0.2.

Defining

$$J_{ij}(q) = I_{ij}(q)[1 - 2sk_c^{ij}\lambda_{ij}] \tag{2.19}$$

we see that $J_{ij}(q)$ verifies the same integral equation as $I_{ij}(q)$ (Eq. (2.13)) but with a renormalized coupling parameter:

$$J_{ij}(q) = \frac{1}{q^2} - \frac{\tilde{\lambda}_{ij}}{2\pi} \int_{|\vec{k}-\vec{q}|<\infty} \frac{\Theta(k-1) J_{ij}(k)}{|\vec{k}-\vec{q}|^2 k^2} d^3\vec{k} \tag{2.20}$$

where

$$\tilde{\lambda}_{ij} = \frac{\lambda_{ij}}{1 - 2sk_c^{ij}\lambda_{ij}} \tag{2.21}$$

with λ_{ij} defined in Eq. (2.14).

Inclusion of the screening, as decribed above, into Eq. (2.8), gives the correlation functions as functionals of $J_{ij}(q)$:

$$g_{ij}(r=0) = \left[1 - 2\tilde{\lambda}_{ij} \int_1^\infty J_{ij}(q) dq\right]^2 \tag{2.22}$$

An analytical approximate solution of the integral equation (2.20) is[5]

$$J_{ij}(q) = \frac{1}{q^2} F_1(\tilde{\lambda}_{ij}) F_2(q; \tilde{\lambda}_{ij}) \tag{2.23}$$

where

$$F_1(\tilde{\lambda}_{ij}) = \left[\sum_{n=0}^{\infty} \frac{1}{n!(n+1)!} (4\tilde{\lambda}_{ij})^n\right]^{-1} \tag{2.24}$$

$$F_2(q; \tilde{\lambda}_{ij}) = 2 \sum_{n=0}^{\infty} \frac{1}{n!(n+2)!} \left(\frac{4\tilde{\lambda}_{ij}}{q}\right)^n \tag{2.25}$$

and hence

$$g_{ij}(r=0) = [F_1(\tilde{\lambda}_{ij})]^2 \tag{2.26}$$

This result corresponds to non-parallel spins. If we consider a paramagnetic plasma we have, in general,

$$g_{ij}(r=0)=\begin{cases}\dfrac{1}{2s_i+1}[F_1(\tilde{\lambda}_{ii})]^2 & \text{for } i=j\\ [F_1(\tilde{\lambda}_{ij})]^2 & \text{for } i\neq j\end{cases} \tag{2.27}$$

where s_i denotes the spin of species i.

III. APPLICATION TO POSITRON ELECTRON MIXTURES

A. Arbitrary positron concentrations

In this section, we specialize the previous results to mixtures of electrons and positrons ($i=e,p$). In this case we have $m_e=m_p$ and $Z_p=-Z_e=1$. We consider that electrons is the species with the largest density, so that $x_e=1$ and $x_p=x=n_p/n_e, x$ ranging between 0 and 1.

The same system was studied by Lantto[11] using the multicomponent Fermi hypernetted-chain (FHNC) theory together with approximate Euler-Lagrange equations for the optimization of the trial wave functions.

In Table I we compare our simple Yasuhara formula (with $s=0.12$ in Eq. (2.21)) to the more laborious Lantto FHNC results. In general, the disagreement increases with the electron density and, for a given r_s, with the positron concentrations.

B. Positron-annihilation rate

Finally, we have determined the positron-annihilation rate considering infinite dilution for the positrons. This is equivalent to consider a single impurity particle (a positron) embedded into an electron gas, which is the model usually utilized for studying the annihilation of positrons in metals[13-18].

Table I Electron-positron correlation function at contact $g_{ep}(r=0)$ in positron-electron mixture as a function of the electron density r_s and positron concentration x. Between parenthesis, the FHNC results of Lantto (Ref. 11)

x/r_s	*1*	*2*	*3*	*4*	*5*
0.0	1.975	3.930	7.713	14.779	27.512
	(2.16)	(4.06)	(7.40)	(13.2)	(23.0)
0.216	1.786	3.184	5.555	9.385	15.252
	(2.02)	(3.70)	(6.49)	(11.0)	(16.9)
0.512	1.695	2.872	4.785	7.770	12.224
	(1.92)	(3.41)	(5.81)	(9.48)	(14.7)
0.729	1.652	2.730	4.449	7.088	10.978
	(1.87)	(3.23)	(5.42)	(8.68)	(13.3)
1.0	1.612	2.601	4.148	6.485	9.892
	(1.81)	(3.08)	(5.05)	(7.98)	(12.1)

The positron-annihilation rate is calculated from the electron-impurity correlation function at the origin using the expression[19]

$$\lambda_p = \frac{12}{r_s} g_{ep}(r=0) \times 10^9 [s^{-1}]. \tag{3.1}$$

The annihilation rate as a function of the electron density, obtained from Eqs. (3.1) and (2.27) (with $x = 0$), is shown in Figure 2. We compare our results with other theoretical treatments and also with experimental data reported by several authors.

From the comparison we conclude that, within the metallic range of electronic densities, our results differ about 5% from the experimental data (and also from the theoretical results of Arponen and Pajanne that reproduce experiments rather well). At lower densities, they show the same deficiency as all those theories based on similar ladder approximations, namely a typical increase of λ_p for values of r_s beyond the metallic range. In favor of our theoretical expressions we remark its simplicity.

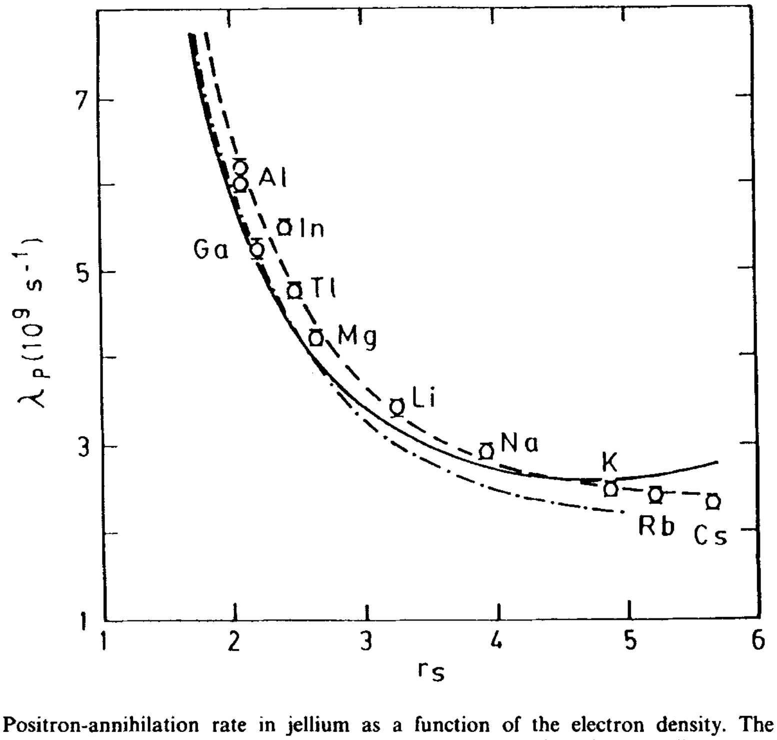

Figure 2 Positron-annihilation rate in jellium as a function of the electron density. The solid line represents the results of the present work. The dashed line and the dotted-dashed line are the results of Arponen and Pajanne (Ref. 18) and of Lantto (Ref. 11), respectively, and are reproduced, as well as the experimental data, from Figure 5 of Ref. 11.

IV. CONCLUSIONS

In this work we have extended the arguments Yasuhara used for the contact electron-electron correlation in the degenerate electron gas, to multicomponent systems of degenerate fermions. The main approximation involved, namely to consider only ladder diagrams in Goldstone formula, is at all unreasonable since our interest is on the pair correlation functions for $r = 0$. At relatively low densities (i.e., at metallic densities), the contact correlations between two particles is dominated by the direct Coulomb interaction, independently of the remaining particles. Under these circumstances, the contribution of ladder diagrams to the contact correlations is fundamental.

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