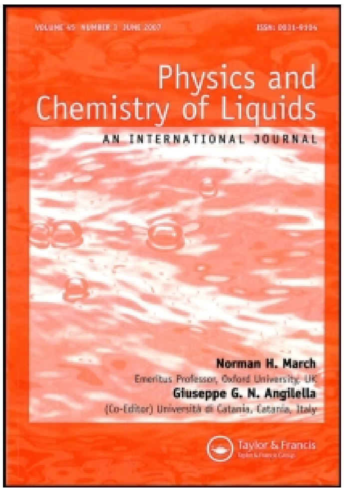

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Pair Function and Structure Factor of an Interacting Electron Liquid

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Pair Function and Structure Factor of an Interacting Electron Liquid

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Recent work on small angle scattering from liquid metals has caused renewed interest in the electron pair function in the uniform interacting electron liquid, jellium. Therefore we have re-examined this problem, starting from an analysis of the exchange hole, in which the only correlations are due to the Pauli Principle and solely therefore between parallel spin electrons. The pair function $g(r)$ of noninteracting Fermions is expressed in terms of the density of the p-component in the free electron density matrix. This motivates the treatment of the Coulomb repulsion via a potential energy $V(r)$. To close the theory, one must either invoke self-consistency to determine $V(r)$, or relate it to the (*direct*) correlation function $c(r)$ as in classical liquids. Both methods are briefly considered; the second has the advantage that here the collective plasma oscillations can be introduced through their zero-point energy.

1 INTRODUCTION

The motivation for the present work on the electron pair correlation function in the uniform interacting liquid known as jellium is two-fold. Firstly, in the course of a study of linear dispersion of plasmons in the simple organic polymers polyacetylene and polydiacetylene,[1] it has proved important to contrast the properties of the exchange hole, and its screening, in quasi-one-dimensional solids with those in isotropic three-dimensional jellium.

The work reported in this paper is concerned solely with jellium. This brings up the second reason for the renewed interest in this area; the recent work on small angle scattering from liquid metals.[2] Summaries of the extensive previous work on the pair function in the jellium model have been presented recently.[3,4]

Starting from the exchange hole, an argument is set out below which allows some account to be taken of the screening of this hole through the introduction of an effective central field potential energy $V(r)$. To close the theory, two methods are then briefly considered for the approximate determination of $V(r)$.

2 SIMPLE RE-INTERPRETATION OF EXCHANGE HOLE

Our starting point is the calculation by Wigner and Seitz[5] of the exchange hole around an electron in noninteracting, or extremely high density, jellium. If we choose to sit on an electron at the origin in an electron liquid of mean number density ρ_0, then relative to this origin the density of electrons, $\rho_0 g(r)$, is determined by

$$g(r) = 1 - \frac{9}{2}\left\{\frac{j_1(k_f r)}{k_f r}\right\}^2, \tag{1}$$

$j_1(x) = (\sin x - x\cos x)/x^2$ being the first-order spherical Bessel function while the Fermi wave number k_f is determined by $\rho_0 = k_f^3/3\pi^2$.

We now utilize the analysis by March and Murray[6] of the free-Fermion first-order density matrix into its orbital angular momentum components to write the diagonal density expansion

$$\rho_0 = \sum_{l=0}^{\infty} (2l+1)n\,(r) \tag{2}$$

All we shall need in what follows is the p-component of the density in Eq. (2), namely

$$n_1(r) = \frac{1}{4\pi^2 r^2}\left\{k + \frac{\sin 2kr}{2r} + \frac{\cos 2kr - 1}{kr^2}\right\} \tag{3}$$

where we have generalized to arbitrary Fermi energy $E = \hbar^2 k^2/2m$. It is now a straightforward matter to re-express Eq. (1) as

$$\begin{aligned} g(r) &= 1 - \frac{9\pi^2}{k_f^4 r^2}\left(\frac{\partial n_1}{\partial k}\right)_{k=k_f} \\ &= 1 - \frac{3\hbar^2}{m\rho_0 r^2}\sigma_1(r, E_f) \end{aligned} \tag{4}$$

where $\sigma_1 = (\partial n_1/\partial E)_{E_f}$ is the local density of states of the p-component at the Fermi level. Equation (4) is another example of the widely accepted view that the properties of a Fermi gas are dominated by the Fermi level behaviour.[7]

From Eq. (4.12) of the work of March and Murray,[6] we can, by differentiation with respect to energy E, obtain a differential equation from which to determine $\sigma_1(r, E)$, in the presence of a potential energy $V(r)$, assumed to be central in isotropic jellium. This equation is explicitly:

$$\frac{1}{8}\frac{\partial^3}{\partial r^3}(r^2\sigma_1) - \frac{1}{r}\frac{\partial}{\partial r}(r\sigma_1) - \frac{1}{2}\frac{\partial V}{\partial r}r^2\sigma_1 - V\frac{\partial}{\partial r}(r^2\sigma_1) + E\frac{\partial}{\partial r}(r^2\sigma_1) = 0. \qquad (5)$$

This can be integrated to yield to second-order in V the result[6]

$$\begin{aligned} f_1(r) = 2kr^2\sigma_1(r, E) = {} & \frac{F_1(r)}{2\pi^2} + \frac{2}{\pi^2 k}\left\{F_1(r)\int_r^\infty V(s)F_2(s)\,\mathrm{d}s \right. \\ & \left. + F_2(r)\int_0^r V(s)\,F_1(s)\,\mathrm{d}s\right\} \\ & + \frac{8}{\pi^2 k^2}\left\{F_2(r)\int_0^r V(s)F_1(s)\int_s^\infty V(t)F_2(t)\,\mathrm{d}t\,\mathrm{d}s \right. \\ & + F_1(r)\int_r^\infty V(s)F_2(s)\int_s^\infty V(t)F_2(t)\,\mathrm{d}t\,\mathrm{d}s \\ & - \tfrac{1}{2}F_1(r)\int_0^r V(s)F_3(s)\int_0^s V(t)F_1(t)\,\mathrm{d}t\,\mathrm{d}s \\ & \left. + \tfrac{1}{2}F_3(r)\int_0^r V(s)F_1(s)\int_0^s V(t)F_1(t)\,\mathrm{d}t\,\mathrm{d}s\right\}, \end{aligned} \qquad (6)$$

where

$$\begin{aligned} F_1 &= k^2r^2j_1^2(kr) \\ F_2 &= k^2r^2j_1(kr)\tilde{n}_1(kr) \\ F_3 &= k^2r^2\tilde{n}_1^2(kr), \end{aligned} \qquad (7)$$

with $\tilde{n}_1$ the first-order sperical Neumann function.

3 METHODS TO DETERMINE EFFECTIVE POTENTIAL $V(r)$

At this stage, we shall assume that $V(r)$ arises from suitable 'screening' of the Coulomb interaction e^2/r. Then the simplest self-consistent field theory leads to the equation:

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(rV) = -\frac{18\rho_0}{k_f^5 r^4}\left\{F_1(r)\int_r^\infty V(s)F_2(s)\,\mathrm{d}s + F_2(r)\int_0^r V(s)F_1(s)\,\mathrm{d}s\right\}. \qquad (8)$$

In the high density limit, Eq. (8) provides an explicit basis for screening the exchange hole which arises solely from Pauli Principle correlations between parallel spin electrons. We have not, to date, obtained an exact analytic solution of Eq. (8), though it seems to us that choice of a suitable integral transform might eventually make this possible.

From Eq. (6), it is evident that second-order corrections can be immediately incorporated in the right-hand-side of Eq. (8) if and when they should be required. Since, however, the resulting equation must obviously be solved numerically, as for the second-order non-linear impurity problem,[8] it is worth noting that the fully non-linear problem posed by solving Eq. (5) simultaneously with Poisson's equation should be tractable by numerical methods. This is now being investigated; we merely note at this point that, since $V(r)$ behaves as e^2/r at sufficiently large r, this Coulomb term will dominate the long-range behaviour in Eq. (5).

In summary, a self-consistent field equation has been proposed for the pair function $g(r)$ of electrons in jellium. In the high density limit, solution of the linear Eq. (8) should be adequate, supplemented as the density is lowered somewhat by the second-order terms exhibited explictly in Eq. (6). Intuitively, we expect $V(r) \simeq -\frac{1}{2}\hbar\omega_p \Delta c(r)$, where ω_p is the plasma frequency, and Δc the direct correlation function difference $c(r) - c(r)_{\text{exchange}}$.

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