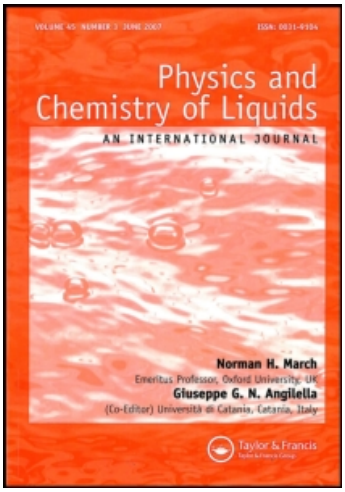

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Homogeneous Fermi liquid with 'artificial' repulsive inverse square law interparticle potential energy

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Homogeneous Fermi liquid with 'artificial' repulsive inverse square law interparticle potential energy

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A good deal is known by now on the so-called jellium model of the homogeneous electron liquid. However, much of the quantitative progress at experimentally realizable densities has come from quantal computer simulation. Therefore, we here consider a homogeneous Fermion liquid with 'artificial' repulsive interaction $\lambda/(r_{ij})^2$ between Fermions i and j at separation r_{ij}. We discuss first of all the way the static structure function $S(q)$, essentially the Fourier transform of the pair correlation function, is changed because of non-zero λ from the 'Fermi hole' form due entirely to Pauli principle effects between parallel spin Fermions. Unlike jellium with e^2/r_{ij} repulsive interactions, $S(q)$ is proportional to q at long wavelengths, whereas the plasmon in jellium annulls the q term and $S(q)$ is quadratic in q as q tends to zero. However for $\lambda/(r_{ij})^2$ interactions, the coefficient of q appearing in the Fermi hole structure factor, is renormalized by particle repulsions. Then some discussion is given of Fermion quasiparticle lifetimes τ as the Fermi surface is approached. Arguments are presented that τ^{-1} is proportional to $|E-E_F|$ as E tends to the Fermi energy. This is already interesting, in fact, in connection with the jellium model and therefore an approximate analytic form of τ is finally derived.

Keywords: Homogeneous Fermion liquids; Structure factor; Quasiparticle lifetime

1. Introduction

Electron liquids in monovalent species as *Na* and *K* are usefully discussed in relation to the so-called jellium model going back to the early work of Sommerfeld on the theory of metals. Because of the weakness of the pseudopotentials in *Na* and *K* in particular, the conduction electrons are relatively uniform throughout most of the unit cell of these

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body-centered-cubic lattices. Thus the jellium model, with its uniform density ρ described conventionally in terms of the interelectronic spacing r_s through

$$\rho = \frac{3}{4\pi r_s^3} \tag{1}$$

is immediately valuable in getting the essence of the behaviour of the interacting conduction electron liquid in the above two alkali metals. However, these are relatively low density metals, with r_s at ambient pressure $\sim$3–4a_0 where a_0 is the Bohr radius $\hbar^2/me^2$. While some important analytic progress is possible for $r_s \ll a_0$ [1,2] for real metallic densities in the range $2 < r_s/a_0 < 5.5$ quantum Monte Carlo simulations pioneered by Ceperley and Alder [3] have yielded to date the definitive quantitative predictions of the jellium model.

Passing from this model, appropriate in the thermodynamical limit, to really small systems, it was pointed out in early work that replacing Coulomb potential energy e^2/r_{ij} allowed analytical progress to be made [4]; see recent work by Capuzzi *et al*. [5]. These latter authors have examined the interplay between harmonic confinement and repulsive potential energy $\lambda/(r_{ij})^2$, with focus on the formation of a Wigner molecule in an artificial two-electron spin-compensated atomic ground state.

Here, we shall, with the above motivation plus later reasons (see below) connected with Fermion quasiparticle lifetimes as the Fermi surface is approached, study a homogeneous Fermion liquid with inverse square law repulsions. Let us begin with the static structure factor $S(q)$.

2. Static structure factor $S(q)$ for homogeneous Fermion liquid with $\lambda/(r_{ij})^2$ repulsive interactions

Let us start the quantitative discussion by recalling the Pauli Principle effect between spin 1/2 Fermions in a spin-compensated uniform Fermion liquid. Then the ground-state wave function is a single Slater determinant formed from plane waves $\Omega^{-1/2}e^{i\mathbf{kr}}$ (Ω being the normalization volume) where $\mathbf{k}$ vectors all lie within the (completely filled) Fermi sphere of radius k_F ($k_F r_s = (9\pi/4)^{1/3}$), related to the Fermi energy E_F by

$$E_F = \frac{\hbar^2 k_F^2}{2m}. \tag{2}$$

Then (see for example the book of Jones and March [6]), the Fermi hole (FH) pair function $g_{FH}(r)$, with corresponding structure factor $S_{FH}(q)$, is given by the closed analytic form

$$S_{FH}(q) = a_1 q + a_3 q^3, \tag{3}$$

for $q \leq 2k_F$. For $q > 2k_F$ one has $S_{FH}(q) = 1$. In equation (3) $a_1 = 3/4k_F$ and $a_3 = -1/16k_F^3$. If we choose to define a corresponding 'direct' correlation function $c(r)$, well known in classical statistical mechanics (see, for instance the book by Ishihara [7]) by

$$h(r) = g(r) - 1 = c(r) + \rho \int h(|\mathbf{r} - \mathbf{r}'|)c(r')\,\mathrm{d}\mathbf{r}', \tag{4}$$

then the Fourier transform, say $\tilde{c}(q)$, of $c(r)$ is immediately given by

$$\tilde{c}(q) = \frac{S(q) - 1}{S(q)}. \tag{5}$$

Inserting the Fermi hole result, equation (3), into equation (5) we immediately find

$$\tilde{c}_{\mathrm{FH}}(q \leq 2k_{\mathrm{F}}) = 1 - \frac{1}{a_1 q + a_2 q^3}, \tag{6}$$

with $\tilde{c}_{\mathrm{FH}}(q > 2k_{\mathrm{F}}) = 0$. Hence the r-space form is obtained by quadrature to read

$$c_{\mathrm{FH}}(r) = \frac{1}{8\pi^3 \rho} \int_0^{2k_{\mathrm{F}}} \left(1 - \frac{1}{a_1 q + a_2 q^3}\right) \frac{\sin(qr)}{qr} 4\pi q^2 \mathrm{d}q. \tag{7}$$

What is important for present purposes, beyond the complete behaviour of $c_{\mathrm{FH}}(r)$, is its long-range form. This is dominated by the small q behaviour in equation (7), the integrand evidently tending to $-1/a_1 q$ as $q \to 0$. This in turn, by Fourier transform (see book by Lighthill [8]) yields for the $r \to \infty$ asymptotic limit:

$$c_{\mathrm{FH}}(r) = -\frac{2}{k_{\mathrm{F}}^2 r^2}. \tag{8}$$

In fact, the complete evaluation of $c_{\mathrm{FH}}(r)$ can be achieved, and is set out in appendix A. Since the full analytic form given there is somewhat lengthy, we note that throughout the entire range of integration in equation (7) embracing the diameter of the Fermi sphere, the term $a_2 q^3$ is fairly small compared with $a_1 q$. The integration is readily completed if we therefore neglect the term $a_2 q^3$, the result being

$$c_{\mathrm{FH}}(r) = \frac{1}{r} \frac{3}{2k_{\mathrm{F}}^3} \left[\frac{\sin(2k_{\mathrm{F}} r) - 2k_{\mathrm{F}} r \cos(2k_{\mathrm{F}} r}{r^2} - \frac{4k_{\mathrm{F}}}{3} \frac{1}{r} [1 - \cos(2k_{\mathrm{F}} r)] \right]. \tag{9}$$

Following Lighthill's account [8], the oscillating terms involving $\cos(2k_{\mathrm{F}} r)$ and $\sin(2k_{\mathrm{F}} r)$ arise from the non-analytic behaviour of $\tilde{c}_{\mathrm{FH}}(q)$ at $q = 2k_{\mathrm{F}}$, whereas the long-range r^{-2} term in equation (8) comes from the non-analyticity at $q = 0$. We will return to the form (8) below after including the effect of the interparticle repulsion energy $\lambda/(r_{ij})^2$.

A. *Beyond the Fermi hole due to repulsive potential energy $\lambda/(r_{ij})^2$*

We now enquire as to the effect on the result in equation (8) of 'switching' on the repulsive interactions $\lambda/(r_{ij})^2$ between the Fermions in the uniform Fermi liquid.

To see this, we proceed intuitively by way of classical statistical mechanics. In the early work of Johnson and March [9] and Johnson *et al.* [10] on pair interactions between ions in liquid metals (see also Reatto [11]), it was pointed out that provided the ions were classical and in an assembly in equilibrium at temperature T, the long-range ($r \to \infty$) behaviour of $c(r)$ was given by

$$c(r) = -\frac{\phi(r)}{k_{\mathrm{B}} T}, \tag{10}$$

where $\phi(r)$ is the pair potential. For the ground-state of jellium, $k_B T$, measuring the thermal energy corresponding to temperature T, is to be replaced by the zero-point energy $\hbar\omega_p/2$ of the plasmon, the frequency ω_p being given by

$$\omega_p = \left(\frac{4\pi\rho e^2}{m}\right)^{1/2}. \tag{11}$$

Hence, by analogy with equation (10), we propose to write the asymptotic form say of $c_\lambda(r)$ as $r \to \infty$ as

$$c_\lambda(r) = -\frac{\lambda}{r^2 E_{\text{char}}}, \tag{12}$$

where E_{char} is a characteristic energy of the inverse power law model. Fourier transformation of the large r limit then gives, as $q \to 0$

$$\tilde{c}_\lambda(q) = \frac{\lambda \times \text{known constant}}{q}. \tag{13}$$

But from equation (6) as $q \to 0$, $\tilde{c}_{\text{FH}}(q) \to -1/a_1 q$, and we see that the interaction between the Fermions 'renormalizes' the coefficient of the q term in $S_{\text{FH}}(q)$ but does not remove it, in marked contrast to jellium where $S_{\text{jellium}}(q) = \frac{1}{2}\hbar(4\pi\rho m e^2)^{-1/2} q^2$ at small q the coefficient of q^2 evidently being determined by the plasma frequency of equation (11).

We show in appendix B how appeal to the work of Gaskell [12] shows that it is plausible to write

$$\tilde{c}(q) = \tilde{c}_{\text{FH}}(q) + \lambda\Delta(q), \tag{14}$$

where, to first-order in λ, Δ is independent of λ. We have argued above that $\Delta(q) \propto q^{-1}$ as q tends to zero [compare equation (13)].

B. *Quasi-particle lifetime in presence of $\lambda/(r_{ij})^2$ repulsive interaction*

Having discussed the static structure factor $S(q)$, we turn now to examine, of course approximately, the form of quasiparticle lifetime τ to be expected when one 'switches on' the repulsive inverse square interaction. We take as starting point the study of Galitskii [13,14].

As background, let us first note that, in many cases one can consider the excited states of a system of interacting Fermi particles as a gas of elementary excitations – quasiparticles. Of course, a description of a system by means of quasiparticles is exact only in the case of an ideal gas. If there is interaction between the particles, the excited states of the 'Fermi type' do not represent the exact stationary states of the systems. This leads to the damping of the quasiparticles. The decay is actually an exciting field [15], due to developments in different spectroscopies.

For a weakly non-ideal Fermi gas with repulsive, short-range interparticle interactions a second-order treatment for the damping was performed by Galitskii [13]. An essential component of his approach is the proper treatment of kinematics in (k, ω) variables. He used the imaginary part of the density-density response function $[\chi_0(k, \omega)]$ of an ideal Fermi system to characterize physically allowed, real transitions [16].

Considering these transitions, for an added fermion with energy $E \geq E_F$ one can [17] write (in Hartree atomic units) for the inverse lifetime the second-order expression

$$\frac{1}{\tau} = \frac{1}{2\pi^2}\frac{1}{\sqrt{2E}}\int_0^{|E-E_F|} d\omega \int_{k^-}^{k^+} dk\, k|V(k)|^2 Im\chi_0(k,\omega), \tag{15}$$

in which $k^{\pm}$ are determined by the energy-momentum conservation law, together with the constraints codified in the density of excitations via the $Im\ \chi_0(k, \omega)$ function.

In his paper of applying methods of quantum field theory, Galitskii used a simple contact ($V = 4\pi f_0$) interaction to equation (15) and obtained

$$\frac{1}{\tau} = \frac{k_F^4}{\pi} f_0^2 \frac{8}{15\sqrt{x}}\left[\Theta(2-x)(2-x)^{5/2} + \frac{5x-7}{2}\right], \tag{16}$$

where $x = E/E_F$ is a shorthand. Notice, that for the physically most important, $\omega_{max} = |E - E_F| \ll E_F$, limit one gets the usual Fermi-liquid form by expansion in equation (16)

$$\frac{1}{\tau} = \frac{4}{\pi} f_0^2 (E - E_F)^2. \tag{17}$$

With our weakly singular $[V(k) = 2\pi^2\lambda/k]$ interaction in equation (15), a straightforward calculation results in the following expression

$$\frac{1}{\tau} = \pi\lambda^2 \frac{4E_F}{3\sqrt{x}}[I_1(x) - I_2(x)], \tag{18}$$

to which the $I_1(x)$ and $I_2(x)$ functions are given by

$$I_1(x) = \left[\ln(x-1) + \left(\frac{8}{3} - 2\ln 2\right)\right], \tag{19}$$

$$I_2(x) = \Theta(2-x)\left[\frac{2}{3}(2-x)^{3/2} + 2(2-x)^{1/2} + \ln\left(\frac{\sqrt{2-x}-1}{\sqrt{2-x}+1}\right)\right]. \tag{20}$$

Finally, for the $\omega_{max} = |E - E_F| \ll E_F$ low-energy limit one gets, by a similar limiting process as the one behind of equation (17), the simple

$$\frac{1}{\tau} = \pi\lambda^2 |E - E_F|, \tag{21}$$

regular form for the inverse-lifetime of a prepared state with energy E close to E_F. A more direct determination of the low-energy limiting forms in equation (17) and equation (21) can be based on equation (15) with $Im\chi_0(k,\omega) = \omega/2\pi k$ and $k^{\pm} = \sqrt{2(E_F + \omega)} \pm k_F$.

3. Summary and proposed future directions

We have studied here the effect of inverse square law repulsive interparticle potential energy $\lambda/(r_{ij})^2$ on a homogeneous Fermion liquid. With the unperturbed structure factor

taken as the Fermi hole form $S_{FH}(q)$ given in equation (3), we have first evaluated the corresponding direct correlation function $c_{FH}(r)$, the Fourier transform of $\tilde{c}_{FH}(q)$ which we have chosen to define through the 'classical' form (5), when $S(q)$ is taken equal to the known $S_{FH}(q)$. The form of $c_{FH}(r)$ in equation (9) is approximate but already useful in showing how the two singularities in $\tilde{c}_{FH}(q)$, at $q=0$ and $q=2k_F$, separately contribute to the asymptotic large r form of $c_{FH}(r)$. At sufficient large r, the dominant contribution comes from q near to zero and is displayed in equation (8). Classical liquid analogy suggests that 'switching on' the interaction $\lambda/(r_{ij})^2$ contributes to the q^{-1} term in $\tilde{c}(q)$ as $q \to 0$, as displayed in equation (13), and also in its r-space equivalent in equation (12).

Turning to low-energy dynamics, we have briefly then estimated the quasiparticle lifetime τ assuming Galitskii's formula [13] as starting point, to treat the interparticle interaction $\lambda/(r_{ij})^2$. The full expression for the lifetime τ is displayed in equation (15), and its simple limiting form as the Fermi energy E_F is approached is $\tau \sim |E - E_F|^{-1}$.

As to future directions, it would be interesting to explore quantitatively the precise form of the characteristic energy entering equation (12), which we except to be revealed by treating the broken symmetry state in which the repulsive interparticle interactions $\lambda/(r_{ij})^2$ eventually drive the Fermions into localized states, to be compared with the Wigner electron crystal induced in jellium at low densities, with $r_s \sim 100\ a_0$ [3,18].

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Appendices

A. Complete evaluation of equation (7) for $c_{\mathrm{FH}}(r)$

As we pointed out in the main text, the 'direct' correlation function $c(r)$ has a compact form with the Fermi hole input. The result is as follows

$$c_{\mathrm{FH}}(r) = \frac{1}{r}\frac{3}{2k_{\mathrm{F}}^3}\left[\frac{\sin(2k_{\mathrm{F}}r) - 2k_{\mathrm{F}}r\cos(2k_{\mathrm{F}}r)}{r^2} - \frac{4k_{\mathrm{F}}}{3}\frac{1}{r}I(r,k_{\mathrm{F}})\right], \tag{22}$$

to which the $I(r,k_{\mathrm{F}}) = I_1(r,k_{\mathrm{F}}) - I_2(r,k_{\mathrm{F}})$ function is given via the expressions

$$I_1(r,k_{\mathrm{F}}) = v\sin(v)[ci(v) - ci(u-v) - ci(u+v)], \tag{23}$$

$$I_2(r,k_{\mathrm{F}}) = v\cos(v)[si(v) + si(u-v) - si(u+v)]. \tag{24}$$

In these expressions the shorthands of $u = 2k_{\mathrm{F}}r$ and $v = \sqrt{3}u$ are used, and the $si(y)$ and $ci(y)$ functions are defined by as usual

$$si(y) = \int_o^y \mathrm{d}t\frac{\sin(t)}{t}, \tag{25}$$

$$ci(y) = -\int_y^\infty \mathrm{d}t\frac{\cos(t)}{t}. \tag{26}$$

B. Density fluctuation $\rho_{\mathbf{k}}$ and a possible variational ground-state wave function for $\lambda/(r_{ij})^2$ interactions

To include interactions in a homogeneous Fermion gas we follow Gaskell [12] by writting

$$\Psi = D\exp\left[-\sum_k d(k)\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\right], \tag{27}$$

where $\rho_{\mathbf{k}}$ denote the Fourier components of the density:

$$\rho_{\mathbf{k}} = \sum_{i=1}^{N}\exp(-i\mathbf{k}\mathbf{r}_i), \tag{28}$$

in which $\mathbf{r}_i$ denote electronic positions. For the homogeneous electron liquid, Gaskell then determined $d(k)$ variationally. For small r_s of the jellium (j) and for long wavelengths

$$d_j(k) \sim \frac{k_F^2 r_s^{1/2}}{k^2}\frac{1}{2}\left[\frac{4}{3\pi}\left(\frac{4}{9\pi}\right)^{1/3}\right]^{1/2}. \tag{29}$$

Returning to the ideal Fermi hole briefly let us rewrite the pair function $g_{\mathrm{FH}}(r)$ as

$$g_{\mathrm{FH}}(x) - 1 = -\frac{3}{2}\int_0^\infty \mathrm{d}\eta\, \eta^2 j_0(\eta x)[1 - S_{\mathrm{FH}}(\eta)], \tag{30}$$

where $\eta = k/k_{\mathrm{F}}$ and $x = k_{\mathrm{F}} r$.

Then the pair function $g_j(r)$ discussed briefly in the main text has, for small r_s, the following approximate form in terms of the direct correlation function

$$g_j(x) - 1 = -\frac{3}{2}\int_0^\infty \mathrm{d}\eta\, \eta^2 j_0(\eta x)\left[1 - \frac{1}{1 - c_{\mathrm{FH}}(\eta) + 4d_j(r_s,\eta)}\right], \tag{31}$$

Motivated partly by the $1 - c_{\mathrm{FH}}(\eta \to 0) = 4/3\eta$ behaviour, it is tempting to try the ansatz that, for the model with which the present article is concerned, to first-order in λ:

$$d_\lambda(k) \sim \text{constant}\frac{\lambda}{\eta}, \tag{32}$$

by attributing in equation (29) the k^{-2} term as resulting from the Fourier transform of the Coulomb interaction to be therefore replaced by $2\pi^2\lambda/k$, the Fourier transform of $\lambda/(r_{ij})^2$.