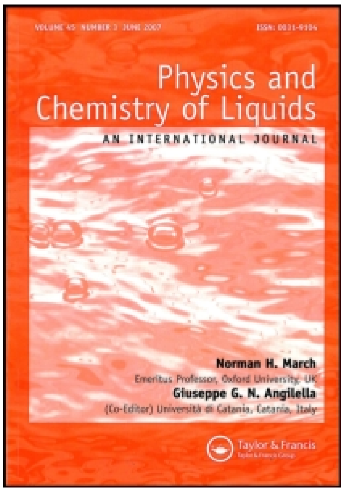

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Boson and fermion many-body assemblies: fingerprints of excitations in the ground-state wave functions, with examples of superfluid ^{4}He and the homogeneous correlated electron liquid

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After a brief summary of some basic properties of ideal gases of bosons and of fermions, two many-body Hamiltonians are cited for which ground-state wave functions allow the generation of excited states. Because of the complexity of ground-state many-body wave functions, we then consider properties of reduced density matrices, and in particular, the diagonal element of the second-order density matrix. For both the homogeneous correlated electron liquid and for an assembly of charged bosons, the ground-state pair correlation function $g(r)$ has fingerprints of the zero-point energy of the plasmon modes. These affect crucially the static structure factor, $S(k)$, in the long wavelength limit. This is best understood by means of the Ornstein–Zernike direct correlation function $c(r)$, which plays an important role throughout this article. Turning from such charged liquids, both boson and fermion, to superfluid ^{4}He, the elevated temperature (T) structure factor $S(k, T)$ is related, albeit approximately, to its zero-temperature counterpart, via the velocity of sound, reflecting the collective phonon excitations and the superfluid density. Finally, some future directions are pointed.

Keywords: superfluid ^{4}He; homogeneous electron liquid; charged bose fluid

1. Background and outline

Many-body ground-state wave functions for both bosons and fermions are undoubtedly complex, even though explicit variational forms exist: for example, the Bijl–Jastrow wave function for a correlated boson assembly [1,2]. However, given an exact many-body ground-state wave function, there are now Hamiltonians which allow, at least in principle, excited states to be generated. Two such Hamiltonians are briefly set out in Appendices 1 and 2 below, and their existence was part of the underlying motivation for the present study. However, we shall usually work with reduced ground-state density matrices [3] rather than N-body wave functions, to achieve quite concrete examples. An early attempt to treat the homogeneous correlated electron liquid using the second-order density matrix (2DM) variationally was made by Young and March [4]. Here we shall consider further in this same so-called jellium model, the ground-state pair correlation function $g(r)$, which is the diagonal element of the 2DM. The related Ornstein–Zernike (OZ) direct correlation function $c(r)$, defined precisely in Equation (2.8) below, will play a key role throughout.

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However, before turning to the major problem of treating strong interactions in many-body assemblies, let us briefly introduce some basic properties distinguishing bosons and fermions by referring first to ideal gases.

1.1. *Contrasts between idealised boson and fermion assemblies*

As background to some of the many-body results to follow, it will be useful to summarise briefly some contrasts in the behaviour of idealised boson and fermion systems.

A number of authors [5] have considered the average separation between two particles at positions x_1 and x_2 when one particle is in state ψ_a and the other ψ_b: the two functions being orthonormal.

(a) *Case of two distinguishable particles*

For distinguishable (d) particles, with wave function $\psi_a(x_1)\psi_b(x_2)$, the mean-square separation is given by

$$\left\langle (x_1 - x_2)^2 \right\rangle_d = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b,$$

where $\langle x \rangle_a = \int \mathrm{d}x\, x |\psi_a(x)|^2$ etc.

(b) *Fermions and bosons*

For spinless fermions, the wave function must be antisymmetrical and for bosons symmetrical. This yields

$$\Psi = \frac{1}{2^{1/2}}[\psi_a(x_1)\psi_b(x_2) \pm \psi_a(x_2)\psi_b(x_1)],$$

the plus sign being for bosons and the minus for fermions. Again, one can calculate the corresponding mean-square separation as

$$\left\langle (x_1 - x_2)^2 \right\rangle_\pm = \left\langle (x_1 - x_2)^2 \right\rangle_d \mp 2\left|\langle x^2 \rangle_{ab}\right|,$$

where $\langle x^2 \rangle_{ab} = \int \mathrm{d}x\, x^2 \psi_a^*(x)\psi_b(x)$. The bosons evidently tend to lie nearer to one another than for distinguishable particles, with the fermions being further apart.

(c) *Elevated temperatures and the virial expansion*

The exact quantal second virial co-efficent $B(T)$ is given by [6]

$$B(T) = \frac{1}{2V}\int [1 - g(r_{12})]\mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2,$$

where V is the volume and g is the pair correlation function already introduced. For ideal spinless fermions and boson assemblies, $B(T)$ has the form [6]

$$B(T) = -\eta\lambda^3/2^{5/2},$$

where $\eta = \pm 1$, the plus sign being for bosons and minus for fermions, while λ is the thermal de Broglie wavelength. Hence, it follows that fermions exert greater pressure and bosons less pressure on the walls of a container than does a classical fluid under the same thermodynamic conditions.

The above pair density $g(r_{12})$ will play a central role in what follows. For ideal boson or fermion fluids at sufficiently high temperature T, $g(r_{12})$ takes the form

$$g(r_{12}, T) = 1 + \eta \exp\left(-2\pi r_{12}^2/\lambda^2\right), \tag{1.1}$$

η being as defined above.

In Appendix 3, we utilise Equation (1.1) for fermions to relate the elevated structure factor $S(k, T)$, which is essentially the Fourier transform (FT) of $g(r_{12}, T)$, to the ground-state structure factor $S(k, 0)$. This anticipates a major theme of this article, but taking into account in the later sections strong particle–particle interactions.

The outline of this article is then as follows. In Section 2, we consider in some detail the boson superfluid ^{4}He. The use of density matrices goes back to the pioneering work of Onsager and Penrose [7] followed by the important study of Yang [8]. We shall again focus on the pair function $g(r)$, or more directly what is the liquid structure factor $S(k)$: essentially the FT of $g(r)$. The main result, albeit approximate, is to relate the elevated temperature structure factor $S(k, T)$ to its ground-state counterpart via the velocity of sound and the superfluid density. Section 3 considers the homogeneous electron liquid already referred to; which has played an important role in the development of the density functional theory of inhomogeneous fermion assemblies [9]. The penultimate Section 4 gives a brief account of a charged homogeneous bose fluid, while Section 5 constitutes a summary, together with some proposals for future studies which should prove fruitful.

2. Superfluid ^{4}He: approximate functional relationship between the elevated temperature structure factor $S(k, T)$ and its ground-state counterpart

The Feynman theory [10] of superfluid ^{4}He clearly recognised the importance of collective phonon modes in the long-wavelength limit $k \to 0$. Then it follows, as a consequence, that the $k \to 0$ limit of the ground-state structure factor $S(k, T = 0)$, denoted below simply by S_0 for notational convenience, involves the velocity of sound c, yielding

$$S_0 = \frac{\hbar k}{2mc} : k \to 0, \tag{2.1}$$

with m the single particle ^{4}He mass. The long-wavelength theory of the structure factor in superfluid ^{4}He was subsequently put on a rigorous footing by Gavoret and Nozieres [11].

Again in the limit $k \to 0$, Equation (2.1) was generalised to elevated temperatures by Feynman and Cohen [12], who obtained the result that

$$S(k, T) = \frac{\hbar k}{2mc} \coth\left(\frac{\hbar kc}{2k_{\mathrm{B}}T}\right) : k \to 0. \tag{2.2}$$

Our objective below, within the present context, is to relate this elevated temperature structure factor to its ground-state counterpart S_0.

The first step in doing so is to use Equation (2.1) in (2.2) to find [13]

$$S(k, T) = S_0 \coth\left(\frac{mc^2}{k_{\mathrm{B}}T} S_0\right). \tag{2.3}$$

This Equation (2.3) shows that the elevated temperature structure factor of superfluid ^{4}He, in the long-wavelength limit $k \to 0$, is characterised by the ground-state structure factor S_0 plus the dimensionless variable measuring the characteristic energy mc^2 in units of the thermal energy $k_{\mathrm{B}}T$.

2.1. *Proposed functional generalisation of $S(k, T)$ related to S_0 beyond the long wavelength limit*

We next propose a functional generalisation of Equation (2.3)

$$S(k, T) = S_0 F\left[S_0; \frac{mc^2}{k_B T}; \frac{\rho_s(T)}{\rho}\right], \tag{2.4}$$

where the constraint of small k is now assumed to be no longer necessary. Here, $F \to \coth((mc^2/k_B T)S_0)$ as $k \to 0$ from Equation (2.3) while also $F \to 1$ as $k \to \infty$ since both $S(k, T)$ and S_0 tend to unity in this limit.

Underpinning the proposal (2.4) lies in the recognition of the importance of the two-fluid model in understanding the superfluid phase of ^{4}He. Thus the superfluid density $\rho_s(T)$ enters the functional form (2.4), as does the normal fluid density $\rho_n(T)$ through the total density ρ given by

$$\rho = \rho_s(T) + \rho_n(T). \tag{2.5}$$

Further motivation for the form (2.4) is presented in Appendix 4, where the separation of the elevated temperature structure factor $S(k, T)$ into a term $[\rho_s(T)/\rho]S_0$ and a remainder proportional to $[\rho_n(T)/\rho]$ is set out following the work of Mayers [14].

2.2. *An approximate correlated ground-state wave function for ground-state of superfluid ^{4}He*

In an early study based on the Bijl–Jastrow wave function [1,2]

$$\Psi_0(\mathbf{r}_1 \ldots \mathbf{r}_2) = \prod_{i<j}^{1,\ldots,N} \exp\{-u(|\mathbf{r}_i - \mathbf{r}_j|)\}, \tag{2.6}$$

Enderby et al. [15] found the long-range form of the two-body function $u(r)$ entering Equation (2.6). Their result that

$$u(r) = \frac{2mc}{\pi^2 \rho \hbar r^2} : r \to \infty, \tag{2.7}$$

where ρ is the density of ^{4}He atoms, was subsequently confirmed by Chester and Reatto [16]. The long-range behaviour (2.7) is now known to be crucial in obtaining a satisfactory overlap with the 'true' ground-state wave function, obtained via quantum Monte Carlo calculations (see also Section 5B below).

It is tempting in the neutral superfluid ^{4}He to compare $u(r)$, certainly at large distances r, with the OZ direct correlation function $c(r)$, which will play a key role in the present study. The OZ definition in a classical liquid was given, starting from the pair correlation function $g(r)$, by [17]

$$h(r) = c(r) + \rho_0 \int h(|\mathbf{r} - \mathbf{r}'|)c(r')\mathrm{d}\mathbf{r}'. \tag{2.8}$$

Here $h(r) = g(r) - 1$ is termed the total correlation function and ρ_0 is now the number density. We recognise that other definitions of $c(r)$ are possible quantally but here retain

Equation (2.8) throughout. Taking the FT of Equation (2.8) readily yields, with $\tilde{c}(k)$ denoting the FT of the structure factor $S(k)$:

$$\tilde{c}(k) = \frac{S(k) - 1}{S(k)}. \tag{2.9}$$

Inserting the Feynman small k-limit (2.1) into Equation (2.8) readily demonstrates that $\tilde{c}(k)$ is proportional to k^{-1} at small k. Using arguments set out fully in Lighthill's book [18], we hence find

$$\underset{r \to \infty}{c\ (r)} = \frac{\text{constant}}{r^2}, \tag{2.10}$$

with FT $\tilde{c}(k)$ proportional to k^{-1} as $k \to 0$. Comparing Equations (2.7) and (2.10) we see a preliminary justification for conjecturing that $u(r)$ is proportional to $c(r)$, which is certainly true at large r.

A corresponding result for the many-fermion Coulombic system jellium will emerge later in Section 3.

2.3. *Can Efimov states result in a further liquid phase transition in ^{4}He at exceedingly low temperatures?*

In early work [19], March discussed the possibility of Efimov states occurring at sufficiently low temperatures in the liquid phase of ^{4}He. This was followed by an interesting comment by Ghassib and Chester [20], and a reply by March [21] emphasising the large area of common ground between [20] and [19]. Subsequent experimental proof of stable dimers [22] and trimers in the gaseous phase makes wholly worthwhile the further study of Efimov states in liquid ^{4}He at the lowest possible temperatures. We also draw attention to the review of Minguzzi et al. [23] which discusses superfluidity with and without a condensate in interacting bose fluids. We re-emphasise, in concluding this section on liquid ^{4}He, the contrast between this liquid below the λ point and the alkali atom gases [23]. Both exhibit superfluidity, but the manifestations of a Bose–Einstein condensate are quite different. Thus, for the atomic vapours, nearly 100% of the atoms are condensed at the lowest temperatures, whereas from (a) neutron scattering and (b) computer simulations in liquid ^{4}He, evidence presently is that the condensate fraction is only 7%. The main conclusion in [23] was that Bose–Einstein condensation and superfluidity are distinct consequences of deeper topological properties of the many-body wave-function.

3. Homogeneous correlated electron liquid

This section concerns the homogeneous correlated electron liquid, or shortly the jellium model. Here, interacting electrons move in a smeared out uniform positive charge non-responsive neutralising background. The essential variable of the jellium model is the number density, say ρ_0, or equivalently one can characterise the model by the mean interelectronic spacing r_s defined by

$$\rho_0 = 3/4\pi r_s^3. \tag{3.1}$$

The Lowdin natural orbitals of this homogeneous electron liquid [3] are plane waves $\exp(i\mathbf{k}\cdot\mathbf{r})$. In the extreme high-density limit, or equivalently as $r_s \to 0$, the kinetic energy dominates the potential terms, and the ground-state wave function Ψ is a determinant of plane waves, where $|\mathbf{k}| \leq k_f$, with k_f denoting the Fermi wave number and the ground state is spin compensated. In turn, k_f is related to the density ρ_0 in Equation (3.1) by

$$\rho_0 = k_f^3/3\pi^2. \tag{3.2}$$

From the determinantal wave function Ψ introduced above, the pair correlation function $g(r)$ can be evaluated, as was first done by Wigner and Seitz [24] and has the form

$$g(r) = 1 - \frac{9}{2}\frac{\{j_1(k_f r)\}^2}{(k_f r)^2}. \tag{3.3}$$

In Equation (3.3), $j_1(x)$ is the first-order spherical Bessel function given by $j_1(x) = (\sin x - x\cos x)/x^2$. Since $j_1(x)$ tends to $(1/3)x$ as x tends to zero, it follows from Equation (3.3) that $g(r=0)$ is 1/2. This has the simple physical interpretation that parallel spins completely avoid each other, meaning that they contribute zero to $g(r=0)$. The antiparallel spins, as r tends to zero, are no longer correlated, and therefore in the spin-compensated ground state $g(r=0) = 1/2$ as given by Equation (3.3).

3.1. *Fermi hole approximation to the ground-state structure factor S(k)*

Equation (3.3) is the Fermi hole (FH) approximation to the ground-state pair correlation function. Below, and following Section 2 on the bose superfluid ^{4}He, we shall frequently work with the electron liquid structure factor $S(k)$, defined explicitly in terms of $g(r)$ in Equation (3.3) by

$$S_{FH}(k) = 1 + \rho_0 \int [g(r) - 1]\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}. \tag{3.4}$$

Inserting Equation (3.3) into Equation (3.4), the result after some manipulation can be written explicitly as

$$\left.\begin{aligned} S_{FH}(k) &= a_1 k + a_3 k^3 : k \leq 2k_f \\ &= 1 : k \geq 2k_f \end{aligned}\right\}. \tag{3.5}$$

In Equation (3.5), $a_1 = 3/4k_f$ and $a_3 = (-(1/16)k_f^3)$ (see, for example, the book of Jones and March [25]).

If it seems strange that Equation (3.3) leads to a piecewise continuous $S_{FH}(k)$ in Equation (3.5), it is easy to show from Equation (3.3) for $g(r) - 1$ that its FT must have singular points at $k = 0$ and $k = 2k_f$, using Lighthill's arguments [18].

3.2. *OZ direct correlation function c(r)*

In Equation (2.7), we gave the OZ definition of $c(r)$, which we adopt throughout the present study. Then, from the consequence of this $\mathbf{r}$ space definition, it follows that

$$\tilde{c}_{FH} = \frac{S_{FH} - 1}{S_{FH}}. \tag{3.6}$$

Inserting Equation (3.5) into Equation (3.6), and taking the FT of the resulting $\tilde{c}_{FH}(k)$ Nagy et al. [26] derive $c_{FH}(r)$ as having the form

$$c_{FH}(r) = \frac{6}{k_f r}\left[j_1(2k_f r) - \frac{I_{FH}(r,k_f)}{3k_f r} \right]. \tag{3.7}$$

In [26], $I_{FH}(r,k_f)$ is given explicitly in terms of $si(x)$ and $ci(x)$ functions, but it will suffice for present purposes to show a plot of this function in Figure 1. Of course, the form (3.7) is only valid in the high-density limit r_s tends to zero, in which Coulomb

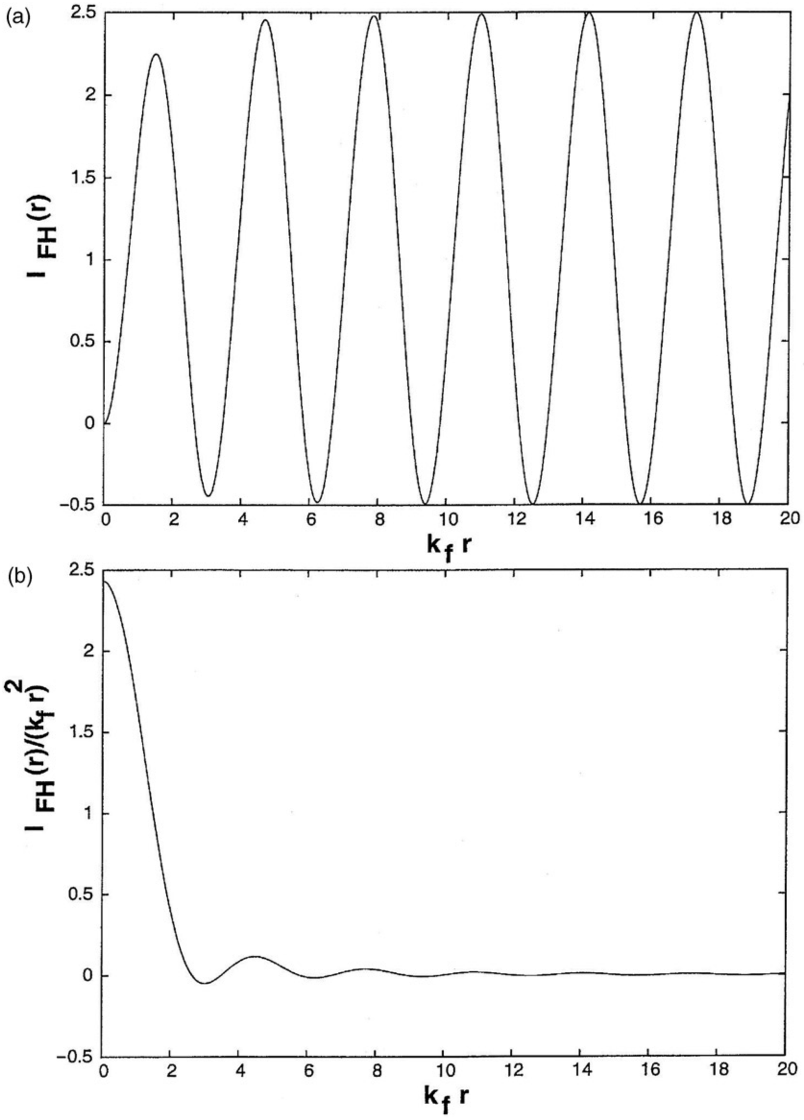

Figure 1. (a) Plot of function $I_{FH}(r,k_f)$ entering Equation (3.7) for the direct OZ correlation function $c_{FH}(r)$ for the Fermi hole of the homogeneous electron gas. (b) Plot of $I_{FH}/(k_f r)^2$ vs. $k_f r$.

correlations are negligible compared with those arising from Fermi statistics (compare Section 1.1 for ideal fermions).

3.3. *Introduction of Coulomb correlations: plasmon zero-point energy and the ground-state structure factor S(k)*

Away from the limiting case r_s tends to zero, represented in the analytical result (3.7), one must have recourse to numerical evaluation of the direct correlation function $c(r, r_s)$. This approach has been adopted in the recent study of Amovilli and March [27]. Their work is based on the modelling of the pair correlation function $g(r, r_s)$ by Gori-Giorgi et al. [28]. These authors have set up a fully quantitative model for the electron structure factors $S(k, r_s)$ and the corresponding pair functions $g(r, r_s)$ for the three-dimensional unpolarised homogeneous electron-liquid. This model appeals not only to known integral and differential properties of the exact pair correlation function, satisfies analyticity requirements both **r** and **k** space, but also accurately interpolates the extensive diffusion Monte Carlo data of Ortiz et al. [29]. Using the model in [28], Amovilli and March [27] have constructed numerically the OZ function $c(r, r_s)$ for jellium for specific values of r_s. Their OZ results are redrawn in Figure 2. We note that these results do not join smoothly onto $c_{FH}(r)$ shown in Figure 1. This is because $S_{FH}(k)$ from Equation (3.5) is proportional to k at small k, whereas the plasmon removes this term completely at $r_s > 0$ and $S(k)$ is proportional to k^2 in the long-wavelength limit, the plasmon zero-point energy $(1/2)\hbar\omega_p$ determining precisely the coefficent of this k^2 term in the long-wavelength limit. Thus again, as with the ground-state of superfluid ^{4}He discussed in Section 2, a collective excitation (phonons for ^{4}He: plasmons for jellium) crucially enters the ground-state structure factor. We pursue this major theme of the present study further when a charged bose fluid is treated in Section 4 below. But before that, let us conclude this discussion of the homogenous electron liquid by referring to a variational ground-state many-fermion wave function used by Gaskell [30]. The focus here will be on the connection of his wave function with the OZ function $c(r, r_s)$; at very least in the long-wavelength limit.

3.4. *Gaskell's variational ground-state wave function and relation to the OZ function c(r, r$_s$)*

To include interactions in a homogeneous fermion liquid let us follow Gaskell [30] by writing the ground-state wave function Ψ as the product of a Slater determinant D of plane waves and a part depending on the density fluctuations $\rho_{\mathbf{k}}$ defined by

$$\rho_{\mathbf{k}} = \sum_{i=1}^{n} \exp(-i\mathbf{k} \cdot \mathbf{r}_i), \tag{3.8}$$

where r_i denote the electronic positions. The explicit form of Ψ is then

$$\Psi = D \exp\left[-\sum_{k} d(k) \rho_{\mathbf{k}} \rho_{\mathbf{k}}^{*} \right] \tag{3.9}$$

and for the homogeneous electron liquid under discussion, Gaskell [30] proposed to determine the quantity $d(k)$ variationally. For high density or equivalently small

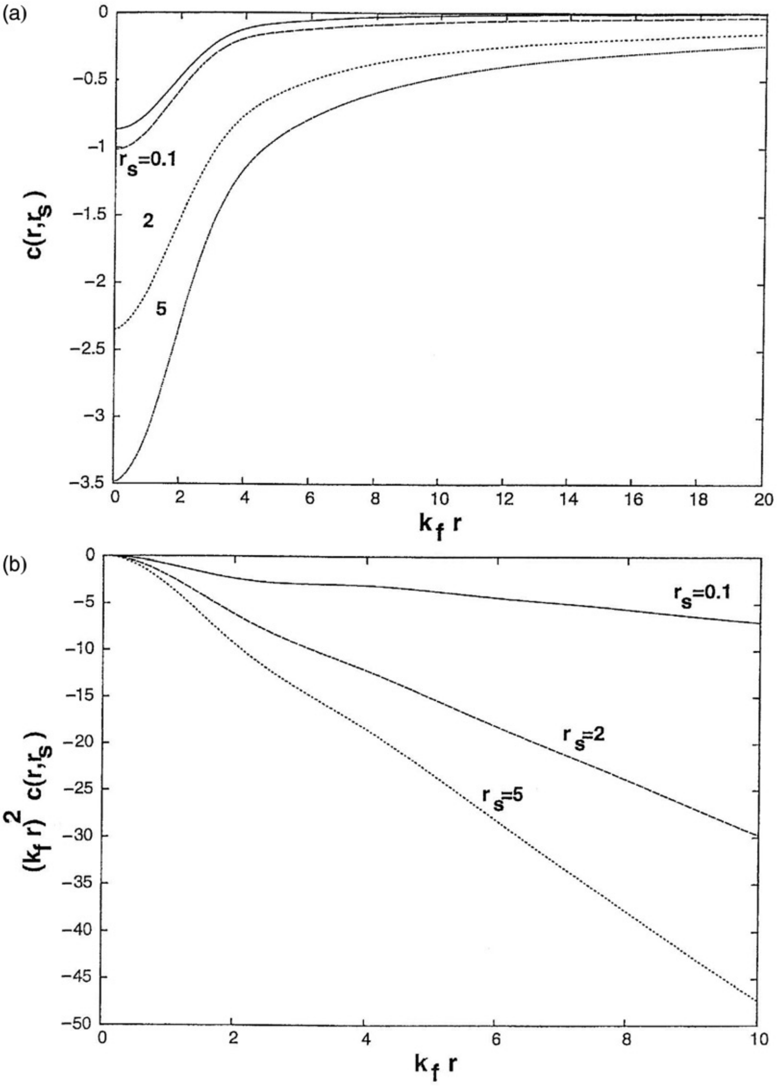

Figure 2. (a) Plot of the OZ direct correlation function $c(r, r_s)$ including Coulombic correlations, where r_s denotes the mean interelectronic spacing in the homogeneous electron liquid having Fermi wave number k_f. The independent variable chosen is $k_f r$. The uppermost curve is the Fermi hole form $c_{FH}(r)$ given in Equation (3.7), with I_{FH} taken from Figure 1. The other three curves correspond to different densities of the homogeneous electron liquid, characterised by $r_s = 0.1$, 2 and 5 atomic units. Note that $2 < r_s < 5$ is the range of the densities of such simple metals as *Aℓ* and *Cs*. (b) Shows how $c(r, r_s)$ times $(k_f r)^2$ *vs.* $k_f r$ rapidly approaches its large r form which is determined by the Coulombic interaction e^2/r. This plot reveals the relative simplicity of the OZ function in this many-fermion case. (Redrawn from Amovilli and March [27].)

interelectronic spacing r_s and for long wavelengths,

$$d(k) \sim \frac{k_f^2 r_s^{1/2}}{k^2} \frac{1}{2} \left[\frac{4}{3\pi} \left(\frac{4}{9\pi} \right)^{1/3} \right]^{1/2}. \tag{3.10}$$

Going back to the Fermi hole discussed in Equations (3.5) and (3.7), let us next write the corresponding pair correlation function $g_{FH}(r)$ given in Equation (3.3) as

$$g_{FH}(x) - 1 = -\frac{3}{2}\int_0^\infty \mathrm{d}t\ t^2 j_0(tx)[1 - S_{FH}(t)] \tag{3.11}$$

where $t = k/k_f$, and $x = k_f r$, and $j_0(x) = \sin x/x$.

Then the pair function $g(r)$, which is the diagonal element of the 2DM, has for high density the following approximate form in terms of the OZ direct correlation function $c_{FH}(r)$, whose FT is written explicitly in Equation (3.7):

$$g(x) = 1 - \frac{3}{2}\int_0^\infty \mathrm{d}t\, t^2 j_0(tx)\left[1 - \frac{1}{1 - c_{FH}(t) + 4d(r_s, t)}\right]. \tag{3.12}$$

We comment a little further in Section 5 below on the interest in studying eventually whether $c_{FH}(t) - 4d(r_s, t)$ entering Equation (3.12) is closely related to the OZ direct correlation function displayed as a function of r_s in Figure 2.

4. Dense charged bose fluid

In this journal some 3.5 decades ago, Fetter [31] studied in detail the low-temperature properties of a dense charged bose fluid. He combined the zero-temperature excitation spectrum $E(k)$ of such a fluid, with particles having mass m and charge e, with the quasiparticle model of Landau, in order to obtain a variety of thermodynamic properties at low temperature. The finite long-wavelength limit, determined by the plasma frequency ω_p discussed in some detail in Section 3 for a charged fermion assembly, leads to a number of important consequences. Two of these are (a) the normal fluid density $\rho_n(T)$ (see also Appendix 4) and (b) the specific heat both vanish as $\exp(-\hbar\omega_p/k_\mathrm{B}T)$ as $T \to 0$. Furthermore, as we emphasised for the charged fermion liquid in the previous section, the zero-temperature structure factor $S(k)$ in the long-wavelength limit now behaves as

$$S(k, T = 0) \propto \frac{k^2}{\hbar\omega_p}, \tag{4.1}$$

leading to a divergence in the OZ direct correlation function in **k** space as

$$\tilde{c}(k) \propto k^{-2} : k \to 0, \tag{4.2}$$

and hence

$$c(r) \propto e^2/r : r \to \infty. \tag{4.3}$$

This demonstrates, just as in a classical liquid [17], that at large distances $c(r)$ reflects the pair interaction, measured in units of a characteristic energy, which in the present case is determined by the zero-point energy of the plasmon modes.

It is of some historical interest to add here a few comments on studies earlier than that of Fetter [31]. Thus, Foldy [32–34] studied a charged bose fluid in a uniform neutralising background, and already showed that in the high-density limit in which the interparticle spacing r_s tends to zero, the depletion of the single-particle mode becomes small and the Coulomb interaction becomes tractable. In fact, before Foldy's work, and as noted by Fetter [31], Ginzburg and Schafroth demonstrated that an ideal charged bose fluid exhibited a Meissner effect below its transition temperature; thereby providing a possible model for a superconductor. Fetter [31] demonstrated that an interacting charged bose fluid also leads to a Meissner effect, but that the general electrodynamics of such a boson assembly was different from that of BCS superconductor.

To conclude this section, the above part of which refers solely to a three-dimensional charged bose gas, it is relevant here to point out (see also [23]) that in two dimensions (2D) the corresponding $S(k)$ at $T=0$ to Equation (4.1) in the long-wavelength limit depends on whether one takes the interaction as $\log r$ (see also Magro and Ceperley [35]) or as e^2/r in 2D. Thus, $S(k) \propto k^{-3/2}$ as k tends to zero for the e^2/r interaction [23], whereas for the $\log r$ case $S(k) \propto k^2/\Omega_p$ where $\Omega_p = \{2\pi\rho e^2/m\}^{1/2}$ is the plasma frequency. The final comment here is that phase fluctuations are enhanced in low-dimensional bose fluids and, in particular, it is straightforward to prove that the ideal bose gas in 2D does not condense at any finite temperature. For 2D, the charged bose fluid with e^2/r interactions, having $S(k) \propto k^{-3/2}$ in the long-wavelength limit as noted above, can be shown to have a condensate at $T=0$, just as in the case of the ideal bose gas.

5. Summary and proposed directions

To begin with the ground-state properties of superfluid ^{4}He, we emphasised at the outset of this article the Bijl–Jastrow wave function (2.6). This was proposed as a variational many-boson wave function characterised by a two-body-like quantity $u(r)$. We stressed in the present context that, at sufficiently large r, this quantity behaves like the OZ direct correlation function $c(r)$. Then, from the fact that in the long-wavelength limit $k \to 0$, the ground-state structure factor $S(k)$ of ^{4}He is proportional to k leads to the Fourier transform $\tilde{c}(k)$ of $c(r)$ diverging as k^{-1}, Enderby et al. [15] derived the result for the long-range function $u(r)$ in Equation (2.7) entering the Bijl–Jastrow form (2.6), namely $u(r) = 2mc/\pi\rho\hbar^2 r^2$ as r tends to infinity, the velocity of sound c entering this long-range behaviour. In turn, this is due to the phonon-like excitations of ^{4}He [15]. We shall return to the above equation when proposing some directions for further work below.

At elevated temperatures, we have put forward an approximate way in which the structure factor $S(k,T)$ may be characterised functionally by the ground-state quantity $S(k,0) \equiv S_0$, plus two dimensionless ratios: mc^2/k_BT, where m is the ^{4}He atomic mass, and also the ratio of the superfluid density $\rho_s(T)$ to the total density $\rho = \rho_s + \rho_n$, where n denotes the normal fluid (see Equation (A4.1); also [14] and [13]).

Turning to the second many-body example treated in detail here, namely the homogeneous electron liquid, the dependence of the zero-temperature structure factor $S(k,0)$ on a collective excitation has been stressed. Via again the OZ direct correlation function, with asymptotic behaviour

$$c(r) \sim \frac{e^2}{r\hbar\omega_p}, \tag{5.1}$$

ω_p being the plasma frequency, we have emphasised that $S(k,0)$ is proportional to k^2 in the long-wavelength limit, to be contrasted with the Hartree–Fock behaviour in Equation (3.5) which is proportional to k as $k \to 0$. We have also written the many-electron wave function proposed variationally by Gaskell [30] in a way which highlights the dependence on the OZ function $\tilde{c}(k)$.

We have then returned finally to a many-boson example, the charged boson gas, and stressed the relevance of Equation (4.3) again, rather than the 'neutral' boson form like Equation (2.10) characteristic of superfluid ^{4}He.

5.1. *Some future directions*

Following the above summary, let us conclude by suggesting a number of future directions which should prove fruitful.

(a) *Overlap of approximate many-body variational wave functions with the true ground state*

In a recent Letter, Mora and Waintal [36] have re-opened the known fact that an intrinsic measure of the quality of a variational wave function is provided by its overlap with the ground state of the many-body assembly under consideration. Denoting the variational wave function by Ψ_v and the true ground state form by Ψ_0, these workers proposed a shift from the procedure of energy minimisation to determine the variables (parameters, or $u(r)$ in the Bijl–Jastrow example) entering Ψ_v. They concentrate on maximising the overlap 0 defined by

$$0 = \frac{|\langle\Psi_v|\Psi_0\rangle|^2}{\langle\Psi_0|\Psi_0\rangle\langle\Psi_v|\Psi_v\rangle}. \tag{5.2}$$

As they emphasise, the idea to maximise the overlap as a variational procedure was already being used by Reatto and co-workers in early studies [37–39]. Already, Reatto had clearly recognised the importance of putting in 'by hand' the long-range behaviour set out in Equation (2.7) in the Bijl–Jastrow wave function (2.6) in order to maximise the overlap 0 in Equation (5.2).

We think in the present context that it would be worthwhile to use the Gaskell wave function written in the form (3.9) to minimise the quantity 0 with respect to $\{c_{FH}(r) - 4d\}$ appearing in $g(r)$ of Equation (3.11), and to compare the result with the OZ direct correlation function shown in Figure 2, for chosen values of the mean interelectronic spacing r_s.

(b) *Test of functional form of elevated temperature structure factor $S(k,T)$ for superfluid ^{4}He*

It would seem of interest to attempt to bring the functional form proposed for the structure factor $S(k,T)$ in superfluid ^{4}He into direct contact with experiment. One point emphasised especially by Mayers [14] is that $S(k,0)$ from present neutron scattering experiments appears to be more 'disordered' than its elevated temperature counterpart $S(k,T)$. Can this be embodied in the functional form (2.4), depending only on $S(k,0)$ and two dimensionless properties mc^2/k_BT and $\rho_s(T)/\rho$?

(c) *Can three-atom-like correlations dramatically affect the behaviour of ^{4}He at extremely low temperatures?*

Finally, we return to the questions concerning Efimov states in superfluid ^{4}He raised in [19–21]. The studies of helium dimers and trimers in free space [22] prompt further conjecture that the chemistry of small helium clusters may have potential importance for constructing, say, a variational many-body wave function for the ground-state of liquid ^{4}He. This could be very instructive in clarifying further issues relating to the possible occurrence of superfluidity in a dense liquid like ^{4}He in the ground state, without a Bose-Einstein condensate.

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Appendix 1. The Sawada Hamiltonian for the high-density limit of the interacting homogeneous electron liquid

As the motivation for the present study, let us consider the Sawada Hamiltonian [40], and in particular the way excited states can be calculated, at least in principle, from knowledge of the ground-state wave function.

The starting-point for simplifying the full Hamiltonian used by Gell-Mann and Brueckner [41] in their calculation of the $\ell n r_s$ term in the correlation energy of high-density jellium was the recognition that many terms in the second quantised Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \in_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{\lambda}{2N} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q},\sigma_1,\sigma_2} u(\mathbf{q}) a^{\dagger}_{\mathbf{k}_1+\mathbf{q}\sigma_1} a^{\dagger}_{\mathbf{k}_2+\mathbf{q}\sigma_2} a_{k_2\sigma_2} a_{\mathbf{k}_1\sigma_1} \tag{A1.1}$$

with $v(\mathbf{q}) = 4\pi/q^2$, contribute only to non-ring diagrams, which can be neglected in the high-density limit.

Elementary excitations

While we have in mind the above Sawada simplification of the Hamiltonian (A1.1), suppose, for a moment more generally, that the ground state of a fermion assembly is given by

$$H\Psi = E\Psi. \tag{A1.2}$$

To construct excited states, let us now consider an operator, Ω_K say, such that

$$\left[H, \Omega_K^{-1}\right]\Psi - \omega_K \Omega_K^{\dagger}\Psi. \tag{A1.3}$$

Using Equations (A1.2) and (A1.3) it then follows readily that

$$H\Omega_K^{\dagger}\Psi = (E + \omega_K)\Omega_K^{\dagger}\Psi. \tag{A1.4}$$

Hence, from this equation, $\Omega_K^{\dagger}\Psi$ is an excited state having excitation ω_K. Furthermore, by taking the conjugate of Equation (A1.3) and using Equation (A1.2), one is led to the result that

$$H\Omega_K\Psi = (E + \omega_K)\Omega_K\Psi. \tag{A1.5}$$

But Equation (A1.2) defines the ground state, and hence from Equation (A1.5) one can write

$$\Omega_K\Psi = 0. \tag{A1.6}$$

The conclusion from the above is that, given a suitable form for the ground state Ψ, one can, in principle, from Equation (A1.4), construct excited state wave functions and their associated excitation energies ω_K.

It is a straightforward matter to show that the above procedure works for independent fermions, where the answer is, of course, well known.

The method can be applied to the Sawada Hamiltonian described above. One again finds by the above procedure an eigenvalue equation for the excitation energies. Thereby, the so-called

Bohn–Pines dispersion relation discussed, for example, by Nozieres and Pines [42] and by Pines [43] emerges.

Appendix 2. Laughlin state as an eigenstate of a model Hamiltonian with particles interacting via a repulsive harmonic force

To press the point made in the previous appendix, we summarise here a different model in which the excited state wave functions can again be generated from a known ground state. The summary below has been motivated by the work of Johnson [44]. There the behaviour of an interacting two-dimensional charged particle assembly in a transverse magnetic field is discussed.

The form of the ground-state wave function for two-dimensional electrons in high-magnetic fields proposed by Laughlin [45] in relation to the fractional quantum Hall effect is the basis of what follows. Laughlin's wave function takes the form

$$\Psi = \prod_{i<j}(z_i - z_j)^n \exp\left\{-\frac{1}{4\ell^2}\sum_i |z_i|^2\right\}, \tag{A2.1}$$

where $z_i = x_i + iy_i$ denotes the complex coordinate of the ith particle, ℓ^2 being defined by

$$\ell^2 = \hbar/m\omega_c : \omega_c = eB/m, \tag{A2.2}$$

with ℓ denoting the magnetic length and ω_c the cyclotron frequency. B is the strength of the magnetic field and m is the electron mass. In Equation (A2.1) n is an odd integer, ensuring that the wave function is antisymmetric under particle exchange.

Although the analytic structure of Ψ in Equation (A2.1) may be anticipated by constructing an antisymmetric determinant built out of single-particle states, it is important to understand the form of Ψ in a way that (a) gives insight into the reason why the electron-electron interactions play a central role and (b) shows why the precise form of interaction is not of major importance in determining the nature of the ground state.

Johnson [44] constructs a model which is solvable, based on repulsive harmonic particle interactions, and in which excited state wave functions can be generated from the ground state. The model is carefully devised so that the Laughlin wave function is an eigenstate of this model. The most general eigenstate of this model Hamiltonian can be constructed essentially from the ground state.

Appendix 3. Ideal fermion fluid: relation between high-temperature pair correlation function and its ground-state counterpart

In Section 1, we have written the pair correlation function $g(r)$ in Equation (1.1) at high-temperature T for ideal bose and fermi fluids. Here, our objective is to relate this elevated temperature result for $g(r,T)$ to its zero-temperature counterpart, $g(r,0)$, for the particular case of an ideal fermion assembly.

Using the total correlation function $h(r)$ defined below Equation (2.8), we can then write, for high temperatures

$$\begin{aligned} h(r,T) &= g(r,T) - 1 \\ &= -\exp\left(-\frac{r^2}{\lambda^2}\right) \end{aligned} \tag{A3.1}$$

and hence

$$\ln\{-h(r,T)\} = -\frac{r^2}{\lambda^2}. \tag{A3.2}$$

Turning to the zero-temperature counterpart of Equation (A3.1), we have from the Wigner–Seitz result (3.3) that

$$h(r, o) = -\frac{9}{2}\left\{\frac{j_1(k_f r)}{k_f r}\right\}^2, \tag{A3.3}$$

where $j_1(x)$ is the first-order spherical Bessel function defined below Equation (3.3) of the main text. Evidently therefore, from insertion of Equation (A3.2) into Equation (A3.3), we can write, since $r^2/\lambda^2 \equiv (k_f r)^2/(k_f\lambda)^2$, the functional relationship for fermions

$$h(r, T=0) = F\left[(k_f\lambda)^2 \ln\{-h(r, T)\}\right], \tag{A3.4}$$

which, we reiterate, is valid when the temperature T on the RHS is sufficiently high to validate Equation (A3.1). This Equation (A3.4) tells us that all the r dependence in $h(r, T)$ is already embedded in the $T=0$ counterpart $h(r, 0)$, the dimensionless product of the thermal de Broglie wavelength and the Fermi wave number k_f crucially entering the relation between the ground-state structure and the high-temperature limit of $h(r, T) = g(r, T) - 1$.

Appendix 4. Elevated temperature liquid structure factor $S(k, T)$ in superfluid ^{4}He and two-fluid behaviour

The purpose of this Appendix is to relate the treatment of the functional form of the elevated temperature structure factor $S(k, T)$ [see [46]] given in Equation (2.4) of the main text to the study of Mayers [14].

Mayers writes (compare his Equation (30))

$$S(k, T) = \frac{\rho_s(T)}{\rho} S_0(k) + \frac{\rho_n(T)}{\rho} S_R(k), \tag{A4.1}$$

where $\rho_s(T)$ is the superfluid density, $\rho_n(T)$ that of the normal fluid and $\rho = \rho_s + \rho_n$. Since $S_R(k)$ in Equation (A4.1) is not known from theory at the time of writing, Mayers sets it equal to the structure factor $S(k, T_\lambda)$ at the superfluid transition. The importance of Equation (A4.1) in the present context is that it strongly suggests that in relating $S(k, T)$ for $T \le T_\lambda$ to the zero-temperature limit $S_0(k)$, the ratio $\rho_s(T)/\rho$ is a further important variable. This then is the reason for introducing $\rho_s(T)/\rho$ into the functional form of $S(k, T)$ proposed in Equation (2.4).