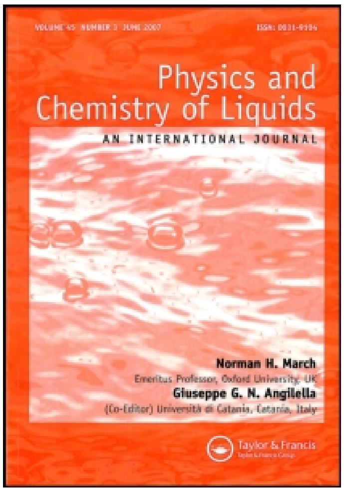

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Superfluidity, Ground-State Wave Function and Bose Condensation in Liquid Helium Four†

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The Bijl-Jastrow product of pairs wave function for the ground-state of He^4 leads inevitably to off-diagonal long-range order. Furthermore, if the pair wave function is constructed to yield the Feynman structure factor $S(k) = \hbar k/2Mc$, then the occupation number n_k of momentum state k diverges as k^{-1} as $k \to 0$. Re-examination by Jackson of the Mook, Scherm and Wilkinson neutron scattering experiment, and more recent neutron inelastic scattering experiments by Cowley and co-workers on liquid He^4 have raised serious doubts as to the existence of a condensate. Superfluidity without a condensate is therefore briefly discussed and appears possible in principle. It is argued here that, *if* there is no condensate in He^4, then the He–He interactions *must* lead to a ground-state wave function which *cannot* be built from a product of pairs, but must include fundamentally three-atom correlations (at least). A study of the pressure dependence of S(k) in He^4 may be helpful in this connection.

1 INTRODUCTION

Recent experiments on liquid He^4 have raised serious doubts as to the existence of a condensate.[1–3] Certainly, it is by now established that the fraction of atoms in any condensate is very much smaller than the original Penrose–Onsager[4] estimates would suggest.

In this paper, we consider some consequences of superfluidity without a

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condensate. This seems possible, at least in principle, as Leggett[5] has argued. Leggett views the basic superfluid property as related to the Hess–Fairbank[6] experiment. In view of this experiment, Leggett takes the basic superfluidity criterion that for a rotating system the equilibrium state is that of zero total angular momentum. On the other hand, the question of the condensate is related to off-diagonal long-range order in the first-order density matrix $\gamma(\mathbf{r}\,\mathbf{r}')$ defined from the ground-state wave function $\Psi(\mathbf{r}_1 \ldots \mathbf{r}_N)$ for N atoms in volume V as

$$\gamma(\mathbf{r}\,\mathbf{r}') = \int \Psi^*(\mathbf{r}\,\mathbf{r}_2 \ldots \mathbf{r}_N)\, \Psi(\mathbf{r}'\,\mathbf{r}_2 \ldots \mathbf{r}_N)\, d\mathbf{r}_2 \ldots d\mathbf{r}_N. \tag{1}$$

We first review what have appeared hitherto to be well established results in the theory of liquid He^4, dividing these however into two groups: (A) not depending on the assumption of a condensate and (B) involving the assumption of a finite fraction ρ_0/ρ atoms in a condensate, ρ being the total number density N/V.

2 (A) FEYNMAN'S STRUCTURE FACTOR S(k) AND ITS CONSEQUENCES

A basic result for the long wavelength limit of the structure factor at $T = 0$, due to Feynman,[7] is that

$$S(k) = \frac{\hbar k}{2Mc} \tag{2}$$

where M is the mass of a He^4 atom while c is the velocity of sound in liquid He^4 at $T = 0$. The result evidently does not involve any condensate property and depends only on the assumption that the dynamical structure factor $S(k\,\omega)$, related to S(k) by

$$S(k) = \int_0^\infty S(k\,\omega)\, d\omega \tag{3}$$

has the form

$$S(k\,\omega) = S(k)\,\delta(\omega - ck) \tag{4}$$

for ground-state and long wavelength properties. The first moment result

$$\int_0^\infty \omega S(k\,\omega) d\omega = \frac{\hbar k^2}{2M} \tag{5}$$

then yields (2) immediately when the form (4) is adopted.

We summarize also two further consequences of (2). The first is that the radial distribution function $g(\mathbf{r}\,\mathbf{r}') \equiv g(|\mathbf{r}-\mathbf{r}'|)$ has the asymptotic form[8]

$$g(r) \sim 1 - \left(\frac{\hbar}{2\pi^2 \rho Mc}\right) r^{-4}. \tag{6}$$

Secondly the Ornstein–Zernike direct correlation function $c(k) = [S(k)-1]/S(k)$ is, from (2), proportional to k^{-1} as $k \to 0$ and hence its Fourier transform $c(r)$ behaves as r^{-2} at large r. We emphasize here that, in a classical liquid, at temperature T, the direct correlation function $c(r) \sim -\phi(r)/k_B T$ at large r, $\phi(r)$ being the pair interaction between atoms. All this shows us that the interacting Bose fluid has "effective interactions" which are of long-range r^{-2} and that the range of the total correlation function $g(r) - 1$ is proportional to r^{-4}. Any acceptable ground-state wave function Ψ must lead to these properties for the pair correlations.

But it is also important to emphasize here that the Landau theory of He^4 does not involve the condensate density ρ_0. Indeed, as pointed out by London,[9] Landau preferred to avoid any appeal to a non-interacting Bose gas but rather to build a two-fluid model for which a condensate plays no role. Thus, the consequences of Landau theory are of kind (A), and not (B) discussed below.

3 (B) OFF-DIAGONAL LONG-RANGE ORDER AND MOMENTUM DISTRIBUTION OF He^4 ATOMS

In this category (B), as we remarked above, our concern is with the off-diagonal properties of the first-order density matrix $\gamma(\mathbf{r}\,\mathbf{r}') \equiv \gamma(|\mathbf{r}-\mathbf{r}'|)$. If a condensate *is assumed*, then the occupation number n_k of the momentum state k as $k \to 0$ is given by[10]

$$n_k = \frac{\rho_0}{\rho}\frac{Mc}{2k} \tag{7}$$

(ρ_0/ρ) being the fraction of atoms in the (assumed) condensate.

From equation (7), since

$$n_k = \int [\gamma(s) - \rho_0] \exp(i\mathbf{k}\cdot\mathbf{s})\,ds \tag{8}$$

it follows that

$$\gamma(|\mathbf{r}-\mathbf{r}'|) - \rho_0 \sim \frac{\text{constant}}{|\mathbf{r}-\mathbf{r}'|^2} \tag{9}$$

at large distances $|\mathbf{r}-\mathbf{r}'|$ from the diagonal. The statement (9) with $\rho_0 \neq 0$ embodies the off-diagonal long-range order. It should be noted in (9) that the constant, from (7) and (8), is itself proportional to (ρ_0/ρ).

It is quite clear that these results (7) and (9), which have hitherto been regarded as having a status comparable with those of category A, in fact hinge on assuming that superfluidity implies a condensate. But as Leggett[5] emphasized, Bose condensation is a sufficient condition for superfluidity, *not* a necessary one. Thus, category A results have a much more basic status than those of category B.

4 RELATION BETWEEN (A) AND (B) PROPERTIES VIA BIJL–JASTROW WAVE FUNCTION

We next emphasize that while the results (7) and (9) refer to the off-diagonal properties of the first-order density matrix $\gamma(|\mathbf{r}-\mathbf{r}'|)$, (A) concerns the diagonal element g of the two-particle (second-order) density matrix Γ. These quantities, g and γ, physically equivalent to the structure factor S(k) and the momentum distribution n_k are related by

$$\gamma(\mathbf{r}\,\mathbf{r}')\ \alpha \int \Gamma(\mathbf{r}\,\mathbf{r}_1\,\mathbf{r}'\,\mathbf{r}_1)\,d\mathbf{r}_1, \tag{10}$$

or, put another way, via the form of the many-body wave function Ψ.

Only for one non-trivial interacting particle wave function, the Bijl–Jastrow form

$$\Psi = \prod_{i<j} f(r_{ij}) \equiv \prod_{i<j} e^{\frac{1}{2}u(r_{ij})} \tag{11}$$

are the relations between S(k) and n_k well established, and we summarize now how the argument goes.

As pointed out by Enderby *et al*,[8] the result (2) of Feynman implies

$$u(r) \sim \left(\frac{-Mc}{\pi^2\rho\hbar}\right) r^{-2} \tag{12}$$

and this long-range form has been built into the pair wave function by Reatto and Chester.[11] But whether or not the result (12) is incorporated, there is no doubt from the work of McMillan[12] that the Bijl–Jastrow wave function implies a condensate: i.e. $\rho_0/\rho \neq 0$. When (12) is built in, then the Feynman result (2) is, of course, a consequence, but also, as Reatto and Chester show, the Gavoret-Nozières result (7) follows, whereas McMillan,[12] without the long-range pair function (12), got n_k finite as $k \to 0$.

5 CONSEQUENCES OF SUPERFLUIDITY WITHOUT A CONDENSATE

Before discussing some of the consequences of superfluidity *without* a condensate, we note additionally that Bogoliubov and Zubarev[13] have shown that the Bijl–Jastrow wave function is the correct form to describe a weakly interacting Bose system, for which case the properties (B) follow, as they demonstrate directly. Secondly, with the *assumption* of a condensate, Gavoret and Nozières show that the (B) results follow to all orders in perturbation theory.

Thus, if superfluidity in He^4 at $T = 0$ does *not* imply a condensate, as experiment now suggests is a possibility, then it seems inescapable that:

a) The momentum distribution n_k cannot be developed by any perturbative theory (even when taken to all orders) from the non-interacting Bose gas. Some "phase transition" must occur as a function of the strength of the atom-atom interactions if there is to be no condensate in the ground-state of liquid He^4.

b) Related to (a), once the coupling strength is sufficient to bring about a transition to a ground-state without a condensate, the Bijl–Jastrow wave function cannot describe such a ground-state. Three-particle correlations (at least) must be directly built into the ground-state wave function. Otherwise, as we have seen, off-diagonal long-range order must follow.

6 SUMMARY

It has been stressed that:

a) Recent neutron inelastic scattering experiments have raised doubts about the conventional assumption that Bose condensation is responsible for the superfluidity (with integral circulation quantization) of liquid He^4.

b) The Feynman structure factor result (2), with its consequences for g(r) and c(r), are basic (A) properties of He^4 at $T = 0$ whereas properties (B) relating to the momentum distribution n_k are based on the assumption of a condensate.

c) If it turns out that in He^4 there is *no* condensate, then the Bijl–Jastrow wave function is inappropriate to describe the ground-state and direct inclusion of three-particle correlations (at least) in Ψ is essential.

It would obviously be of considerable interest in furthering our understanding of liquid He^4 if an experiment could be carried out to measure the three-atom correlations. Such experiments have been proposed, but never to our knowledge directly implemented. However it is of interest to note that, in classical liquids, some handle on three-particle correlations is provided by studying the pressure dependence of the structure factor S(k).[14] But, at best, this will be useful to test models.

Our final comment concerns the question as to whether pair force interactions will be adequate to describe the ground-state of liquid He^4, should it turn out to have *no* condensate. It seems to us possible (though not probable) that inclusion of three-particle correlations in the ground-state wave function may, at the same time, point to the need for introducing three-body forces. Such many-body forces are known to play a significant role in determining the crystal structures of the inert gases: a matter presumably related to higher-order atom correlations.

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