

Bose-Einstein Condensation, Phase Coherence, and Two-Fluid Behavior in ^4He

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It is shown that the assumption that the many particle wave functions describing superfluid ^4He have some phase coherence properties of correlated basis functions provides a new explanation of the link between Bose-Einstein condensation and two fluid behavior. This assumption also implies that the condensate fraction is proportional to the superfluid fraction, in agreement with experiment, and provides a simple quantitative explanation of the anomalous reduction in spatial order and liquid density, observed as the temperature is lowered in superfluid ^4He .

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Convincing evidence that two fluid behavior in ^4He [1] is linked to Bose-Einstein condensation (BEC) is provided by neutron scattering measurements [2–7] and path integral Monte Carlo calculations [8,9], which both show that a finite Bose condensate fraction appears at the same temperature as a finite superfluid fraction. However, the only existing microscopic derivation of this link is based on the properties of the weakly interacting Bose gas [10–12], whereas liquid helium is a strongly interacting system. Another approach to the theory of liquid helium is to expand the many particle wave function in terms of correlated basis functions (CBF's). CBF's incorporate the spatial correlations of the ground state and, hence, do include strong interactions. This method has been used by numerous workers [13–19] to accurately calculate both the ground state and the excited state properties of superfluid ^4He . It is shown that the phase coherence properties of CBF's provide a new explanation of two fluid behavior and also of the reduction in spatial order [20–22] and liquid density [23], observed in superfluid ^4He as the temperature is reduced. This uniquely anomalous behavior has been much discussed previously [24–29], but there is at present no agreement as to why it occurs or how it is linked to BEC.

We consider an N particle system at volume V and temperature T , in the limit $N \rightarrow \infty$, at constant N/V . Denoting an arbitrarily chosen particle coordinate as \vec{r} and the coordinates of all other particles as \vec{s} , the N particle wave functions are

$$\Psi_i(\vec{r}, \vec{s}) = |\Psi_i(\vec{r}, \vec{s})| \exp[i\Phi_i(\vec{r}, \vec{s})]. \quad (1)$$

In ^4He the condensate fraction f is generally taken as the probability that an arbitrarily chosen particle occupies a single particle momentum state $\exp(i\vec{k}_j \cdot \vec{r})/\sqrt{V}$, which for simplicity is taken as $\vec{k}_0 = 0$. It then follows from the standard definition of the single particle density matrix [30,31] in terms of the states $\Psi_i(\vec{r}, \vec{s})$ that f can be expressed as [32,33]

$$f(T) = \frac{1}{V} \sum_i \eta_i(T) \int d\vec{s} \left| \int \Psi_i(\vec{r}, \vec{s}) d\vec{r} \right|^2, \quad (2)$$

where $\eta_i(T)$ is the probability that state i is occupied at temperature T . The condensation temperature T_B is defined by the condition $f = 0$ for $T \geq T_B$.

It has been shown previously [34] that if $f \neq 0$, i.e., for $0 \leq T < T_B$, Eq. (2) implies that occupied states $\Psi_i(\vec{r}, \vec{s})$ in ^4He , considered as functions of \vec{r} , must have the following properties. (a) $\Psi_i(\vec{r}, \vec{s})$ must be nonzero within a volume $\propto V$. (b) The phases $\Phi_i(\vec{r}, \vec{s})$ and $\Phi_i(\vec{r}', \vec{s})$ are correlated as $|\vec{r} - \vec{r}'| \rightarrow V^{1/3}$. Furthermore, in the presence of BEC, the ground state $\Psi_0(\vec{r}, \vec{s})$ must be “phase coherent”; i.e., the phase $\Phi_0(\vec{r}', \vec{s})$ is precisely determined by the phase $\Phi_0(\vec{r}, \vec{s})$ for all \vec{r}, \vec{r}' . This is true because the phase of the ground state wave function $\Psi_0(\vec{r}, \vec{s})$ of any Bose system is independent of \vec{r}, \vec{s} [35]. Note that in this sense a Bose condensed system *must* occupy a coherent state at $T = 0$, even though N is fixed [36]. In contrast, for $T \geq T_B$, Eq. (2) implies that occupied states $\Psi_i(\vec{r}, \vec{s})$ must be “phase incoherent”; i.e., the phases $\Phi_i(\vec{r}, \vec{s})$ and $\Phi_i(\vec{r}', \vec{s})$ are randomly oriented when $|\vec{r} - \vec{r}'| > r_C$, where r_C is a finite “coherence length.”

We consider the way in which this change from phase coherence at $T = 0$ to phase incoherence for $T \geq T_B$ occurs in CBF's. The CBF wave function is essentially a product of the exact many particle ground state wave function $\Psi_0(\vec{r}, \vec{s})$, with the ideal Bose gas wave function $\Theta_i(\vec{r}, \vec{s})$.

$$\Psi_i(\vec{r}, \vec{s}) = C_i \Theta_i(\vec{r}, \vec{s}) \Psi_0(\vec{r}, \vec{s}), \quad (3)$$

where C_i is a normalization constant [37],

$$\Theta_i(\vec{r}_1, \vec{s}) = \frac{1}{\sqrt{N_P V^N}} \sum_P \exp(ik_0 \cdot \vec{r}_1) \times \exp(ik_1 \cdot \vec{r}_2) \dots \exp(ik_J \cdot \vec{r}_N), \quad (4)$$

$\vec{r}_2 \dots \vec{r}_N$ is denoted as \vec{s} , and the sum is over the N_P permutations of the N particle coordinates in the occupied states \vec{k}_j . $\Theta_i(\vec{r}_1, \vec{s})$ can be rearranged into the form

$$\Theta_i(\vec{r}_1, \vec{s}) = \sum_j \alpha_{ij}(\vec{s}) \exp(i\vec{k}_j \cdot \vec{r}_1), \quad (5)$$

where $\alpha_{ij}(\vec{s}) \exp(i\vec{k}_j \cdot \vec{r}_1)$ is the sum of the terms in (4)

containing the factor $\exp(i\vec{k}_j \cdot \vec{r}_1)$. It follows from (3) and (5) that

$$\Psi_i(\vec{r}, \vec{s}) = \Psi_{iC}(\vec{r}, \vec{s}) + \Psi_{iR}(\vec{r}, \vec{s}), \quad (6)$$

where

$$\Psi_{iC}(\vec{r}, \vec{s}) = C_i \alpha_{i0}(\vec{s}) \Psi_0(\vec{r}, \vec{s}) \quad (7)$$

and

$$\Psi_{iR}(\vec{r}, \vec{s}) = C_i \sum_{j \neq 0} \alpha_{ij}(\vec{s}) \exp(i\vec{k}_j \cdot \vec{r}_1) \Psi_0(\vec{r}, \vec{s}). \quad (8)$$

The phase of $\Psi_{iR}(\vec{r}, \vec{s})$ varies randomly with \vec{r} , over distances $r_C \sim 1/\Delta k \sim (V/N)^{1/3}$, where Δk is the range of values of \vec{k}_j included in (8). Hence $\Psi_{iR}(\vec{r}, \vec{s})$ is phase incoherent and does not contribute to f [34,38]. It, therefore, follows from (2), (6), and (7) that

$$f(T) = \sum_i \eta_i(T) \int |C_i \alpha_{i0}(\vec{s})|^2 f_0(s) d\vec{s}, \quad (9)$$

where

$$f_0(\vec{s}) = \frac{1}{V} \left| \int \Psi_0(\vec{r}, \vec{s}) d\vec{r} \right|^2. \quad (10)$$

Equation (9) gives the mean value of the condensate fraction. Fluctuations from the mean are due to the range of values of $|C_i \alpha_{i0}(\vec{s})|^2$ and $f_0(s)$ corresponding to probable i and \vec{s} . It is assumed that fluctuations in $f(T)$ are negligible, as is generally the case as $N \rightarrow \infty$. This implies that $|C_i \alpha_{i0}(\vec{s})|^2$ and $f_0(s)$ must be the same for all probable i and \vec{s} at a given T and that $|C_i \alpha_{i0}(\vec{s})|^2$ is effectively a function only of T .

$$|C_i \alpha_{i0}(\vec{s})|^2 = w_C(T). \quad (11)$$

It follows from Eqs. (9) and (11) that

$$f(T) = w_C(T) f(0). \quad (12)$$

Thus, at $T = 0$, $w_C(T) = 1$, and $\Psi_i(\vec{r}, \vec{s}) = \Psi_0(\vec{r}, \vec{s})$ is phase coherent, whereas for $T \geq T_B$, $w_C(T) = 0$, and $\Psi_i(\vec{r}, \vec{s}) = \Psi_{iR}(\vec{r}, \vec{s})$ is phase incoherent, as required.

It follows from Eq. (6) that

$$\int |\Psi_i(\vec{r}, \vec{s})|^2 d\vec{r} = w_{iC}(s) + w_{iR}(s) + X_i(\vec{s}), \quad (13)$$

where

$$w_{iC}(s) = \int |\Psi_{iC}(\vec{r}, \vec{s})|^2 d\vec{r} \quad (14)$$

with an analogous expression for $w_{iR}(s)$ and

$$X_i(\vec{s}) = \int \Psi_{iC}(\vec{r}, \vec{s}) \Psi_{iR}(\vec{r}, \vec{s}) d\vec{r} + \text{CC}, \quad (15)$$

and CC denotes complex conjugate. Dividing the total volume V into M volumes V_m , each of size r_C^3 , where r_C is the coherence length of $\Psi_{iR}(\vec{r}, \vec{s})$, Eq. (15) can be formally expressed as

$$X_i(\vec{s}) = \sum_{m=1}^M |A_m(\vec{s})| \exp[i\varphi_m(\vec{s})] + \text{CC}, \quad (16)$$

where by definition of the V_m , the phase $\varphi_m(\vec{s})$ varies randomly with m and

$$|A_m(\vec{s})| = \left| \int_{V_m} \Psi_{iC}(\vec{r}, \vec{s}) \Psi_{iR}(\vec{r}, \vec{s}) d\vec{r} \right| \quad (17)$$

is the amplitude of the contribution from region m . It follows from condition (a) above that $\Psi_0(\vec{r}, \vec{s})$ and, hence from Eqs. (7) and (8), $\Psi_{iC}(\vec{r}, \vec{s})$ and $\Psi_{iR}(\vec{r}, \vec{s})$ must be nonzero within a macroscopic volume $\propto V$. Thus, it follows from (14) that on average

$$|A_m(\vec{s})| \propto \sqrt{w_{iC}(\vec{s}) w_{iR}(\vec{s})} \frac{r_C^3}{V} = \frac{\sqrt{w_{iC}(\vec{s}) w_{iR}(\vec{s})}}{M}. \quad (18)$$

Since, according to (16), $X_i(\vec{s})$ is the sum of M randomly phased contributions, it follows from (18) that

$$X_i(\vec{s}) \sim \sqrt{M} |A_m(\vec{s})| \sim \frac{\sqrt{w_{iC}(\vec{s}) w_{iR}(\vec{s})}}{\sqrt{M}} \propto \frac{1}{\sqrt{N}}. \quad (19)$$

Providing that $w_{iC}(\vec{s}) \sim w_{iR}(\vec{s})$, $X_i(\vec{s})$ is negligible compared to both $w_{iC}(\vec{s})$ and $w_{iR}(\vec{s})$ in the limit $N \rightarrow \infty$. Note that this is not true in the limit $T \rightarrow 0$, when $w_{iR}(\vec{s}) \rightarrow 0$ or in the limit $T \rightarrow T_B$, when $w_{iC}(\vec{s}) \rightarrow 0$.

However, not too close to $T = 0$ or $T = T_B$, it follows from (13) and (19) that as $N \rightarrow \infty$

$$\sum_i \eta_i(T) \int |\Psi_i(\vec{r}, \vec{s})|^2 d\vec{r} d\vec{s} = w_C(T) + w_R(T) = 1, \quad (20)$$

where

$$w_C(T) = \sum_i \eta_i(T) \int |\Psi_{iC}(\vec{r}, \vec{s})|^2 d\vec{r} d\vec{s} \quad (21)$$

with an analogous expression for $w_R(T)$. It follows from (20) that $w_C(T)$ can be interpreted as the weight of the coherent component and $w_R(T)$ as the weight of the incoherent component.

It follows from similar arguments that other integrals of $\Psi_i(\vec{r}, \vec{s})$ over \vec{r}, \vec{s} split into two independent components of weights $w_C(T)$ and $w_R(T)$. In particular, the fluid flow [38]

$$\begin{aligned} F &= \frac{\hbar N}{M} \sum_i \eta_i(T) \int |\Psi_i(\vec{r}, \vec{s})|^2 \frac{\partial}{\partial \vec{r}} \Phi_i(\vec{r}, \vec{s}) d\vec{r} d\vec{s} \\ &= w_C(T) F_C + w_R(T) F_R, \end{aligned} \quad (22)$$

where Eqs. (7) and (11) imply that $F_C = F_0$ is the ground state flow, while F_R is the flow associated with elementary excitations. Similarly, the total fluid energy is

$$E = w_C E_0 + w_R E_R, \quad (23)$$

the entropy is

$$S = \left(\frac{\partial E}{\partial T} \right)_V = w_C S_0 + w_R S_R, \quad (24)$$

and the pressure is

$$P = \left(\frac{\partial E}{\partial V} \right)_T = w_C P_0 + w_R P_R, \quad (25)$$

where E_0 , S_0 , and P_0 are the ground state values. The entropy of the coherent component $S_0 = (\partial E_0 / \partial T)_V = 0$ while $S_R \neq 0$. Clearly the two components have identical properties to the superfluid and the normal fluid of ^4He . Hence, $w_C(T)$ can be identified with the superfluid fraction $\rho_S(T)$ and $w_R(T)$ with the normal fluid fraction $\rho_N(T)$.

$$\rho_S(T) = w_C(T), \quad \rho_N(T) = w_R(T). \quad (26)$$

This identification has a number of implications, which can be tested by experiment.

It follows from Eqs. (12) and (26) that $\rho_S(T)$ is proportional to f .

$$f(T)/f(0) = \rho_S(T). \quad (27)$$

Figure 1 compares neutron scattering measurements of $f(T)/f(0)$ in superfluid ^4He with tabulated values [39] of $\rho_S(T)$. It can be seen that within experimental error, Eq. (27) is satisfied in superfluid ^4He . It should be stressed that (27) is not valid as $T \rightarrow 0$ [40,41] or as $T \rightarrow T_B$ [42], as mentioned following Eq. (19).

At a given T and V , Eqs. (25) and (26) also imply that

$$P(T, V) = \rho_S(T, V)P_0(V) + \rho_N(T, V)P_R(T, V), \quad (28)$$

where $P_0(V)$ is the ground state pressure. For comparison of (28) with experiment, the approximation was made that $P_R(T, V) = P(T_B, V)$. Numerical values of $\rho_S(T, V)$, $P_0(V)$, and $P(T_B, V)$ were taken from the tabulated values

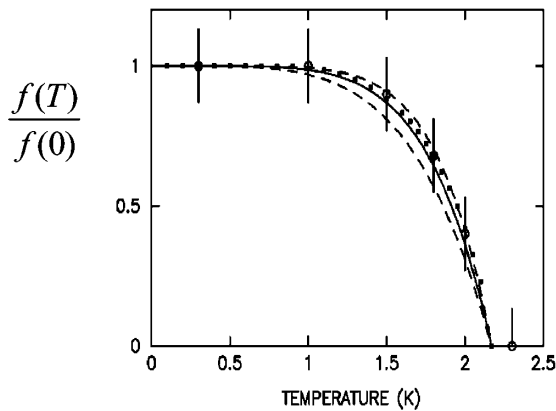


FIG. 1. The points \blacksquare give the superfluid fraction [39]. Glyde *et al.* [7] give $f(T)/f(0) = 1 - (T/T_\lambda)^\gamma$, with $\gamma = 5.5 \pm 1.0$, and the solid line was calculated from this expression while the dashed lines define the corresponding error. The points \circ and corresponding errors are taken from measurements of f by Sosnick *et al.* [5].

of Maynard [43] and used to calculate $P(T, V)$ from (28). The ratio $R(T, P) = V(0, P)/V(T, P)$, of the liquid density at T to that at $T = 0$ was calculated by linear interpolation of the calculated $P(T, V)$ table and is shown as the solid lines in Fig. 2. The directly measured [43] values of $R(T, P)$, shown as the points, are in good agreement with the calculation. Thus, the anomalous density variation of the superfluid with temperature can be attributed to the different partial pressures exerted by the superfluid and normal fluid components in (28).

The static structure factor $S(\vec{q})$ can be expressed as [44]

$$S(\vec{q}) = 1 + (N - 1) \sum_i \eta_i(T) \int |\Psi_i(\vec{r}_1, \vec{s})|^2 \times \exp[i\vec{q} \cdot (\vec{r}_1 - \vec{r}_2)] d\vec{r}_1 d\vec{s}. \quad (29)$$

The cross terms between $\Psi_{iC}(\vec{r}_1, \vec{s})$ and $\Psi_{iR}(\vec{r}_1, \vec{s})$ in the integral over \vec{r}_1 in (29) are negligible. Thus (6), (7), (11), (26), and (29) imply that

$$S(\vec{q}) = \rho_S(T)S_0(\vec{q}) + \rho_N(T)S_R(\vec{q}), \quad (30)$$

where $S_0(\vec{q})$ is the static structure factor at $T = 0$. For comparison with experiment the approximation was made that $S_R(\vec{q}) = S_B(\vec{q})$, where $S_B(\vec{q})$ is $S(\vec{q})$ at the superfluid transition. $S_0(\vec{q})$ was taken as the 1 K result obtained by Sears and Svensson [20]. The solid line in Fig. 3 shows $[S(\vec{q}) - 1]/[S_B(\vec{q}) - 1]$ calculated from (30), with these assumptions. The points with errors were also taken from Ref. [20]. It can be seen that the measurements of $S(q)$ are consistent with (30) and that the reduction in spatial order as the temperature is lowered can therefore be attributed to the increasing weight of the superfluid, which is more disordered than the normal fluid, for reasons discussed previously [38]. To summarize, the assumption that in the presence of BEC the wave function in ^4He , like CBF's, can be divided into coherent and incoherent components, provides a new explanation of

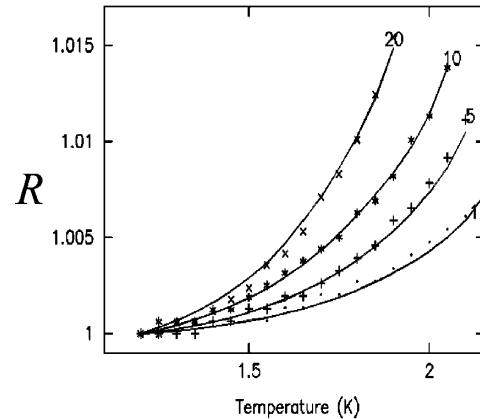


FIG. 2. Shows the ratio R of the density at temperature T to that at $T = 0$, at pressures \bullet , 1 bar; $+$, 5 bar; $*$, 10 bar; and \times , 20 bar. The solid lines were calculated from (28). The points were calculated from tabulated values of $V(T, P)$ [43].

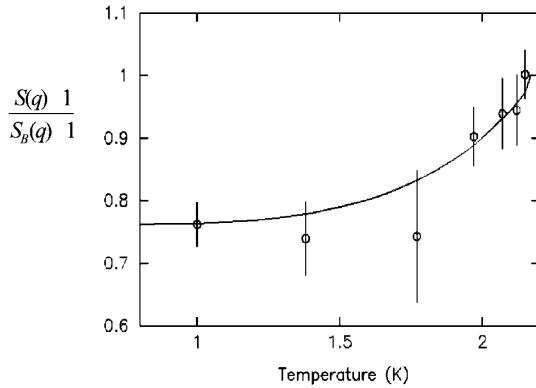


FIG. 3. The solid line is calculated from Eq. (30). The points were obtained from the experimental work of Sears and Svensson [20].

two fluid behavior and leads to the three new predictions illustrated in Figs. 1–3, which agree well with experiments on ^4He .

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