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Abstract

It is shown that the assumption of a Bose-Einstein condensation of a macroscopic number of particles into a single momentum state necessarily implies that the many particle wavefunction describing the system contains a component with phase coherence over the sample volume. This component has all the properties usually associated with the 'condensate wavefunction' which is postulated to account for coherent phase effects in superconductors and superfluid ^{4}He. The derivation is completely general, independent of assumptions about the form of the particle interaction, isotropy or anisotropy, translational invariance or temperature. It is shown that the condensate part of the wave function makes no contribution to the static pair correlation function $g(\vec{r})$, thus explaining the reduction in amplitude of the oscillations in $g(\vec{r})$ which are observed in neutron scattering measurements on ^{4}He, as the temperature is reduced below the the λ point.

London [1] first suggested over 50 years ago that the presence of superfluidity in liquid ^{4}He at low temperatures is linked with the phenomemon of Bose-Einstein condensation. In an ideal Bose gas there is a macroscopic occupation of a single momentum state at temperatures below the condensation temperature

$$T_B = \frac{2\pi\hbar^2}{Mk_B}\left(\frac{\rho}{2.612}\right)^{2/3}$$ (1)

where M is the particle mass, $\rho = N/V$ where N is the number of particles, V is the sample volume, $\hbar$ is Planck's constant and k_B is the Boltzmann constant. The value of T_B predicted from the known density and mass of ^{4}He atoms is 3.1K, very close to the temperature of the observed λ transition temperature in ^{4}He (2.17K). The arguments of Bogoliobov [2] and Feynman [3] have lead to the general acceptance that the λ transition involves a Bose condensation of the ^{4}He atoms, and that superfluidity (and superconductivity) is linked to the macroscopic occupation of a single momentum state. However no direct demonstration of the linkage has ever been made. There is overwhelming experimental evidence that coherence effects in superconductors and superfluids (e.g. flux quantisation and Josephson effects) can be well described by the concept of the 'condensate wavefunction'. However at present the existence of a condensate wavefunction with the requisite properties in ^{4}He has no microscopic justification and is regarded as a postulate [4].

Another as yet unresolved question is whether the presence of a condensate has any effect on the spatial correlations of particles in a Bose fluid. Intuitively one might expect that Bose condensation implies a loss of spatial ordering, as the localisation in momentum space implies that in some way the wavefunction for each particle has a component which is spread uniformly over the sample volume. If this is the case, the condensate component will not contribute to the pair correlation function $g(\vec{r})$. Hyland et al [5] have suggested that the pair correlation function $g_n(\vec{r})$ of ^{4}He above the λ transition and the corresponding function $g_s(\vec{r})$ in the superfluid are related by

$$\left[g_n(\vec{r}) - \rho\right] = (1-f)^2\left[g_s(\vec{r}) - \rho\right]$$ (2)

Although their derivation is not generally accepted [6,7], this formula describes experimental data very well. Experimental determinations of the condensate fraction from neutron scattering measurements of $g(\vec{r})$ obtained from equation 2 [8] are in good agreement with theoretical predictions and measurements of the condensate fraction by other methods.

In this paper it is shown that if there is a Bose condensation of a macroscopic number of particles into a single momentum state, of momentum $\vec{p}_T$, then the Bose symmetry of the wavefunction necessarily implies that a particle with index n contributes a component

$\exp(i\vec{p}_T . r_n)$ to the total wavefunction and that the components from each particle add coherently to produce a macroscopic wavefunction with coherent phase throughout the volume of the sample. It is also shown that the postulate that the condensate component makes no contribution to $g(\vec{r})$ is correct. Although we specifically consider [4]He we note that the argument applies equally well to Cooper pairs in superconductors, although it does not address the origin of the binding of electrons into Cooper pairs.

In an ideal Bose gas all particles have zero momentum at zero temperature T. However in real systems the fraction f of particles occupying the condensate is less than 100% even at $T=0$. Theory [9,10] and experiment [11] both suggest that at $T=0$, $f \sim 10\%$ in [4]He and that as the temperature is raised, f decreases, becoming zero at the λ point . We first consider a Bose condensed fluid with no centre of mass motion. The momentum distribution $n(\vec{p})$ is then,

$$n(\vec{p}) = f\delta(\vec{p}) + (1-f)n_{nc}(\vec{p}) \tag{3}$$

where f is the condensate fraction , $n_{nc}(\vec{p})$ is the momentum distribution of uncondensed atoms and $\delta(\vec{p})$ is the Dirac δ function. We examine the consequences of a momentum distribution of the form given in equation (3) for the wavefunctions of a Bose system.

The momentum distribution of atoms in a many particle system is [12]

$$n(\vec{p}) = \frac{1}{8\pi^3} \int \rho_1(\vec{r}_1, \vec{r}_1') \exp\left[i\vec{p}.(\vec{r}_1 - \vec{r}_1')\right] d\vec{r}_1 d\vec{r}_1' \tag{4}$$

where the one particle density matrix $\rho_1(\vec{r}_1, \vec{r}_1')$ is defined in terms of the wavefunction by

$$\rho_1(\vec{r}_1, \vec{r}_1') = \int \Psi^*(\vec{r}_1, \vec{r}_{N-1}) \Psi(\vec{r}_1', \vec{r}_{N-1}) d\vec{r}_{N-1} \tag{5}$$

and the wavefunction is normalised,

$$\int \Psi^*(\vec{r}_1, \vec{r}_{N-1}) \Psi(\vec{r}_1, \vec{r}_{N-1}) d\vec{r}_1 d\vec{r}_{N-1} = 1 \tag{6}$$

The N-1 coordinates $\vec{r}_2, \vec{r}_3 .... \vec{r}_{N-1}, \vec{r}_N$ and volume elements $d\vec{r}_2 d\vec{r}_3 .... d\vec{r}_{N-1} d\vec{r}_N$ are denoted by $\vec{r}_{N-1}$ and $d\vec{r}_{N-1}$ respectively. Combining equations 4 and 5 we obtain,

$$n(\vec{p}) = \frac{1}{8\pi^3} \int d\vec{r}_{N-1} \left| \int \Psi(\vec{r}_1, \vec{r}_{N-1}) \exp(i\vec{p}.\vec{r}_1) d\vec{r}_1 \right|^2 \tag{7}$$

$\Psi(\vec{r}_1, \vec{r}_{N-1})$ can be thought of as the amplitude for particle 1 to be at $\vec{r}_1$, with all other particles fixed at the positions $\vec{r}_{N-1}$. The modulus squared of the Fourier transform of each such amplitude makes a real, positive contribution to $n(\vec{p})$ with a weighting determined by the probability of the different configurations in the 3(N-1) dimensional $\vec{r}_{N-1}$ space.

It follows from equations 3 and 7 that for some configurations $\vec{r}_{N-1}$ the function $\Psi(\vec{r}_1, \vec{r}_{N-1})$ must contain a component which contributes to the δ function and which is therefore independent of $\vec{r}_1$.

$$\Psi(\vec{r}_1, \vec{r}_{N-1}) = \Phi_1(\vec{r}_1, \vec{r}_{N-1}) + c(\vec{r}_{N-1}) \tag{8}$$

where $\Phi_1(\vec{r}_1, \vec{r}_{N-1})$ contains all parts of the wavefunction which have an $\vec{r}_1$ dependence and $c(\vec{r}_{N-1})$ includes all those parts of the wavefunction which have no dependence on $\vec{r}_1$.

Substituting in equation 7 gives,

$$n(\vec{p}) = \frac{1}{8\pi^3} \int \left| \tilde{\Phi}_1(\vec{p}, \vec{r}_{N-1}) + 8\pi^3 c(\vec{r}_{N-1}) \delta(\vec{p}) \right|^2 d\vec{r}_{N-1} \tag{9}$$

where

$$\tilde{\Phi}_1(\vec{p}, \vec{r}_{N-1}) = \int \Phi_1(\vec{r}_1, \vec{r}_{N-1}) \exp(i\vec{p}.\vec{r}_1) d\vec{r}_1. \tag{10}$$

and we assume that the sample is contained in a box of (in the limit infinite) volume V so that

$$\delta(\vec{p}) = \frac{1}{8\pi^3} \int \exp(i\vec{p}.\vec{r}_1) d\vec{r}_1 \tag{11}$$

and

$$[\delta(\vec{p})]^2 = (V/8\pi^3)\delta(\vec{p}) \tag{12}$$

The crucial observation required for calculating the pair correlation function is that, if the condensate fraction is finite, the cross terms between the condensate and non condensate terms in equation 9 are negligible, since $\tilde{\Phi}_1(\vec{p}, \vec{r}_{N-1})$ is negligible compared with $\delta(\vec{p})$ at $\vec{p} = 0$. It is known from neutron Compton scattering measurements of the momentum distribution in ^{4}He (recently extended to momentum transfers of 150 Å^{-1} [13]) that the width of the momentum distribution of the uncondensed component is $\sim \hbar/a$ where a is the interparticle separation. This is what one would expect from the uncertainty principle if each atom is enclosed in a 'cage' composed of surrounding atoms. Thus it follows that for configurations of the particles which have significant probability amplitude (i.e. where each atom is surrounded by a 'cage' of width $\sim a$) $\tilde{\Phi}_1(0, \vec{r}_{N-1}) \sim \sqrt{a/\hbar}$, whereas $\delta(0) \sim \sqrt{L/\hbar}$, where L is a length of the order of the sample dimensions. Thus $\tilde{\Phi}_1(0, \vec{r}_{N-1})/\delta(0) \sim 1/\sqrt{N}$, where N is the number of particles and for $N \to \infty$ the product $\tilde{\Phi}_1(\vec{p}, \vec{r}_{N-1})\delta(\vec{p})$ is negligible compared to $[\delta(\vec{p})]^2$.

Thus for a macroscopically large system,

$$\left|\tilde{\Phi}_1(\vec{p},\vec{r}_{N-1})+8\pi^3 c(\vec{r}_{N-1})\delta(\vec{p})\right|^2 = \left|\tilde{\Phi}_1(\vec{p},\vec{r}_{N-1})\right|^2 + \left|8\pi^3 c(\vec{r}_{N-1})\delta(p)\right|^2 \tag{13}$$

and from equations 9 and 12,

$$n(\vec{p}) = \frac{1}{8\pi^3}\int\left|\tilde{\Phi}_1(\vec{p},\vec{r}_{N-1})\right|^2 d\vec{r}_{N-1} + V\delta(p)\int\left|c(\vec{r}_{N-1})\right|^2 d\vec{r}_{N-1} \tag{14}$$

Comparing with equation 3 we obtain,

$$V\int\left|c(\vec{r}_{N-1})\right|^2 d\vec{r}_{N-1} = \int\left|c(\vec{r}_{N-1})\right|^2 d\vec{r}_N = f \tag{15}$$

where $d\vec{r}_N = d\vec{r}_1 d\vec{r}_{N-1}$. The absence of cross terms in equation 13 also implies that,

$$\left|\Psi(\vec{r}_N)^2\right| = \left|\Phi_1(\vec{r}_N)\right|^2 + \left|c(\vec{r}_{N-1})\right|^2 \tag{16}$$

The analagous argument in $\vec{r}$ space is that $c(\vec{r}_{N-1})/\Phi_1(\vec{r}_N) \approx 1/\sqrt{N}$ for values of $\vec{r}_1$ which give significant amplitude for $\Phi_1(\vec{r}_N)$.

The static structure factor $S(\vec{q})$ is defined in terms of the wave function as [14]

$$S(\vec{q}) - 1 = \frac{1}{N}\sum_{n\neq m}\int\left|\Psi(\vec{r}_N)\right|^2 \exp\left[i\vec{q}.(\vec{r}_n - \vec{r}_m)\right]d\vec{r}_N \tag{17}$$

where the double summation is over all particles and the pair correlation function $g(\vec{r})$ is defined by,

$$g(\vec{r}) = \rho + \frac{1}{8\pi^3}\int\left[S(\vec{q}) - 1\right]\exp(-i\vec{q}.\vec{r})d\vec{q} \tag{18}$$

We consider the contribution to $S(\vec{q})$ coming from particles with indices 1 and 2. This is

$$S_{12}(\vec{q}) = \frac{2}{N}\int\left|\Psi(\vec{r}_N)\right|^2 \exp\left[i\vec{q}.(\vec{r}_1 - \vec{r}_2)\right]d\vec{r}_N \tag{19}$$

From equations 16 and 18 we obtain

$$S_{12}(\vec{q}) = \frac{2}{N}\int\left[\left|\Phi_1(\vec{r}_N)\right|^2 + \left|c(\vec{r}_{N-1})\right|^2\right]\exp\left[i\vec{q}.(\vec{r}_1 - \vec{r}_2)\right]d\vec{r}_N$$

$$= \frac{2}{N}\int\left|\Phi_1(\vec{r}_N)\right|^2 \exp\left[i\vec{q}.(\vec{r}_1 - \vec{r}_2)\right]d\vec{r}_N + 8\pi^3\delta(\vec{q})\int\left|c(\vec{r}_{N-1})\right|^2 \exp\left[-i\vec{q}.\vec{r}_2\right]d\vec{r}_{N-1} \tag{20}$$

Thus the part containing $c(\vec{r}_{N-1})$ appears only at $q = 0$ and makes no contribution to $S(\vec{q})$. The same argument can be applied to all terms in the sum, e.g. for $S_{nm}(\vec{q})$ we divide the wavefunction into two parts, one of which has no dependence upon $\vec{r}_n$. We could equally well choose $\vec{r}_m$.

If we assume that the scattering from the uncondensed component of the wavefunction is identical to that from the normal fluid, but reduced by a factor $(1-f)^2$, i.e. that

$$\frac{1}{N}\sum_{n\neq m}\int|\Phi_1(\vec{r}_N)|^2\exp[i\vec{q}.(\vec{r}_n-\vec{r}_m)]d\vec{r}_N=(1-f)^2[S_n(\vec{q})-1] \tag{21}$$

where $S_n(\vec{q})$ is the structure factor of the normal fluid, then the Hyland et al [5] result follows directly from equations 16,17 and 18. The justification of the factor $(1-f)^2$ is as follows. For given values of all particle coordinates except for $\vec{r}_1$ and $\vec{r}_2$, the function

$|\Phi_1(\vec{r}_N)|^2$ in equation 20 can be regarded as the probability distribution of the uncondensed component of particles *1* and *2* with the other *N-2* particles fixed in position. Each atom contributes only a fraction $(1-f)$ of the scattering density of a normal fluid as there is a probability f of the atom being in the condensate. As each term in equation 21 is the product of amplitudes from two atoms the total scattering intensity is reduced by the factor $(1-f)^2$. In fact the assumption that $g(\vec{r})$ of the uncondensed component is identical to that of atoms in the normal fluid seems to have no sound theoretical basis and is not really necessary. The argument presented here predicts only that

$(1-f)^2(g_s(\vec{r})-\rho)=[g_{nc}(\vec{r})-1]$ where $g_{nc}(\vec{r})$ is the pair correlation function of atoms not in the condensate. The question of whether $g_{nc}(\vec{r})$ and $g_n(\vec{r})$ are identical can be decided experimentally by high precision neutron scattering measurements.

We next consider the case where the fluid is in uniform motion with momentum $\vec{p}_T$ per atom . In this case equation 3 is modified to

$$n(\vec{p})=f\delta(\vec{p}-p_T)+(1-f)n_{nc}(\vec{p}-p_T) \tag{22}$$

and equation 8 to

$$\Psi(\vec{r}_1,\vec{r}_{N-1})=\Phi_1^{p_T}(\vec{r}_1,\vec{r}_{N-1})+c(\vec{r}_{N-1})\exp(i\vec{p}_T.r_1) \tag{23}$$

The same division of the wavefunction can be made for any other label n, i.e.,

$$\Psi(\vec{r}_N)=\Phi_n^{p_T}(\vec{r}_n,\vec{r}_{N-n})+c(\vec{r}_{N-n})\exp(i\vec{p}_T.\vec{r}_n)$$

and we can express $\Psi(\vec{r}_N)$ in the form,

$$\Psi(\vec{r}_N)=\frac{1}{N}\sum_n\Phi_n^{p_T}(\vec{r}_n,\vec{r}_{N-n})+\frac{1}{N}\sum_n c(\vec{r}_{N-n})\exp(i\vec{p}_T.\vec{r}_n) \tag{24}$$

This is the sum of two terms, both of which satisfy Bose symmetry. The first term is the non-condensate part of the wave function and the second term is the condensate part. From equation 6 and taking account of the fact that there is no overlap in configuration space $\vec{r}_N$ between the condensate and non condensate, or between terms from different atoms in the condensate, we obtain

$$\int|\Psi(\vec{r}_N)|^2d\vec{r}_N=\frac{1}{N}\sum_{n,m}\int\Phi_n^{p_T*}(\vec{r}_n,\vec{r}_{N-n})\Phi_m^{p_T}(\vec{r}_m,\vec{r}_{N-m})d\vec{r}_N+\frac{1}{N}\sum_n\int|c(\vec{r}_{N-n})|^2d\vec{r}_N \tag{25}$$

Referring to equation 15 we find that the wavefunction in 24 gives the probability f for a particle to be in the condensate.

Thus we obtain a remarkably simple picture. The total wavefunction is a superposition of states in which each atom makes a contribution to the 'condensate wavefunction' with an amplitude which depends upon the configuration of all other particles. At zero temperature all contributions must add in phase, as the wavefunction of a Bose system at $T=0$ must be real and therefore $c(\vec{r}_{N-n})$ contains no phase factors. Thus the phase of he macroscopic wavefunction varies through the sample volume as $\exp(i\vec{p}_T.\vec{r})$. This is not necessarily true at higher temperatures where the phase coherence will be reduced, perhaps contributing to the reduction of the condensate fraction in ^{4}He with temperature. The converse of the derivation of equation 24 is that if the condensate wavefunction has an $\vec{r}$ dependence of the form $\exp(i\vec{p}_T.\vec{r})$, this implies that all atoms and not just the condensate component have a momentum $\vec{p}_T$. This is the origin of the previously somewhat mysterious linkage of the condensate wavefunction with the motion of all atoms in the liquid.

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