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Preprint
RAL-P-97-006

5w9729

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Submitted for publication to J Low Temperature Physics (Accepted)

June 1997

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ISSN 1361-4762

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A New Approach to Bose Condensation and Superfluidity in ^4He

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Abstract

An investigation is made of the implications that the presence of a Bose condensate (BC) has for the form of the many particle Schrödinger wavefunction. It is shown that many particle wavefunctions of states which contribute to the BC, contain long range structure in the position space of each particle. It follows from the requirement that the wavefunction is single valued that, in the presence of a BC, the angular momentum of each particle must be quantised over macroscopic length scales. The paper thus provides a new and simple proof from first principles, that Bose condensation implies macroscopic quantum behaviour. It is shown that this behaviour can be described in terms of the occupation by each particle of the same single particle-like macroscopic wavefunction. The structure in position space of this wavefunction is investigated, using a well known model of the many particle wavefunction for the ground state of ^4He . The model predicts that the probability density of each particle is delocalised in the presence of a BC, occupying all spaces in the sample volume, from which the particle is not excluded by the hard core interaction with other particles.

Pacs Numbers 67.40-w

1.Introduction

London ¹ first suggested over 50 years ago that the presence of superfluidity in liquid ⁴He at low temperatures, is linked with the phenomenon of Bose-Einstein condensation, i.e. to the macroscopic occupation of a single momentum state. In an ideal Bose gas a Bose condensate (BC) is present at temperatures below the condensation temperature

$$T_B = \frac{2\pi\hbar^2}{Mk_B} \left(\frac{N}{2.612V} \right)^{2/3} \quad (1.1)$$

where M is the particle mass, N is the number of particles, V is the sample volume, $\hbar$ is Planck's constant and k_B is Boltzmann's constant. The value of T_B predicted for an ideal gas, with the density and mass of liquid ⁴He, is 3.1K, very close to the temperature of the observed λ transition (2.17K).

Since the seminal paper of London it has gradually become accepted that Bose condensation is the key to superfluidity in ⁴He. However in contrast to an ideal Bose gas, only a fraction f of particles occupy the zero momentum state at $T=0$. Penrose and Onsager ² provided the first theoretical estimate of an 8% BC fraction in liquid helium at $T=0$. Subsequent variational calculations, refined this estimate to $f=9\%$ ³. Perhaps the most convincing evidence for the link between a BC and superfluidity has been provided by Path Integral Monte Carlo calculations, ^{4,5} which show a singularity in the specific heat close to 2.17K, which coincides with the development of a BC. These calculations also give $f=9\%$. A number of experimental methods have been used in attempts to measure the BC fraction in liquid helium and although the interpretation of these measurements relies upon assumptions which are difficult to verify, they all give $f\sim 9\%$, at $T=0$. The situation until 10 years ago was reviewed by Sears ⁶. The main advance since then has been the Deep Inelastic Neutron Scattering measurements of Sokol et al, ⁷ which also give $f\sim 9\%$, although Sokol has emphasised

that his experimental data is consistent with the assumption that superfluid ^4He contains no condensate.^{7, 8}

It is now generally accepted that in the presence of a BC all particles occupy the same single particle wavefunction which extends over macroscopic length scales and that the phase of this wavefunction governs the macroscopic momentum distribution of the fluid. If one accepts this as a postulate, most of the exotic behaviour of bulk superfluid ^4He , including superfluidity and the occurrence of quantised vortices, can be explained⁹. However the link between Bose condensation and superfluidity is often characterised as ill understood. Most textbooks on liquid helium concentrate on the work of Landau¹⁰ and Feynman¹¹ to explain the physical basis of superfluidity in ^4He and Bose condensation does not play a central role in either of these treatments. The presence of a BC is a basic assumption of field theoretical treatments, but these treatments have not been well represented in text books on liquid helium, partly because they use advanced many body formalism, which does not readily yield any physical picture of the processes underlying superfluidity.

Field theoretical treatments have however yielded a considerable and hard won understanding of superfluidity in ^4He . These methods are particularly valuable for investigating the form of the excitation spectrum in the liquid. The work of Bogoliobov¹² first showed that a BC can exist in an interacting system and how the presence of a BC in an interacting gas can change the dispersion relation from particle-like to phonon-like at low energies. This work was crucial as a microscopic basis for superfluidity via the well known Landau criterion.¹⁰ Subsequent work^{13,14,15} showed how the two fluid equations are a natural consequence of a Bose broken symmetry. More recent work^{16,17,18,19} has lead to an understanding of how density fluctuations mix with the single particle spectrum, a realisation of the qualitative differences between the spectrum exhibited at $T=0$ and finite temperatures and an understanding of how the excitations of the superfluid merge with those of the normal

fluid, as the liquid passes through the transition temperature. There is now a large body of field theoretical literature on liquid helium which has been extensively reviewed in two recent textbooks^{20,21}.

Despite extensive theoretical and experimental work on liquid helium during the past 50 years, there are a number of long standing questions, relating to the nature of the macroscopic wavefunction in ^4He and the link with Bose condensation, which still have no clear answer.

- (1) How can a particle in a strongly interacting many body system, such as liquid helium, occupy a single particle wavefunction?
- (2) Why in the presence of a BC does this wavefunction extend over macroscopic length scales?
- (3) How can every particle in superfluid helium at $T=0$ occupy the same single particle wavefunction when only $\sim 9\%$ occupy a single momentum state?

The approach taken in this paper is to investigate the implications that the presence of a BC has for the structure in position space of the many particle Schrödinger wavefunction. The approach is rigorously based and provides clear answers to questions 1-3 above. It is also relatively simple and has a clear physical interpretation. It can be understood by anyone with a basic knowledge of elementary quantum mechanics, probability theory and Fourier transforms, at a level which can be found in the introductory chapters of most modern textbooks on quantum mechanics²².

Section 2 presents definitions and notation. Section 3 gives a definition of a “conditional wavefunction” (CW) for a single particle, in terms of the many particle Schrödinger wavefunction. It is shown that the momentum of particles is determined by the phase of the CW in an identical way to that familiar from single particle quantum mechanics. In section 4 it is shown that when the many particle wavefunction contributes to the BC, the CW extends over macroscopic length scales and can be

identified with the macroscopic wavefunction, postulated to explain macroscopic quantum behaviour. In section 5, a model wavefunction is used to infer the spatial structure of the CW. It is shown how in the presence of a BC all particles can occupy the same macroscopic CW, even though the BC fraction may be much less than unity. In section 7 a summary and conclusions are given. The appendix discusses the connection between the CW and the "order parameter", a central concept of other microscopic theories of ^4He , which assume that a BC is present.

2. Notation and Definitions

We consider a system of N particles in a rectangular box of volume V . Using periodic boundary conditions, with $\hbar = 1$, each momentum state occupies a discrete element of volume $1/V$ in momentum space. The probability that a particular momentum state is occupied is defined as $n_{\vec{p}} / V$ and

$$\frac{1}{V} \sum_{\vec{p}} n_{\vec{p}} = 1 \quad (2.1)$$

The Schrödinger N particle wavefunction corresponding to a state i with energy E_i is $\Psi_i(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N-1}, \vec{r}_N)$. The coordinates of an arbitrarily chosen particle are denoted as $\vec{r}$ and those of all other particles by $\vec{s}$, ie

$$\Psi_i(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N-1}, \vec{r}_N) = \Psi_i(\vec{r}, \vec{s}) \quad (2.2)$$

The wavefunctions are normalised ,

$$\int |\Psi_i(\vec{r}, \vec{s})|^2 d\vec{r} d\vec{s} = 1 \quad (2.3)$$

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

²³

$$\rho_1(\vec{r}, \vec{r}') = \sum_i B_i \int \Psi_i^*(\vec{r}, \vec{s}) \Psi_i(\vec{r}', \vec{s}) d\vec{s} \quad (2.4)$$

where $B_i \propto \exp(-E_i / k_B T)$ is the thermal probability that a state of energy E_i is occupied. The momentum distribution of the atoms is

$$n_{\vec{p}} = \int \rho_1(\vec{r}, \vec{r}') \exp[i\vec{p} \cdot (\vec{r} - \vec{r}')] d\vec{r} d\vec{r}' \quad (2.5)$$

Combining equations 2.4 and 2.5 gives ²³

$$n_{\vec{p}} = \sum_i B_i \int d\vec{s} \left| \int \Psi_i(\vec{r}, \vec{s}) \exp(i\vec{p} \cdot \vec{r}) d\vec{r} \right|^2 \quad (2.6)$$

In the presence of a Bose Condensate (BC) the momentum distribution of the atoms has the form

$$n_{\vec{p}} = (1-f)u_{\vec{p}} + fV\delta_{\vec{p}0} \quad (2.7)$$

The probability that an atom occupies the $\vec{p} = 0$ momentum state is

$$\frac{n_0}{V} = f \quad (2.8)$$

$u_{\vec{p}}$ is the momentum distribution for $p \neq 0$. In the presence of a BC, $f \sim 1$ and $n_0 / n_{\vec{p}} \sim N$, whereas in the absence of a BC, $f \sim 1/N$ and $n_0 / n_{\vec{p}} \sim 1$.

3. Definition of Conditional Wavefunction(CW)

In this section a “conditional wavefunction” (CW) for a single particle is defined in terms of the many particle wavefunction. It will be shown in the following two sections that, for states which contribute to the BC, the CW has all the properties of the macroscopic wavefunction, postulated to explain the exotic macroscopic properties of superfluid ^4He . In particular the CW has structure over macroscopic length scales and its phase governs the momentum of the particle.

The standard interpretation of the N particle wavefunction is

$$|\Psi_i(\vec{r}, \vec{s})|^2 = P_i(\vec{r}, \vec{s})$$

(3.1)

where $P_i(\vec{r}, \vec{s})$ is the probability for state i that there is a particle at $\vec{r}$ and the other $N-1$ particles are at $\vec{s}$. It follows from the basic axioms of probability theory²² that,

$$P_i(\vec{r}, \vec{s}) = P_i(\vec{r}|\vec{s})P_i(s)$$

(3.2)

where $P_i(\vec{r}|\vec{s})$ is the probability that there is a particle at $\vec{r}$ if the other particles are at $\vec{s}$.

$$P_i(\vec{s}) = \int P_i(\vec{r}, \vec{s}) d\vec{r} = \int |\Psi_i(\vec{r}, \vec{s})|^2 d\vec{r}$$

(3.3)

is the probability that the other $N-1$ particles are at $\vec{s}$.

We define the "conditional wavefunction" (CW) of a single particle for configuration $\vec{s}$ and state i as

$$\psi_i(\vec{r}|\vec{s}) = \Psi_i(\vec{r}, \vec{s}) / \sqrt{P_i(\vec{s})}$$

(3.4)

Equations 3.3 and 3.4 define the conditional wavefunction, $\psi_i(\vec{r}|\vec{s})$, in terms of the many particle wavefunction $\Psi_i(\vec{r}, \vec{s})$. The CW shares a number of properties with the single particle wavefunction, familiar from elementary quantum mechanics. From equations 3.2 and 3.4,

$$|\psi_i(\vec{r}|\vec{s})|^2 = P_i(\vec{r}|\vec{s})$$

(3.5)

i.e. the modulus squared of the CW gives the probability distribution in position space of the particle. It follows from the identification of $P_i(\vec{r}|\vec{s})$ and $P_i(\vec{s})$ as probability distribution functions that the CW is normalised.

$$\int P_i(\vec{s}) d\vec{s} = \int P_i(\vec{r}|\vec{s}) d\vec{r} = \int |\psi_i(\vec{r}|\vec{s})|^2 d\vec{r} = 1$$

(3.6)

It follows from equations 2.6 and 3.4 that

$$n_{\vec{p}} = \sum_i B_i \int |\tilde{\psi}_{i\vec{p}}(\vec{s})|^2 P_i(\vec{s}) d\vec{s} = \sum_i B_i \int n_{i\vec{p}}(\vec{s}) P_i(\vec{s}) d\vec{s}$$

(3.7)

where

$$\tilde{\psi}_{i\vec{p}}(\vec{s}) = \int \psi_i(\vec{r}|\vec{s}) \exp(i\vec{p} \cdot \vec{r}) d\vec{r}$$

(3.8)

and

$$n_{i\vec{p}}(\vec{s}) = |\tilde{\psi}_{i\vec{p}}(\vec{s})|^2$$

(3.9)

$n_{i\vec{p}}(\vec{s})$ is the momentum distribution of the particle of interest in the state i , when all other particles are in configuration $\vec{s}$. It can be seen from equations 3.8 and 3.9 that the relation between the CW and the momentum distribution $n_{i\vec{p}}(\vec{s})$ is identical to that between a single particle wavefunction and the corresponding momentum distribution in elementary quantum mechanics. The inverse of 3.8 is

$$\psi_i(\vec{r}|\vec{s}) = \frac{1}{V} \sum_{\vec{p}} \tilde{\psi}_{i\vec{p}}(\vec{s}) \exp(-i\vec{p} \cdot \vec{r}) \quad (3.10)$$

It follows from 3.6, 3.8 and Parseval's theorem that the momentum distribution $n_{i\vec{p}}(\vec{s})$ is normalised, i.e.

$$\frac{1}{V} \sum_{\vec{p}} |\tilde{\psi}_{i\vec{p}}(\vec{s})|^2 = \frac{1}{V} \sum_{\vec{p}} n_{i\vec{p}}(\vec{s}) = 1 \quad (3.11)$$

It also follows from the fact that $\psi_i(\vec{r}|\vec{s})$ is the Fourier transform of $\tilde{\psi}_{i\vec{p}}(\vec{s})$ ²⁴, that the expectation value of $\vec{p}$ can be calculated as

$$\int \vec{p} n_{i\vec{p}}(\vec{s}) d\vec{p} = \int \psi_i(\vec{r}|\vec{s})^* (-i\nabla) \psi_i(\vec{r}|\vec{s}) d\vec{r} \quad (3.12)$$

i.e. $\vec{p}$ can be replaced by $-i\nabla$ in the way familiar from elementary single particle quantum mechanics. In particular, if the CW changes from $\psi_i(\vec{r}|\vec{s})$ to $\psi_i(\vec{r}|\vec{s}) \exp[iS(\vec{r})]$, where $S(\vec{r})$ is an arbitrary real function, then the momentum at $\vec{r}$ changes by $\nabla S(\vec{r})$.

The primary motivation for the introduction of the CW is that, as the following two sections show, when a BC is present the CW has identical properties to the postulated single particle-like macroscopic wavefunction in superfluid helium. The introduction of the CW also allows one to rewrite some well known expressions (e.g. for the momentum distribution, condensate fraction and density matrix) in a simple form, which makes direct contact with elementary probability theory. However the essential feature of the CW is that it describes the behaviour of the many particle wavefunction

$\Psi_i(\vec{r}, \vec{s})$ as a function of $\vec{r}$, for fixed $\vec{s}$. The function $P_i(\vec{s})$ is essentially a normalisation factor.

4. The Macroscopic Wavefunction and Superfluidity

In order to obtain an expression for the condensate fraction, we divide $\psi_i(\vec{r}|\vec{s})$ into its $\vec{p} = 0$ and $\vec{p} \neq 0$ components, i.e

$$\psi_i(\vec{r}|\vec{s}) = \Delta\psi_i(\vec{r}|\vec{s}) + \bar{\psi}_i(\vec{s}) \quad (4.1)$$

where from equations 3.8 and 3.10

$$\bar{\psi}_i(\vec{s}) = \frac{\tilde{\psi}_{i0}(\vec{s})}{V} = \frac{1}{V} \int \psi_i(\vec{r}|\vec{s}) d\vec{r} \quad (4.2)$$

and

$$\Delta\psi_i(\vec{r}|\vec{s}) = \frac{1}{V} \sum_{\vec{p} \neq 0} \tilde{\psi}_{i\vec{p}}(\vec{s}) \exp(-i\vec{p} \cdot \vec{r}) \quad (4.3)$$

$\bar{\psi}_i(\vec{s})$ is the mean value of $\psi_i(\vec{r}|\vec{s})$ over the volume V . The function $\Delta\psi_i(\vec{r}|\vec{s})$ is the deviation from the mean and has only $\vec{p} \neq 0$ Fourier components. The weight of the $\vec{p} = 0$ component of $n_{i\vec{p}}(\vec{s})$ is (from 3.9 and 4.2)

$$\frac{n_{i0}(\vec{s})}{V} = \frac{|\tilde{\psi}_{i0}(\vec{s})|^2}{V} = V |\bar{\psi}_i(\vec{s})|^2 = f_i(\vec{s}) \quad (4.4)$$

Equation 4.4 defines $f_i(\vec{s})$, the condensate fraction for configuration $\vec{s}$ in state i .

It follows from equations 2.8, 3.7 and 4.4 that

$$f = \sum_i B_i \int f_i(\vec{s}) P_i(\vec{s}) d\vec{s} \quad (4.5)$$

i.e. the condensate fraction f is a weighted average of $f_i(\vec{s})$ over all possible configurations $\vec{s}$ and occupied states i . It is obvious that if f is finite, then equation 4.5 implies that $f_i(\vec{s})$ will also be finite for a significant number of occupied states i and configurations $\vec{s}$. Macroscopic quantum behaviour follows from this trivial observation.

It can be inferred from the definition of $f_i(\vec{s})$ via equations 4.2 and 4.4 and from the fact that $\psi_i(\vec{r}|\vec{s})$ is normalised (equation 3.6), that if $f_i(\vec{s})$ remains finite as $V \rightarrow \infty$ then $\psi_i(\vec{r}|\vec{s})$ must have structure in $\vec{r}$ which extends over distances comparable to the sample size. Considering first the groundstate, for which the many particle wavefunction $\Psi_0(\vec{r},\vec{s})$ and hence $\psi_i(\vec{r}|\vec{s})$ can be taken as real and positive²⁶, if $|\psi_i(\vec{r}|\vec{s})|^2$ is distributed over a region of volume $\sim v$, then for normalisation, the amplitude of $\psi_i(\vec{r}|\vec{s})$ must be $\sim 1/\sqrt{v}$. It follows from equation 4.2 that $\bar{\psi}_i(\vec{s}) \sim \sqrt{v}/V$ and from equation 4.4 that $f_i(\vec{s}) \sim v/V$. This point can be illustrated by considering an unrealistic but simple normalised Gaussian form for $\psi_i(\vec{r}|\vec{s})$, i.e,

$$\psi_i(\vec{r}|\vec{s}) = \frac{1}{(2\pi)^{3/4} \sqrt{\sigma_x \sigma_y \sigma_z}} \exp \left[\frac{-x^2}{4\sigma_x^2} + \frac{-y^2}{4\sigma_y^2} + \frac{-z^2}{4\sigma_z^2} \right] \quad (4.6)$$

Substituting this form in equations 4.2 and 4.4 gives $f_i(\vec{s}) = (8\pi)^{3/2} (\sigma_x \sigma_y \sigma_z) / V$. Unless the product $\sigma_x \sigma_y \sigma_z$ scales as V , then $\bar{\psi}_i(\vec{s})$ and hence $f_i(\vec{s}) \rightarrow 0$ as $V \rightarrow \infty$. Thus the volume over which the amplitude of $\psi_i(\vec{r}|\vec{s})$ is significant must be $\sim V$, if state i contributes to the BC. (In the following section a model which incorporates a more realistic spatial structure for $\psi_i(\vec{r}|\vec{s})$ in the ground state of liquid helium is examined. For this model f is exactly equal to v/V .) In excited states $\Psi_i(\vec{r},\vec{s})$, the CW is not necessarily real or positive, but this does not affect the conclusion that a finite value of $f_i(\vec{s})$ as $V \rightarrow \infty$ implies long range structure in $\psi_i(\vec{r}|\vec{s})$, since any variation in the phase of $\psi_i(\vec{r}|\vec{s})$ with $\vec{r}$ will decrease rather than increase the mean value of $\psi_i(\vec{r}|\vec{s})$. Long range structure will still be required to give a finite value of $f_i(\vec{s})$.

The delocalisation of the CW in the presence of a BC is the central result of this paper. It can be restated without reference to the CW as follows. *Many particle wavefunctions which contribute to the BC, contain long range structure in the position space of each particle. More precisely, if we consider the spatial behaviour of $\Psi_i(\vec{r},\vec{s})$ as a function of $\vec{r}$, the coordinate of an arbitrarily chosen particle, for a*

fixed configuration $\vec{s}$ of all other particles, there will be many probable configurations $\vec{s}$ for which $\Psi_i(\vec{r}, \vec{s})$ contains long range structure in $\vec{r}$.

One direct consequence of the long range structure in $\Psi_i(\vec{r}, \vec{s})$ is macroscopic quantisation of angular momentum. Writing $\psi_i(\vec{r}|\vec{s}) = A_i(\vec{r}, \vec{s}) \exp[i\mathcal{G}_i(\vec{r}, \vec{s})]$, where $A_i(\vec{r}, \vec{s})$ and $\mathcal{G}_i(\vec{r}, \vec{s})$ are real functions. $\psi_i(\vec{r}|\vec{s})$ (and hence $\Psi_i(\vec{r}, \vec{s})$) is single valued only if

$$\oint \nabla \mathcal{G}_i(\vec{r}, \vec{s}) \cdot d\vec{r} = 2\pi n \quad (4.7)$$

where n is an integer and the integral is taken around any closed loop. A transition to a state with different phase $\mathcal{G}_i'(\vec{r}, \vec{s})$ is possible, providing that

$$S_i(\vec{r}, \vec{s}) = \mathcal{G}_i(\vec{r}, \vec{s}) - \mathcal{G}_i'(\vec{r}, \vec{s}) \text{ satisfies} \\ \oint \nabla S_i(\vec{r}, \vec{s}) \cdot d\vec{r} = 2\pi m \quad (4.8)$$

$\psi_i(\vec{r}|\vec{s})$ remains single valued, providing that m is an integer. It was shown in section 3 that in order to calculate single particle momentum properties from $\psi_i(\vec{r}|\vec{s})$, one can substitute $\vec{p} = -i\hbar\nabla$. It follows that a change of phase of $\psi_i(\vec{r}|\vec{s})$ by $S_i(\vec{r}, \vec{s})$, corresponds to a change in momentum of $\Delta\vec{p} = \hbar\nabla S_i$. Thus from equation 4.8

$$\oint \Delta\vec{p}(\vec{r}, \vec{s}) \cdot d\vec{r} = m\hbar \quad (4.9)$$

Due to the long range structure of $\psi_i(\vec{r}|\vec{s})$, equation 4.9 must be satisfied for integration loops of macroscopic size, in states i which contribute to the BC. Thus any change in the angular momentum of the fluid (due for example to forces between a tube wall and flowing fluid) must be quantised over macroscopic length scales if a BC is present.

Classical viscous processes rely upon the fact that in classical fluids, small volume elements (but still large compared to atomic sizes) can be set into motion independently of each other. However this is no longer true in the presence of a BC.

Any change in the motion of the fluid must be correlated over macroscopically large length scales. Otherwise, some choices of integration loop within the fluid, would not satisfy equation 4.9 and the states i which contribute to the BC could not be occupied. In particular the macroscopic velocity gradients, which are necessary for classical viscous processes to occur, cannot be established and these processes are therefore prohibited when a BC is present. Processes which do satisfy equation 4.9 in ^4He include the creation of phonons and rotons ($m=0$) and the creation of quantised vortices ($m>0$). As shown by Landau¹⁰ below a minimum critical flow velocity, such processes cannot occur. Thus at lower velocities shear forces are unable to introduce rotational flow into the fluid without exciting a macroscopic number of particles out of the condensate. Such processes have negligible probability in a sufficiently large system at finite f . Since irrotational flow is in a sense the most fundamental property of superfluids²⁵ one can say that superfluidity is a direct consequence of the presence of a BC.

We emphasise that quantisation of angular momentum and the absence of classical viscous processes depends only upon the proviso that a macroscopic number of particles occupy the condensate. Macroscopic quantum effects will occur, at any value of f , providing that $fN \rightarrow \infty$ as $N \rightarrow \infty$. In particular, as the temperature is raised and f decreases, irrotational flow will be maintained for all values of f up to the transition temperature, which corresponds to $f=0$. It also follows from the Bose symmetry of the wavefunction that the angular momentum of *every* particle in the fluid must be quantised over macroscopic length scales for *any* finite f . It is worth noting that the link between the phase of the macroscopic wavefunction and the momentum distribution in the liquid is established in a new way in this paper. This link follows directly from the fundamental quantum expression for the momentum distribution in equation 2.6 and unlike derivations which rely on considerations of the Galilean transformation²⁶, links the phase directly with the canonical momentum rather than the velocity of the particles.

To summarise the main arguments of this section, if a BC exists at any temperature, *some* wavefunctions $\Psi_i(\vec{r}, \vec{s})$ containing long range structure must be occupied.

Wavefunctions with long range structure can only be occupied in the presence of macroscopic quantisation of angular momentum. Otherwise the particles would be described by a many particle wavefunction which is not single valued. Thus Bose condensation (at any temperature) implies that momentum of every particle must be quantised over macroscopic length scales.

5. Model Wavefunction

In this section the spatial structure of the CW in liquid helium is investigated with the aid of a well known model wavefunction introduced by Feynman¹¹ and used by Penrose and Onsager², in the first calculation of the condensate fraction in ⁴He at zero temperature. The model "hard sphere" ground state wavefunction for spheres of radius R has the form

$$\begin{aligned} \Psi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N-1}, \vec{r}_N) &= C \quad \text{if } |\vec{r}_n - \vec{r}_m| > 2R \quad \text{for all } n, m, n \neq m \\ &= 0 \quad \text{if } |\vec{r}_n - \vec{r}_m| < 2R \quad \text{for any } n, m, n \neq m \end{aligned} \quad (5.1)$$

The wavefunction has a constant value C providing that two spheres do not overlap and is zero otherwise.

The form of the CW, $\psi_0(\vec{r}|\vec{s})$, is especially simple for a many particle wavefunction of the form given in equation 5.1. An allowed configuration $\vec{s}$ is one in which $N-1$ particles are positioned with their centres at arbitrary positions within the sample volume, with the condition that none of the particle centres lie within a distance $2R$ of each other. Figure 1 shows a possible configuration of $N-1$ hard spheres (black circles)

with centres at the points $\vec{r}_2, \vec{r}_3, \dots, \vec{r}_N$. Around each of the $N-1$ particles is a region of radius $2R$, (white circles) which the particle of interest cannot enter without hard core overlap. It follows from equation 5.1 that $\psi(\vec{r}|\vec{s})$ is zero if $\vec{r}$ lies within one of these exclusion regions and has a constant value $c(\vec{s})$ otherwise. The CW occupies the gray shaded region illustrated in figure 1.

Let the volume from which the particle is not excluded by the presence of other particles be $v(\vec{s})$. Then since $\psi(\vec{r}|\vec{s})$ is normalised

$$\int |\psi_0(\vec{r}|\vec{s})|^2 d\vec{r} = 1 = v(\vec{s})|c(\vec{s})|^2 \quad (5.2)$$

Thus the normalisation constant $|c(\vec{s})|^2$ has the value $1/v(\vec{s})$. It also follows that

$$\bar{\psi}_0(\vec{s}) = \frac{1}{V} \int \psi_0(\vec{r}|\vec{s}) d\vec{r} = \frac{c(\vec{s})v(\vec{s})}{V} \quad (5.3)$$

and (from 4.4) that the condensate fraction in this configuration is

$$f_0(\vec{s}) = V|\bar{\psi}_0(\vec{s})|^2 = \frac{V|c(\vec{s})|^2 v(\vec{s})^2}{V^2} = \frac{v(\vec{s})}{V} \quad (5.4)$$

Thus we obtain the simple result that for the model wavefunction, the condensate fraction for configuration $\vec{s}$ is equal to the fraction of the total volume, from which the particle of interest is not excluded by the hard core of other particles.

Since f is just the fraction of the total volume available for occupation by the CW, the problem of calculating the condensate fraction in this model is equivalent to finding the fraction of the volume available for the insertion of an extra hard sphere, when $N-1$ hard spheres are already randomly positioned within a volume V . We note that as the number of particles increases (at a constant ratio of N/V) this fraction will become precisely defined. Random fluctuations in the volume available for occupation by another particle, due to random variations of the positions of the other $N-1$ particles, will be $\sim V/\sqrt{N}$. Thus the condensate fraction will be determined very

precisely in a macroscopic system, with $\Delta f / f \sim 1/\sqrt{N}$ and will be the same for the overwhelming majority of configurations $\bar{s}$. It is also worth noting that any change in the thermodynamic properties of the liquid, due to the presence of the long range structure, will be related to macroscopic averages of the CW over space. These averages will also be independent of the precise configuration $\bar{s}$, since in a sufficiently large volume, all possible local configurations of atoms will be sampled. Thus the $\bar{s}$ dependence of $\psi_0(\vec{r}|\bar{s})$ is essentially irrelevant.

It can also be seen that any two particles have the same CW to within terms $\sim 1/N$. If we consider a configuration of $N-2$ particles and add a particle, then the CW of this particle will occupy the entire sample volume, except for the regions which it cannot enter due to the hard core potential of the other particles already present. If we add a second particle the same comment applies, except that the CW of the second particle is excluded from $N-1$ rather than $N-2$ hard core regions. In the limit of large N this difference can be neglected and the CWs of any two particles are identical to within terms $\sim 1/N$. Since CWs of different particles occupy the same region of space when a BC is present, only Bose particles can form such a state. In the absence of macroscopic quantisation effects, the CWs of different particles are not identical. As discussed below, in this case the CW of each particle is localised and different CWs will occupy different regions of space.

For a particular configuration $\bar{s}$ the momentum distribution of the particle of interest is given by equations 3.8 and 3.9. In the presence of a condensate, $v(\vec{s}) \sim V$ and $\psi_0(\vec{r}|\bar{s})$ is distributed over a large number ($\sim N$) of randomly positioned regions (see Figure 1). The $\vec{p} = 0$ component of $\psi_0(\vec{r}|\bar{s})$ is $\sim \sqrt{N}$ times larger than the $\vec{p} \neq 0$ components, since all contributions in momentum space add coherently at $\vec{p} = 0$ and with random phase at $\vec{p} \neq 0$. (There is a close analogy with the power spectrum of "shot noise" ²⁷). It follows that the probability that the zero momentum state is occupied is $\sim N$ times larger than that of other momentum states, i.e. a BC is present.

We note that the probability that a particular momentum state is occupied is given by the modulus square of the corresponding Fourier amplitude of $\psi_0(\vec{r}|\vec{s})$, in an identical way to elementary quantum mechanics. It is in this sense that a fraction f of the particles occupy the zero momentum state. In fact every particle is simultaneously in both condensate and non-condensate. There is a strong analogy with single particle quantum mechanics, where unless the wavefunction is an eigenstate of momentum, the particle has an amplitude to be in a number of different momentum states simultaneously.

As the radius R of the particles is reduced, the probability that each particle occupies the zero momentum state increases smoothly, approaching 1 as the particle radius shrinks to zero. For $R=0$ all particles occupy the zero momentum state and the model reduces to an ideal gas. The model suggests that the presence of long range structure and the associated BC in the ground state, is favoured in liquid helium due to two connected features.

- (i) The low mass of the helium atoms means that the liquid has a high kinetic energy of zero point motion and this can be significantly reduced by the formation of a state with long range structure in position space.
- (ii) The low density of the liquid, which is the result of the large zero point motion, combined with the weak attractive interactions between atoms, means that there is sufficient space between particles for the formation of an extended CW, without hard core overlap between atoms. Thus although the potential energy increases when a BC is formed⁶, this increase is not large and is outweighed by the decrease in kinetic energy.

The latter consideration also provides a simple qualitative explanation of the fact that the formation of a BC is favoured by low density and weak interactions between particles. One would also expect that the BC fraction in ^4He will decrease with increasing pressure, in agreement with calculation and experiment^{28,29} since there will

be less space available for occupation by the CW, without hard core overlap with other particles.

It was shown in the previous section that the presence of long range structure in the CW implies macroscopic quantum effects. Thus the absence of such effects implies that the only occupied states are those which have no long range structure in the CW. The width of calculated and observed momentum distributions in normal ^4He is consistent with the assumption that the only thermally occupied states are those in which the volume occupied by the CW is $\sim V/N$. In this case all Fourier components of $\psi_i(\vec{r}|\vec{s})$ are of comparable amplitude and the width of the momentum distribution is $\sim \hbar\sqrt{N/V}$, as is observed.

Although the results in this section rely on an oversimplified model wavefunction, they are also valid with minor modifications for more realistic variational wavefunctions, such as Jastrow functions. The latter are defined as

$$\Psi(\vec{r}_1, \vec{r}_2 \dots \vec{r}_N) = C \prod_{i < j} f(\vec{r}_i - \vec{r}_j) \quad (5.5)$$

where C is a normalisation constant and $f(\vec{r})$ goes smoothly to zero at small $\vec{r}$ and to a constant value at large $\vec{r}$. (The model wavefunction is in fact a special case of a Jastrow function with $f(\vec{r}) = 0$ for $\vec{r} < 2R$ and constant for $\vec{r} > 2R$). The Jastrow CW is (neglecting the normalisation constant)

$$\Psi(\vec{r}|\vec{s}) = \prod_i f(\vec{r} - \vec{r}_i) \quad (5.6)$$

The sharp cut off in the model CW at the boundaries of the hard core exclusion regions of the other particles is unphysical and will introduce spurious higher momentum components into the momentum distribution. In more realistic wavefunctions, where $f(\vec{r})$ goes to zero smoothly with decreasing $\vec{r}$, the amplitude of the CW will fall off gradually in the vicinity of another particle. In addition the

condensate fraction will no longer be given simply by the volume outside the hard core exclusion regions. Apart from this the physical picture provided by the hard core model will be essentially unchanged by the use of a more realistic wavefunction for the ground state of liquid helium. In particular the conclusion that every particle occupies the same CW to within terms $\sim 1/N$ is unchanged.

6. Summary and Conclusions

This paper has presented a new approach to the phenomena of superfluidity and macroscopic quantum behaviour in ^4He , based on an examination of the implications of the presence of a Bose condensate (BC), for the form of the many particle wavefunction. In the introduction three specific questions were raised;

1. *How can a particle in a strongly interacting many body system such as superfluid helium occupy a single particle wavefunction?* A way of approaching this question has been given in section 3, where it was shown that in any many particle system (independent of the form of particle interactions or whether the particles are Bose or Fermi) a “conditional wavefunction” (CW) can be defined in terms of the many particle Schrödinger wavefunction. The CW has many properties in common with a single particle wavefunction, including those attributed to the macroscopic single particle-like wavefunction in superfluid helium.

2. *Why does this single particle wavefunction extend over macroscopic length scales in the presence of a BC?* It was shown in section 4 that structure in the CW over macroscopic length scales is a mathematical consequence of the fundamental expression for the momentum distribution in a many particle system (equation 2.6) and the presence of a BC. When a BC is present the CW has identical properties to the macroscopic wavefunction, postulated to explain superfluidity and hence can be identified with the macroscopic wavefunction. The physical nature of the long range structure in the macroscopic wavefunction was investigated in section 5 using a model many particle wavefunction for the ground state. It was shown that in this model, the probability density of each particle occupies every part of the sample volume from which it is not excluded by its hard core interaction with other particles. It will be shown in a subsequent paper³⁰ that this delocalisation has significant implications for the form of the pair correlation function.

3. *How can every particle occupy the same single particle state at $T = 0$, when only a fraction f are in the same momentum state?* The model wavefunction indicates that in the presence of a BC, the CW of each particle occupies the same region of space to within terms $\sim 1/N$. Hence in this sense one can say that every particle occupies the same macroscopic wavefunction. The probability f that the zero momentum state is occupied in this state, is given by the modulus squared of the zero momentum Fourier component of the CW and will be less than one. (The close analogy with single particle quantum mechanics is obvious.) However the long range structure in the CW, when a BC is present implies that the occupation of the zero momentum state is much greater than that of other momentum states. i.e. $f \sim 1$.

In conclusion, this paper has presented a new approach to understanding the phenomenon of superfluidity in ^4He . The main result of the paper was derived in section 4, where it was shown that in the presence of a BC, the angular momentum of each particle must be quantised over macroscopic length scales. This result is valid at all temperatures where f is non-zero and is independent of the form of the many particle wavefunction. Macroscopic quantisation of angular momentum implies that processes which create rotational flow. (except for quantised vortices) are forbidden in the presence of a BC. Since irrotational flow is the most fundamental property of superfluids²⁵, the paper provides a new and simple proof from first principles that Bose condensation implies superfluidity.

Appendix. The Order Parameter

A central concept of previous microscopic theories of superfluidity which take the presence of a BC as their central assumption, is a non-zero value of the "order parameter" in the superfluid phase²⁶. The order parameter can be defined via the Penrose-Onsager criterion for the presence of a BC.²

$$\rho_1(\vec{r}, \vec{r}') \rightarrow \langle \psi^*(\vec{r}) \rangle \langle \psi(\vec{r}') \rangle \neq 0 \quad \text{as } |\vec{r} - \vec{r}'| \rightarrow \infty$$

(A.1)

This implies that "off diagonal long range order" (ODLRO) exists in the one particle density matrix. In the absence of a BC $\rho_1(\vec{r}, \vec{r}') \rightarrow 0$ as $|\vec{r} - \vec{r}'| \rightarrow \infty$. The "order parameter" or "condensate wavefunction" is usually identified as the function $\langle \psi(\vec{r}) \rangle$.

Equation A.1 follows very simply from the formalism of sections 3 and 4. From equations 2.4 and 3.4, the one particle density matrix can be written as,

$$\rho_1(\vec{r}, \vec{r}') = \sum_i B_i \int P(\vec{s}) \psi_i(\vec{r}|\vec{s}) \psi_i^*(\vec{r}'|\vec{s}) d\vec{s}$$

(A.2)

Expanding $\psi_i(\vec{r}|\vec{s})$ and $\psi_i^*(\vec{r}'|\vec{s})$ into their Fourier components via equations 4.1-4.3 and multiplying out the components we find a constant component $f(\vec{s})/V$ and a sum of products of different Fourier components. The latter averages to zero for $|\vec{r} - \vec{r}'| \rightarrow \infty$ and after performing the integration over $\vec{s}$, we obtain the result

$$\rho_1(\vec{r}, \vec{r}') \rightarrow f/V \quad \text{as } |\vec{r} - \vec{r}'| \rightarrow \infty$$

(A.3)

An explicit link between the order parameter and the conditional wavefunction, defined in sections 4 and 5 is given by equations 4.4, 4.5 and A.1,

$$\langle \psi^*(\vec{r}) \rangle \langle \psi(\vec{r}') \rangle = \sum_i B_i \int |\bar{\psi}_i(\vec{s})|^2 P(\vec{s}) d\vec{s} = \frac{f}{V} \quad \text{as } |\vec{r} - \vec{r}'| \rightarrow \infty$$

(A.4)

i.e. in a system with zero net momentum, the order parameter is the r.m.s. value of $\bar{\psi}_i(\bar{s})$ averaged over all configurations $\bar{s}$ and thermally occupied eigenstates i . As shown in section 4, $\bar{\psi}_i(\bar{s})$ is non zero only when the many particle wavefunction contains long range spatial structure. Thus a non-zero order parameter implies long range structure in the many particle wavefunction and hence irrotational flow.

The physical origin of ODLRO in liquid helium can be illustrated using the model of section 5. The model CW has uniform amplitude within the occupied volume fV and is zero elsewhere. Hence for normalisation (equation 3.6), $\psi_i(\vec{r}|\bar{s})$ must have amplitude $1/\sqrt{fV}$, where it is non-zero. If we consider an arbitrary point within the fluid, the probability that the point is occupied by the CW is f . If we consider a second point, displaced from the first by a distance $\vec{r} - \vec{r}'$, then the probability that this point is occupied is also f , providing that $|\vec{r} - \vec{r}'|$ is greater than $2R$. The average over all possible positions $\bar{s}$ of the product $\psi_i(\vec{r}|\bar{s})\psi_i^*(\vec{r}'|\bar{s})$ is therefore $f^2[1/\sqrt{fV}]^2 = f/V$, if $|\vec{r} - \vec{r}'| > 2R$, in agreement with equation A.4.

Figure1

A schematic illustration of the conditional wavefunction (CW) for the model of section 5. The black circles are $N-1$ particles of radius R positioned at arbitrary points $\bar{s}$ within the sample volume. The white circles are exclusion regions of radius $2R$. The centre of another particle could not be placed in the white or black circles without hard core overlap. $\psi_0(\vec{r}|\bar{s})$ is constant within the grey region, i.e. it occupies every part of the sample volume from which it is not excluded by hard core overlap with other atoms.

¹ F. London, Nature **141** 643 (1938)

² O. Penrose and L. Onsager Phys Rev **104** 576 (1956)

-
- ³ W. L. Macmillan Phys Rev **A138**, 442 (1965) . See E. Manoukis in "Momentum Distributions", ed P.E. Sokol and R.N. Silver (Plenum Press, New York 1989) for a recent review of variational calculations in ^4He .
- ⁴ D.M Ceperly and E. L. Pollock Phys Rev Lett **56** 351 (1986), E.L. Pollock and D.M. Ceperly, Phys Rev B **36** 8343 (1987).
- ⁵ D.M Ceperly Rev. Mod. Phys. **67** 279 (1995)
- ⁶ V.F. Sears Phys Rev B **28** 5109 (1983)
- ⁷ T. R. Sosnick, W.M. Snow and P.E. Sokol Phys Rev B **41** 11185 (1990)
- ⁸ P.E. Sokol "Bose Einstein Condensation", ed A. Griffin and D.W. Snoke (Cambridge University Press, 1995)
- ⁹ D.R. Tilley and J. Tilley "Superfluidity and Superconductivity" (Adam Hilger, New York, 1990)
- ¹⁰ L.D. Landau J. Phys. Moscow **5** 71 (1941), J. Phys. Moscow **11** 91
- ¹¹ R.P Feynmann Phys Rev **91** 1291 (1953), **91** 1301 (1953), **94** 262 (1954)
- ¹² N.N. Bogoliobov J Phys Moscow **11** 23 (1947)
- ¹³ P.C. Hohenberg and P.C. Martin Ann. Phys. **34** 291 (1965).
- ¹⁴ S.T. Belaviev Sov Phys JETP **7** 289 (1959)
- ¹⁵ P.W. Anderson Rev Mod Phys **38** 298 (1966) .
- ¹⁶ S. K. Ma, H. Gould and V. K. Wong, Phys Rev A **3** 1453 (1971)
- ¹⁷ V. K. Wong and H. Gould Ann. Phys **83** 252 (1974), Phys Rev B **14** 3961 (1976)
- ¹⁸ A. Griffin and T. Cheung Phys Rev A **7** 2086 (1973)
- ¹⁹ P. Szepfalusy and I. Kondor, Ann. Phys. **82** 1
- ²⁰ A. Griffin "Excitations in a Bose Condensed Liquid" (Cambridge University Press, 1993) and references therein.

-
- ²¹ H.R. Glyde " Excitations in Liquid and Solid Helium", (Oxford University Press,1994)
- ²² See for example L. E. Ballantine " Quantum Mechanics ", (Prentice Hall, London, 1979), Chapters 1 and 5.
- ²³ L. D. Landau and E.M. Lifshitz, " Statistical Physics", 3rd Edition, (Pergamon Press 1978), pages192-197.
- ²⁴ E Merzbacher, "Quantum Mechanics", (John Wiley and Sons,1970), Section 8.1.
- ²⁵ P. Nozieres and D. Pines " Theory of Quantum Fluids, Vol II", (Addison-Wesley, 1990), Chapter 4, P50, " the neatest way of characterising superfluidity is in terms of irrotational flow, rather than by the absence of resistance".
- ²⁶ See for example K.Huang, " Statistical Mechanics", (John Wiley and Sons, New York, 1987), Chapters 12 and 13 and Appendix A.
- ²⁷ D.C. Champeney "Fourier Transforms and their Physical Applications", (Academic Press, 1973), section 7.3and Appendix L.
- ²⁸ W. M. Snow, Y. Yang and P. E. Sokol, Europhys Lett **19** 403 (1992) and references therein.
- ²⁹ J. H. Root and E. C. Svensson Physica B **169** 505 (1991)
- ³⁰ J. Mayers to be published