



Temperature Dependence of the Physical Properties of Bose-Einstein Condensed Gases and Liquids

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Temperature dependence of the physical properties of Bose-Einstein condensed gases and liquids

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Abstract

Gases and liquids in the presence of Bose-Einstein condensation (BEC) have unique and very striking macroscopic physical properties. For example they exhibit flow without viscosity, quantised vortices and two-fluid behaviour. Macroscopic quantum interference effects in the form of density oscillations are observed when two or more clouds of ultra-cold Bose-Einstein condensed atoms overlap. The microscopic properties of Bose-Einstein condensed liquid ^4He are also uniquely anomalous, and unexplained. Neutron and X-ray scattering measurements show that liquid ^4He in its superfluid phase is the only known liquid in which pair correlations between atomic positions decrease upon cooling. The liquid also shows an anomalous thermal expansion upon cooling. Inelastic neutron scattering shows that it is also the only known liquid which has sharp peaks in its dynamic structure factor. It is shown here that all the above phenomena can be explained in a physically transparent and quantitative way by two simply stated postulates. The first is that in the presence of BEC at finite temperature, the many particle wave functions of occupied states can be written as the sum of a component which is localized in coordinate space and a component which is delocalized. The second is that the delocalized component is identical to the ground state wave function. It is argued that these postulates are in fact forced by basic quantum mechanics, existing theoretical treatments of BEC and a wide range of experimental measurements of Bose-Einstein condensed liquid ^4He .

1. Introduction

Experiment shows that in the presence of Bose-Einstein condensation (BEC), ultra-cold gases and liquid ^4He have uniquely anomalous physical properties. For example liquid ^4He flows without viscosity [1] and exhibits quantised vortices [2]. Quantised vortices are also observed in ultra-cold gases [3,4]. Macroscopic density oscillations are observed when two or more Bose-Einstein condensed clouds of atoms overlap [5]. It is widely accepted that these phenomena are due to the fact that BEC implies macroscopic single particle quantum behaviour (MSPQB) – that is in the presence of BEC every particle behaves as if it occupies the same single particle quantum state, with a single particle wave function which is non-zero over macroscopic length scales.

It was shown in a previous paper [6] that in gases and liquids at zero temperature, MSPQB is a necessary consequence of BEC. This paper considers the behavior of gases and liquids in the presence of BEC at finite temperature. The best known finite temperature effect associated with BEC is "two fluid" behaviour. Bose-Einstein condensed liquid ^4He behaves as if it were two fluids, "freely intermingling, with no viscous interaction"[1]. As is well known the "superfluid" component has zero entropy and no viscosity, whereas the "normal" fluid has entropy and behaves viscously. As the temperature is raised the superfluid fraction diminishes, vanishing at the condensation temperature T_C . Although two-fluid behaviour has yet to be observed in Bose-Einstein condensed gases, it is generally accepted on theoretical grounds [7] that it must also occur in weakly interacting systems.

Many other fundamental experimental properties of liquid ^4He in the presence of BEC are both highly anomalous and unexplained. For example neutron [8] and X-ray [9] measurements show that ^4He in its superfluid phase is the only known liquid in which pair correlations between atomic positions reduce as the liquid is cooled. The liquid also undergoes an anomalous thermal expansion as it is cooled [10]. It is also the only known liquid which has very narrow peaks in its dynamic structure factor, measured by inelastic neutron scattering. [11, 12,13]. The highest resolution measurements [14] show that these peaks have apparently zero widths as $T \rightarrow 0$. In

all other liquids such peaks have widths in wave vector transfer of $\Delta q \sim 1/a$ where a is the average nearest-neighbour distance between atoms.

It is shown in this paper that all these phenomena can be explained quantitatively by two simply stated postulates. The first is that at finite T in the presence of BEC, the many particle Schrödinger wave functions of occupied states are a superposition of a component which is delocalized in coordinate space and a component which is localized. The second postulate is that the delocalized component is identical to the ground state wave function. It is argued that these postulates are in fact forced by basic quantum mechanics, existing theory of BEC and a wide range of experimental data on liquid ^4He .

In section 2 the terms "delocalization" and "localization" of the many particle wave function Ψ are given a precise definition. The "conditional wave function" is also defined in terms of Ψ . Section 3 summarizes previously obtained [6] results at zero temperature. In section 4 it is shown that as the temperature is raised in the presence of BEC, the many particle wave functions of occupied states must change from delocalized functions at zero temperature to localized functions as T approaches the transition temperature. Section 5 presents the two basic postulates as to how this change occurs. Sections 6 and 7 derive the physical consequences of these postulates and show that these consequences agree quantitatively with measurements. In section 8 it is argued that the two postulates are forced by extensive experimental data on liquid ^4He and by generally accepted theoretical treatments of BEC.

2. Definitions

2a. Localization and delocalization of the wave function

We consider the Schrödinger wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N)$ of a system of N identical Bose particles, contained within a volume $V \propto N$. Denoting one of the particle coordinates as \mathbf{r} and

the other $N - 1$ coordinates as \mathbf{s} , the wave function is written as $\Psi(\mathbf{r}, \mathbf{s})$. The wave function $\Psi(\mathbf{r}, \mathbf{s})$ is defined as;

"delocalized" if for every \mathbf{s} that occurs [15], the function $\Psi(\mathbf{r}, \mathbf{s})$ is a non-zero function of \mathbf{r} over a volume $\sim V$ containing $\sim N$ atoms.

"Localized" if for every \mathbf{s} that occurs [15], the function $\Psi(\mathbf{r}, \mathbf{s})$ is a non-zero function of \mathbf{r} only over a volume $\sim V / N$ containing ~ 1 atoms.

In any Bose system of identical particles $\Psi(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N)$ is unchanged under interchange of particle coordinates. Hence if Ψ is delocalized (localized) in any single coordinate \mathbf{r} it must be delocalized (localized) in all coordinates. The difference between localized and delocalized forms of $\Psi(\mathbf{r}, \mathbf{s})$ is illustrated schematically in Figure 1.

2b The conditional wave function

According to its standard physical interpretation, $|\Psi(\mathbf{r}, \mathbf{s})|^2$ is the probability distribution function (pdf) for the N coordinates \mathbf{r}, \mathbf{s} . Hence Ψ must be normalized

$$\int |\Psi(\mathbf{r}, \mathbf{s})|^2 d\mathbf{r} d\mathbf{s} = 1 \quad (2.1)$$

It is convenient to define the "conditional wave function" (CWF) $\psi_{\mathbf{s}}(\mathbf{r})$ [16] as

$$\psi_{\mathbf{s}}(\mathbf{r}) = \Psi(\mathbf{r}, \mathbf{s}) / \sqrt{P(\mathbf{s})} \quad (2.2)$$

where

$$P(\mathbf{s}) = \int |\Psi(\mathbf{r}, \mathbf{s})|^2 d\mathbf{r} \quad (2.3)$$

is the pdf for \mathbf{s} . The coordinates \mathbf{s} are included as a subscript in $\psi_{\mathbf{s}}(\mathbf{r})$ to emphasize that

wherever $\psi_{\mathbf{s}}(\mathbf{r})$ is used we consider its \mathbf{r} dependence at a given \mathbf{s} . If $\Psi(\mathbf{r}, \mathbf{s})$ is delocalized,

$\psi_{\mathbf{s}}(\mathbf{r})$ must be a non-zero function of \mathbf{r} over a macroscopic volume $\sim V$. If $\Psi(\mathbf{r}, \mathbf{s})$ is localized, $\psi_{\mathbf{s}}(\mathbf{r})$ is a non-zero function of \mathbf{r} only over a microscopic region of volume $\sim V/N$. Localized and delocalized forms of $\psi_{\mathbf{s}}(\mathbf{r})$ are also illustrated in Figure 1.

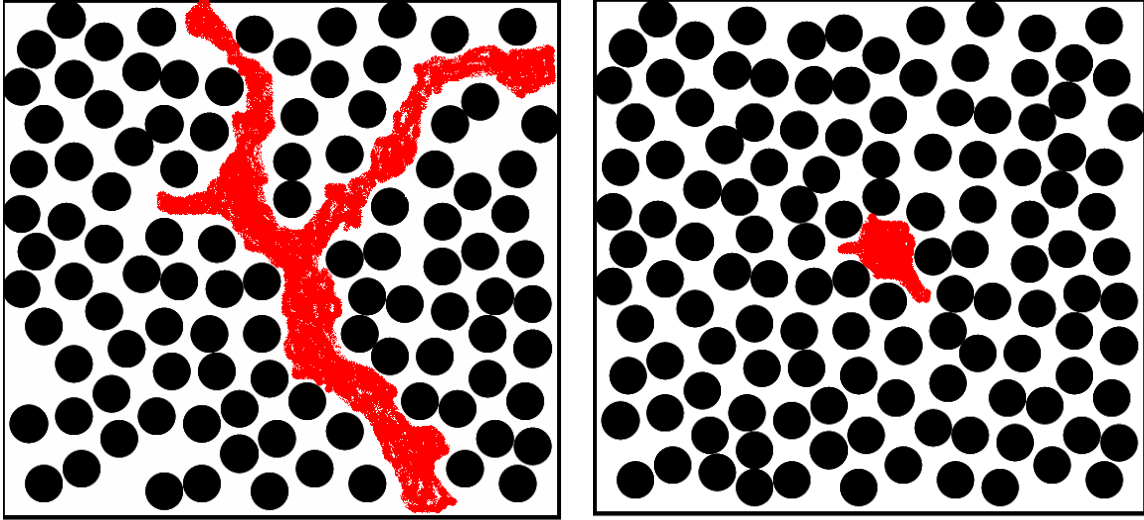


Figure 1. The left hand figure illustrates a delocalized form of $\Psi(\mathbf{r}, \mathbf{s})$ and the right hand figure a localized form. The black circles indicate $N - 1$ atoms at a particular \mathbf{s} , for which $\Psi(\mathbf{r}, \mathbf{s})$ is non-zero. Assuming hard core repulsion between atoms, $\Psi(\mathbf{r}, \mathbf{s})$ must be zero if \mathbf{r} is too close to any of the atoms at \mathbf{s} . Regions of \mathbf{r} for which $\Psi(\mathbf{r}, \mathbf{s}) \neq 0$ are sketched in red. $\Psi(\mathbf{r}, \mathbf{s})$ can be a delocalized function of \mathbf{r} if there is sufficient space in the fluid structure, as illustrated on the left. In the right hand figure $\Psi(\mathbf{r}, \mathbf{s})$ is localized, because there is only a single space which can be occupied without hard-core overlap with atoms at \mathbf{s} . The figure also illustrates the form of the conditional wave function $\psi_{\mathbf{s}}(\mathbf{r})$ in the two cases.

In many respects $\psi_{\mathbf{s}}(\mathbf{r})$ can be treated as a single particle wave function which is conditional upon \mathbf{s} [6]. For example it follows from eqs. (2.1)-(2.3) that $\psi_{\mathbf{s}}(\mathbf{r})$ is a normalized function of \mathbf{r}

$$\int |\psi_{\mathbf{s}}(\mathbf{r})|^2 d\mathbf{r} = 1 \quad (2.4)$$

It also follows from the probability interpretation of $|\Psi(\mathbf{r}, \mathbf{s})|^2$ that $|\psi_{\mathbf{s}}(\mathbf{r})|^2$ is the conditional pdf for coordinate \mathbf{r} , given \mathbf{s} . It is shown in section 6 and ref [6] that the conditional density, momentum distribution, flow, total kinetic energy and total potential energies can similarly be expressed in terms of standard single particle expressions, with $\psi_{\mathbf{s}}(\mathbf{r})$ replacing the single particle wave function. The measurable values of these quantities are obtained from an average over \mathbf{s} , weighted by $P(\mathbf{s})$.

3. Zero Temperature

This paper considers only physical properties which are averages over a region of space containing $N_{\Omega} \gg 1$ atoms. It was shown in [6] that for the calculation of such properties, the ground state Schrödinger wave function $\Psi_0(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N)$ in the presence of BEC can be approximately factorized into a single particle product.

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \cong \prod_{n=1}^N \eta_0(\mathbf{r}_n) \quad (3.1)$$

where

$$|\eta_0(\mathbf{r})|^2 = \bar{\rho}_0(\mathbf{r}) \quad (3.2)$$

and $N\bar{\rho}_0(\mathbf{r})$ is the macroscopic particle density at $T = 0$. The symbol \cong means equal to within terms $\sim 1/\sqrt{N_{\Omega}}$.

It was also shown in [6] that, to within terms $\sim 1/\sqrt{N_{\Omega}}$, the time dependence of $\eta_0(\mathbf{r})$ is given by the single particle Schrödinger equation,

$$\frac{\hbar^2}{2m} \frac{\partial^2 \eta_0(\mathbf{r}, t)}{\partial \mathbf{r}^2} + V_{eff}(\mathbf{r}, t) \eta_0(\mathbf{r}, t) + \Xi(\mathbf{r}) \eta_0(\mathbf{r}, t) \cong i\hbar \frac{\partial}{\partial t} \eta_0(\mathbf{r}, t) \quad (3.3)$$

where m is the atomic mass, $\Xi(\mathbf{r})$ is an externally applied potential and $V_{eff}(\mathbf{r}, t)$ is an effective single particle potential, equal to the ground state energy per atom at the local density $\rho_0(\mathbf{r}, t)$.

It was shown in [6] that at $T = 0$, eqs (3.1)-(3.3) are a necessary consequence of two properties of liquids and gases in the presence of BEC;

- (a) BEC implies that the many particle ground state wave function is delocalized, in the sense defined in section 2. Hence integrals of the ground state CWF $\psi_{0S}(\mathbf{r})$ are possible over macroscopic regions of \mathbf{r} space containing $N_{\Omega} \gg 1$ atoms.
- (b) In liquids and gases there are by definition no long range correlations between particle positions. This leads to randomness in the \mathbf{r} dependence of $\psi_{0S}(\mathbf{r})$ (see Figure 1). The central limit theorem then implies that the integral of any functional of $\psi_{0S}(\mathbf{r})$ over a region containing $\sim N_{\Omega}$ atoms [6] is precisely defined to within terms $\sim 1/\sqrt{N_{\Omega}}$. Eqs (3.1) -(3.3) are thus accurate only when $N_{\Omega} \gg 1$. For example they accurately describe the t and \mathbf{r} dependence of the fluid density $\rho_0(\mathbf{r}, t)$ over macroscopic length scales, but are not accurate over length scales comparable to the separation between atoms [17].

It follows from eq (3.2) that $\eta_0(\mathbf{r})$ is non-zero wherever the fluid density is non-zero. Thus if N is sufficiently large, η_0 is a non-zero function of \mathbf{r} over macroscopic length scales. Hence eqs (3.1)-(3.3) imply the presence of macroscopic single particle quantum behavior; for example superfluid flow, quantized vortices and interference fringes between overlapping condensates (see section 7).

4. Finite Temperature

At zero temperature only the ground state is occupied and the system has the unique wave function $\Psi_0(\mathbf{r}, \mathbf{s})$. In contrast, if the number of atoms is large, a vast number of different N particle states can be occupied at finite T . As is well known, measurable physical properties are

obtained by performing a thermal average over these occupied states. For example the total energy at temperature T is

$$U(T) = \sum_i B_i(T) E_i \quad (4.1)$$

where $B_i(T)$ is the Boltzmann probability that state i is occupied and

$$E_i = \int \Psi_i^*(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N) \hat{H} \Psi_i(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N) d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_N \quad (4.2)$$

is the energy of state i , where \hat{H} is the N particle Hamiltonian operator and Ψ_i is the wave function of state i .

As the temperature is changed different N particle states will be populated and the properties of the wave functions Ψ_i of these states will therefore change, as is implicit in eqs (4.1) and (4.2).

In particular the localisation properties must change with temperature. It was shown in [6] that at $T = 0$ the wave function must be delocalized in the presence of BEC. It was also shown in [6] that if the wave function is delocalized, MSPQB must occur, in the precise sense that eqs (3.1)-(3.3) are satisfied over macroscopic length scales. Extensive experimental data and the existing theory of BEC both demonstrate that MSPQB does not occur for $T \geq T_C$. Hence wave functions of occupied states cannot be delocalized at $T = T_C$. It follows that wave functions of occupied states must change from delocalized to localized functions as the temperature is raised from zero to T_C .

5. Basic Postulate

In the rest of the paper we consider one of the states i which can be occupied at a given T . All the results obtained can be trivially generalized to measurable properties, by summing over occupied states as in (4.1). To simplify notation the subscript i is dropped and the wave function of this "typical" state is denoted as $\Psi(\mathbf{r}, \mathbf{s})$ [18].

The basic postulate of this paper is that the necessary change in Ψ from delocalization to localization as T is raised in the presence of BEC occurs in the following way. In the presence of BEC at temperature T , the wave function $\Psi(\mathbf{s}, \mathbf{r})$ of a typical occupied state has the form [19]

$$\Psi(\mathbf{s}, \mathbf{r}) = \alpha(T)\Psi_D(\mathbf{s}, \mathbf{r}) + \beta(T)\Psi_L(\mathbf{s}, \mathbf{r}) \quad (5.1)$$

where,

- (1) $\Psi_D(\mathbf{s}, \mathbf{r})$ is a delocalized function of all coordinates, $\Psi_L(\mathbf{s}, \mathbf{r})$ is a localized function.
- (2) $\Psi(\mathbf{s}, \mathbf{r})$, $\Psi_D(\mathbf{s}, \mathbf{r})$ and $\Psi_L(\mathbf{s}, \mathbf{r})$ are all normalized and Bose symmetric under interchange of particle coordinates.
- (3) As the temperature is raised, $\alpha(T)$ decreases from unity at $T = 0$ to zero at $T = T_C$.

A subsidiary postulate is that the delocalized component is identical to the ground state wave function.

$$\Psi_D(\mathbf{s}, \mathbf{r}) = \Psi_0(\mathbf{s}, \mathbf{r}) \quad (5.2)$$

For a wave function of the form in eq (5.1), it follows straightforwardly that the CWF can be split into a component $\psi_{DS}(\mathbf{r})$ which is delocalized in \mathbf{r} and a component $\psi_{LS}(\mathbf{r})$ which is localized.

$$\psi_S(\mathbf{r}) = a_S(T)\psi_{DS}(\mathbf{r}) + b_S(T)\psi_{LS}(\mathbf{r}) \quad (5.3)$$

$\psi_{DS}(\mathbf{r})$ and $\psi_{LS}(\mathbf{r})$ are defined in terms of $\Psi_D(\mathbf{s}, \mathbf{r})$ and $\Psi_L(\mathbf{s}, \mathbf{r})$ in an analogous way to eqs (2.2) and (2.3). Eq (5.2) implies that $\psi_{DS}(\mathbf{r})$ is identical to the CWF of the ground state.

$$\psi_{DS}(\mathbf{r}) = \psi_{0S}(\mathbf{r}) \quad (5.4)$$

Equations (5.3) and (5.4) are similar to the postulate adopted in previous work [20,21]. The only difference is that $\psi_{LS}(\mathbf{r})$ is here assumed to be localized whereas previously the function $\psi_{LS}(\mathbf{r})$ was assumed to be delocalized in \mathbf{r} , but with phase correlations only over distances $\sim (V/N)^{1/3}$. It is now clear that the latter assumption cannot be correct. The basic condition

that must be satisfied for MSPQB to occur (eq 6.4 of ref [6]) is that the integral of $|\psi_{\mathbf{s}}(\mathbf{r})|^2$ over a volume containing N_{Ω} atoms, is the same for all \mathbf{s} that occur [15] to within terms $\sim 1/\sqrt{N_{\Omega}}$. Clearly the phase of $\psi_{\mathbf{s}}(\mathbf{r})$ has no bearing upon whether or not this condition is satisfied. It was shown in [6] that all that is required in any liquid or gas, is that $\psi_{\mathbf{s}}(\mathbf{r})$ is a delocalized function of \mathbf{r} . If $\psi_{L\mathbf{s}}(\mathbf{r})$ is delocalized and phase incoherent, eq (5.3) implies that MSPQB will still occur at $T = T_C$.

Since existing theory and a wide range of experimental data show that MSPQB does not occur at $T = T_C$, $\psi_{L\mathbf{s}}(\mathbf{r})$ must be a localized function of \mathbf{r} . In fact this follows from more general arguments. If $\psi_{L\mathbf{s}}(\mathbf{r})$ is delocalized for any \mathbf{s} that occurs [15], it is easily shown that the requirement that $\Psi(\mathbf{r}, \mathbf{s})$ is single valued implies quantization of angular momentum over macroscopic length scales - that is MSPQB. Hence $\psi_{L\mathbf{s}}(\mathbf{r})$ must be a localized function of \mathbf{r} for all \mathbf{s} that occur. It will be shown in the following section that all the results obtained in [20,21] are equally valid if $\psi_{L\mathbf{s}}(\mathbf{r})$ is localized, rather than delocalized and phase incoherent.

6. Physical consequences of the basic Postulates.

6a. Two fluid behavior

It follows from standard results of quantum mechanics and the definition of $\psi_{\mathbf{s}}(\mathbf{r})$ in eqs (2.2)-(2.3), that the particle density $\rho(\mathbf{r})$ is [6]

$$\rho(\mathbf{r}) = N \int |\psi_{\mathbf{s}}(\mathbf{r})|^2 P(\mathbf{s}) d\mathbf{s} \quad (6.1)$$

The macroscopic particle density $\bar{\rho}(\mathbf{r})$ is defined as a "coarse grained average" [6] of $\rho(\mathbf{r})$ over a region $\Omega(\mathbf{r})$, centered at \mathbf{r} , of volume Ω and containing $N_{\Omega} \gg 1$ particles.

$$\bar{\rho}(\mathbf{r}) = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} \rho(\mathbf{r}') d\mathbf{r}' = N \int P(\mathbf{s}) d\mathbf{s} \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} |\psi_{\mathbf{s}}(\mathbf{r}')|^2 d\mathbf{r}' \quad (6.2)$$

It follows from eq. (5.3) that

$$\int_{\Omega(\mathbf{r})} |\psi_S(\mathbf{r}')|^2 d\mathbf{r}' = |a_S|^2 \int_{\Omega(\mathbf{r})} |\psi_{0S}(\mathbf{r}')|^2 d\mathbf{r}' + |b_S|^2 \int_{\Omega(\mathbf{r})} |\psi_{LS}(\mathbf{r}')|^2 d\mathbf{r}' + CT \quad (6.3)$$

where the "cross-terms" have the form

$$CT = a_S^* b_S \int_{\Omega(\mathbf{r})} \psi_{0S}^*(\mathbf{r}') \psi_{LS}(\mathbf{r}') d\mathbf{r}' + CC \quad (6.4)$$

The functions $\psi_{0S}(\mathbf{r})$ and $\psi_{LS}(\mathbf{r})$ have very different amplitudes, as illustrated schematically in

Figure 2a. This must be the case, since both are normalized functions of \mathbf{r} , but while $\psi_{0S}(\mathbf{r})$ is

non-zero over a volume $\sim V \propto N$, $\psi_{LS}(\mathbf{r})$ is non zero only within a volume $\sim V/N$. Hence

$$|\psi_{0S}(\mathbf{r})| \sim 1/\sqrt{V} \quad (6.5)$$

whereas

$$|\psi_{LS}(\mathbf{r})| \sim \sqrt{N/V} \quad (6.6)$$

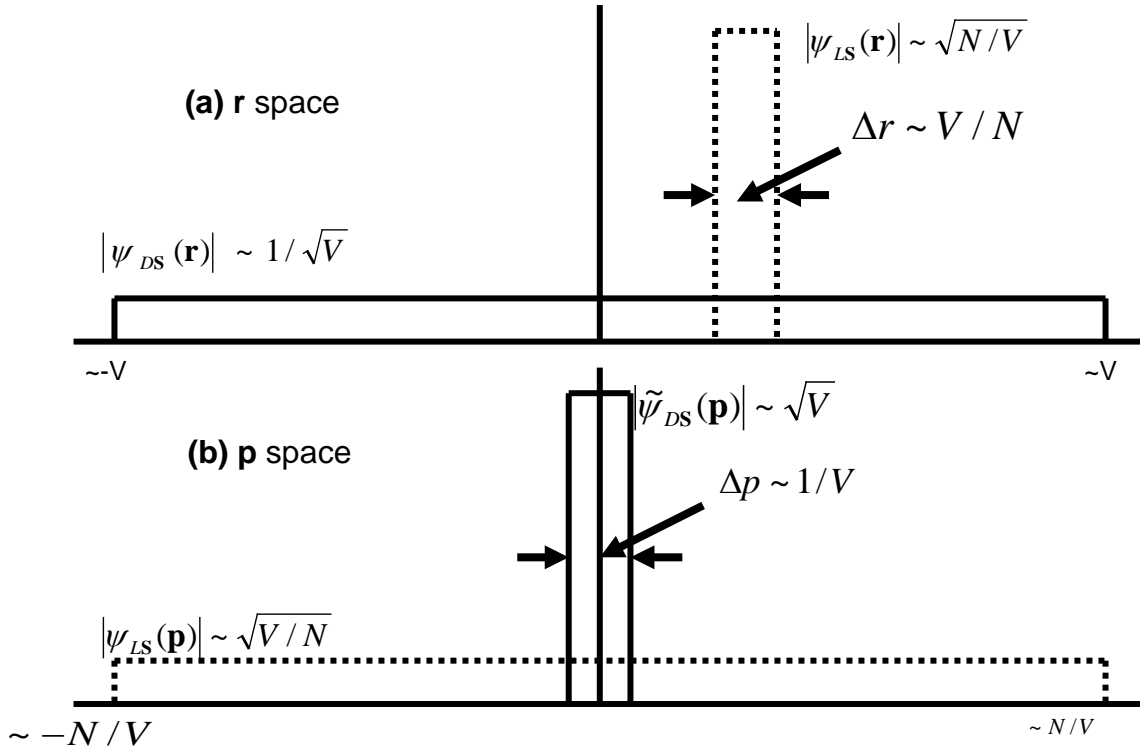


Figure 2 shows schematically the relationship between the amplitudes of localized and delocalized components of ψ_s in position (\mathbf{r}) space and momentum (\mathbf{p}) space. ψ_D and ψ_L are normalized in both \mathbf{r} and \mathbf{p} whereas the integrated product $|\psi_D||\psi_L|$ is $\sim 1/\sqrt{N}$ in both \mathbf{r} and \mathbf{p} space.

In the calculation of the terms in eq (6.3) there are two possibilities;

(i) $\psi_{LS}(\mathbf{r})$ is localized within the integration volume $\Omega(\mathbf{r})$. It then follows from eqs (6.5) and (6.6) that the cross-terms (6.4) are $\sim 1/\sqrt{N}$ compared with the contribution of the second term on the right in eq (6.3).

(ii) $\psi_{LS}(\mathbf{r})$ is localized outside the volume Ω . In this case only the first term on the right in eq (6.3) is non-zero.

In either case the contribution of the cross-terms in (6.3) is at most $\sim 1/\sqrt{N}$ compared to the sum of the other terms. This is intuitively obvious from consideration of Fig 2a.

Hence to within terms $\sim 1/\sqrt{N}$,

$$\bar{\rho}(\mathbf{r}) = \bar{\rho}_0(\mathbf{r}) + \bar{\rho}_L(\mathbf{r}) \quad (6.7)$$

where

$$\bar{\rho}_0(\mathbf{r}) = \int P(\mathbf{s}) d\mathbf{s} |a_s|^2 \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} |\psi_{0s}(\mathbf{r}')|^2 d\mathbf{r}' \quad (6.8)$$

with a similar expression for $\bar{\rho}_L(\mathbf{r})$.

Similar arguments can be applied to the fluid flow. This can be expressed in the form [6]

$$\mathbf{F}(\mathbf{r}) = \int P(\mathbf{s}) \frac{\hbar}{m} |\psi_s(\mathbf{r})|^2 \nabla \theta_s(\mathbf{r}) d\mathbf{s} \quad (6.9)$$

where θ_s is the phase of ψ_s . It follows from almost identical arguments to those used in the

derivation of eq (6.7) that, to within terms $\sim 1/\sqrt{N}$, $\mathbf{F}(\mathbf{r})$ also separates into two components.

$$\bar{\mathbf{F}}(\mathbf{r}) = \bar{\mathbf{F}}_0(\mathbf{r}) + \bar{\mathbf{F}}_L(\mathbf{r}) \quad (6.10)$$

Furthermore, by the arguments given in [6] and summarized in section 3, the flow $\bar{\mathbf{F}}_0$ of the delocalized component must exhibit MSPQB. There is no such requirement for the flow $\bar{\mathbf{F}}_L$ of the localized component.

It is clear that the delocalized component can be identified with the superfluid in the two-fluid model and the localized component with the normal fluid. Evidently the superfluid fraction is

$$w_D(T) = |\alpha(T)|^2 \quad (6.11)$$

and the normal fluid fraction is

$$w_L(T) = |\beta(T)|^2 \quad (6.12)$$

where $\alpha(T)$ and $\beta(T)$ are the amplitudes in eq (5.1).

6b. Thermodynamic Properties

The consequences of eq (5.1) are in fact much wider than two-fluid behavior. The very different amplitudes and regions of coordinate space occupied by Ψ_D and Ψ_L , imply that all overlap integrals between Ψ_D and Ψ_L , in the calculation of any physical quantity, are at most $\sim 1/\sqrt{N}$ compared to other terms. Hence the delocalized (superfluid) and localized (normal fluid) components of the wave function contribute independently to all physical properties, in the limit $N \rightarrow \infty$. For example the energy density at \mathbf{r} can be expressed as [6]

$$E(\mathbf{r}) = N \int P(\mathbf{s}) E_s(\mathbf{r}) d\mathbf{s} \quad (6.13)$$

where the conditional energy density is

$$E_s(\mathbf{r}) = \kappa_s(\mathbf{r}) + v_s(\mathbf{r}) \quad (6.14)$$

The conditional kinetic energy density is [6]

$$\kappa_s(\mathbf{r}) = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} \psi_s^*(\mathbf{r}') \frac{-\hbar^2}{2m} \frac{\partial^2 \psi_s(\mathbf{r}')}{\partial \mathbf{r}'^2} d\mathbf{r}' \quad (6.15)$$

and the conditional potential energy density is

$$v_s(\mathbf{r}) = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} V_s(\mathbf{r}') |\psi_s(\mathbf{r}')|^2 d\mathbf{r}' \quad (6.16)$$

where $V_s(\mathbf{r}')$ is the potential energy of interaction of a particle at \mathbf{r}' with the other $N - 1$ particles at \mathbf{s} .

It follows from similar arguments to those used in the derivation of eq. (6.7) that to within terms $\sim 1/\sqrt{N}$, $\kappa_s(\mathbf{r})$ and $v_s(\mathbf{r})$ and hence $E_s(\mathbf{r})$ divide into independent contributions from the localized and delocalized components of $\psi_s(\mathbf{r})$. Hence

$$E_s(\mathbf{r}) = a_s E_{0s}(\mathbf{r}) + b_s E_{Ls}(\mathbf{r}) \quad (6.17)$$

It follows from (6.13) and (6.17) that to within terms $\sim 1/\sqrt{N}$ the two components contribute separately to the total energy density of the fluid.

$$E(\mathbf{r}) = w_D E_0(\mathbf{r}) + W_L E_L(\mathbf{r}) \quad (6.18)$$

Eq (6.18) implies [20,21] that all thermodynamic properties are the sum of two independent contributions from the superfluid and the normal fluid.

Eq (6.18) provides a simple physical explanation of the anomalous thermal expansion of superfluid ^4He upon cooling [10]. Eq (6.18) implies that the pressure exerted by the fluid is the sum of separate contributions from the two components. The superfluid exerts more pressure than the normal fluid. Hence as the liquid cools and the superfluid fraction increases, the liquid expands. It was shown in refs [20,21] that this reasoning gives quantitative agreement with measurements on superfluid ^4He .

6c. The momentum distribution.

The momentum distribution $n(\mathbf{p})$ of the atoms can be expressed in the form [6]

$$n(\mathbf{p}) = \int P(\mathbf{s}) n_s(\mathbf{p}) d\mathbf{s} \quad (6.19)$$

where

$$n_s(\mathbf{p}) = \frac{1}{\hbar^3} |\tilde{\psi}_s(\mathbf{p})|^2 \quad (6.20)$$

and

$$\tilde{\psi}_s(\mathbf{p}) = \int \psi_s(\mathbf{r}) \exp(i\mathbf{p}\cdot\mathbf{r} / \hbar^3) d\mathbf{r} \quad (6.21)$$

Substituting eq. (5.3) and (5.4) gives

$$\tilde{\psi}_s(\mathbf{p}) = a_s \tilde{\psi}_{0s}(\mathbf{p}) + b_s \tilde{\psi}_{LS}(\mathbf{p}) \quad (6.22)$$

where $\tilde{\psi}_{0s}(\mathbf{p})$ and $\tilde{\psi}_{LS}(\mathbf{p})$ are defined in a similar way to eq. (6.21) . Hence

$$n_s(\mathbf{p}) = |a_s|^2 |\tilde{\psi}_{0s}(\mathbf{p})|^2 + |b_s|^2 |\tilde{\psi}_{LS}(\mathbf{p})|^2 + CT_p \quad (6.23)$$

where the "cross-terms" are

$$CT_p = a_s^* b_s \tilde{\psi}_{0s}^*(\mathbf{p}) \tilde{\psi}_{LS}(\mathbf{p}) + a_s b_s^* \tilde{\psi}_{0s}(\mathbf{p}) \tilde{\psi}_{LS}^*(\mathbf{p}) \quad (6.24)$$

It follows from Parseval's theorem for Fourier transforms that if the cross-terms CT in eq (6.3)

are $\sim 1/\sqrt{N}$, the cross-terms CT_p in eq (6.23) must also be $\sim 1/\sqrt{N}$. Hence to within terms

$\sim 1/\sqrt{N}$,

$$n_s(\mathbf{p}) = |a_{DS}|^2 |\tilde{\psi}_{0s}(\mathbf{p})|^2 + |a_{LS}|^2 |\tilde{\psi}_{LS}(\mathbf{p})|^2 \quad (6.25)$$

It follows from eqs (6.25) and (6.19) that the two components contribute separately to the measured momentum distribution. This is also intuitively obvious from consideration of Figure 2,

which demonstrates that the integral of $|\psi_D \psi_L|$ is $\sim 1/\sqrt{N}$ compared with the integrals of

$|\psi_D|^2$ and $|\psi_L|^2$ in both \mathbf{r} and \mathbf{p} space.

6d The condensate fraction and the superfluid fraction

In the presence of BEC at $T = 0$, a fraction $f_0 \sim 1$, of the weight of the distribution $n(\mathbf{p})$ is in

the $\mathbf{p} = 0$ state. Since momentum states have volume in \mathbf{p} space of $\sim \hbar^3 / V$ this implies that

$$|\tilde{\psi}_{0s}(0)| \sim (V / \hbar^3)^{1/2} \quad (6.26)$$

In contrast since $\psi_{LS}(\mathbf{r})$ is localized within a region of volume $\sim V/N$, it follows from standard Fourier transform theory that $\tilde{\psi}_{LS}(\mathbf{p})$ must occupy a volume $\sim \hbar^3 N/V$ in \mathbf{p} space. Hence since $\tilde{\psi}_{LS}(\mathbf{p})$ is normalized in \mathbf{p} space (see Figure 2a),

$$|\tilde{\psi}_{LS}(0)| \sim \left[(V/N\hbar^3) \right]^{1/2} \quad (6.27)$$

Comparing eqs (6.26) and (6.27) $|\tilde{\psi}_{LS}(0)|$ is a factor $\sim 1/\sqrt{N}$ smaller than $|\tilde{\psi}_{0S}(0)|$. Thus to within terms $\sim 1/\sqrt{N}$, only the delocalized component contributes to the zero momentum state. Again this is intuitively obvious from consideration of Figure 2b.

The assumption (5.2) that the delocalized component is identical to the ground state, further implies that the condensate fraction $f(T)$ at finite temperature T , is proportional to the superfluid fraction, with a proportionality constant equal to the condensate fraction at $T = 0$ [19,20]

$$f(T) = w_0(T) f_0 \quad (6.28)$$

It has been shown previously (see Fig 3 of ref [21]) that eq (6.28) is accurately obeyed by state of the art data on the condensate fraction [22] in superfluid ^4He .

6f. Static Structure factor

The contribution of a state with wave function Ψ to the static structure factor $S(\mathbf{q})$ is [23,24].

$$S(\mathbf{q}) = \int |\Psi(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N)|^2 \frac{1}{N} \sum_{n,m} \exp[i\mathbf{q} \cdot (\mathbf{r}_n - \mathbf{r}_m)] d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_N \quad (6.29)$$

It follows by similar arguments to those used in section 6a that, to within terms $\sim 1/\sqrt{N}$, $S(\mathbf{q})$ is the sum of independent contributions from the delocalized and delocalized components of Ψ . Eq (5.2) implies that the structure factor of the delocalized component is identical to the ground state structure factor $S_0(\mathbf{q})$. Hence

$$S(\mathbf{q}) = w_D S_0(\mathbf{q}) + w_L S_L(\mathbf{q}) \quad (6.30)$$

where $S_L(\mathbf{q})$ is the structure factor of the localized component.

Eq (6.30) provides a simple physical explanation of the uniquely anomalous increase in spatial correlations, observed as T is raised in superfluid ^4He . More spaces between atoms are required for the wave function to delocalize, as illustrated in Figure 1. More spaces imply reduced pair correlations between atomic positions. Hence the delocalized (superfluid) component has reduced pair correlations compared with the localized (normal fluid) component. It follows that as T is lowered and the superfluid fraction increases, pair correlations will decrease. It was shown in refs [23,24] that this reasoning is in quantitative agreement with measurements of the static structure factor and the atomic size and the packing density in superfluid ^4He . It would be a remarkable coincidence if this agreement was accidental, since only a $\sim 10\%$ change in the atomic diameter is necessary to remove this agreement [24].

6g. Dynamic Structure factor

The contribution of a state with wave function Ψ to the dynamic structure factor $S(\mathbf{q}, \omega)$ is

$$S(\mathbf{q}, \omega) = \sum_f |A_f|^2 \delta(\hbar\omega + E_f - E) \quad (6.31)$$

where

$$A_f(\mathbf{q}) = \int \Psi^*(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N) \sum_n \exp(i\mathbf{q}\mathbf{r}_n) \Psi_f(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N) d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_N \quad (6.32)$$

The sum in (6.31) is over all final states of energy E_f , E is the energy of the state with wave function Ψ , $\hbar\omega$ is the energy transfer and \mathbf{q} is the wave vector transfer. Due to the Bose symmetry of the wave function, every n makes the same contribution to A_f which can therefore be written in the form [25]

$$A_f(\mathbf{q}) = N \int \Psi^*(\mathbf{r}, \mathbf{s}) \exp(i\mathbf{q}\mathbf{r}) \Psi_f(\mathbf{r}, \mathbf{s}) d\mathbf{r} d\mathbf{s} \quad (6.33)$$

It follows from eq (5.1) that there are two contributions to A_f , that from the localized component of the wave function

$$A_{Lf}(\mathbf{q}) = N \int \Psi_L^*(\mathbf{r}, \mathbf{s}) \exp(i\mathbf{q} \cdot \mathbf{r}) \Psi_f(\mathbf{r}, \mathbf{s}) d\mathbf{r} d\mathbf{s} \quad (6.34)$$

and that from the delocalized component, $A_{Df}(\mathbf{q})$, defined in an analogous way to eq (6.34).

Furthermore since $\Psi_L(\mathbf{r}, \mathbf{s})$ is a localized function of \mathbf{r} , non zero only within a region of dimension $a \sim (V/N)^{1/3}$, it follows from eq (6.33) and elementary Fourier transform theory that the contribution to $A_{Lf}(\mathbf{q})$ must have width in \mathbf{q} of at least $\Delta q \sim 1/a$. In contrast the delocalized component $A_{Df}(\mathbf{q})$ can contain peaks with width in \mathbf{q} , $\Delta q \sim 1/V^{1/3}$. Thus any peaks in $S(\mathbf{q}, \omega)$ with widths $\Delta q \ll 1/a$ must be contributed only by the delocalized component. Eq (5.2) then implies that the intensity of such peaks must be proportional to the weight of the delocalized component - that is to the superfluid fraction. This prediction agrees (within the experimental error of ~2%) with neutron scattering measurements [11,13] of the intensity of such peaks.

7. Interference between Condensates

We consider two clouds of Bose-Einstein condensed gas which are initially confined in a potential which allows a very small overlap between the clouds (See Figure 3). At time $t = 0$, the potential is switched off and the clouds are allowed to expand and overlap.

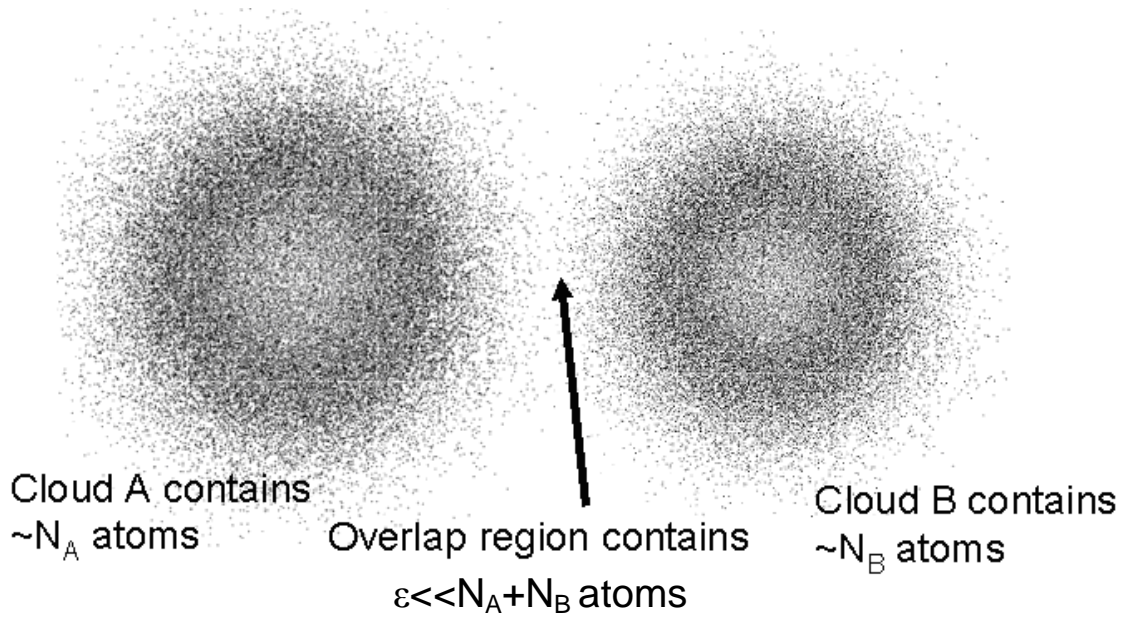


Figure 3 . Illustrates two clouds of Bose-Einstein condensed atoms confined by an external potential such that there is a small overlap between clouds. The left hand cloud has the density distribution $\rho_A(\mathbf{r})$ and the right hand cloud the distribution $\rho_B(\mathbf{r})$.

7a Zero Temperature

In the ground state, the presence of BEC implies that the macroscopic behavior of the two clouds is determined by eqs (3.1)-(3.3). The initial density distribution has the form (see Figure 3)

$$\rho(\mathbf{r},0) = \rho_A(\mathbf{r}) + \rho_B(\mathbf{r}) \quad (7.1)$$

It is assumed that the potential is such that the overlap region (that is the region where both $\rho_A(\mathbf{r})$ and $\rho_B(\mathbf{r})$ are non-zero) contains $\epsilon \ll N$ atoms. ϵ can in principle be vanishingly small, provided enough time is allowed for atoms in the two clouds to reach thermal equilibrium before the potential is switched off.

It then follows from eq. (7.1) that the function $\eta_0(\mathbf{r},0)$, defined in eq (3.2) has the form

$$\eta_0(\mathbf{r},0) = \eta_A(\mathbf{r}) + \eta_B(\mathbf{r}) \quad (7.2)$$

where to within terms $\sim \epsilon$,

$$|\eta_{A(B)}|^2 = \rho_{A(B)} \quad (7.3)$$

It follows from eq. (3.1) that the phase of η is $\phi = \Phi_0 / N$ where Φ_0 is the phase of Ψ_0 . Φ_0 has a constant value in the ground state of any Bose system [26]. Hence the phases of η_A and η_B in eq. (7.2) have the same constant (that is independent of \mathbf{r}) value

$$\phi_A = \phi_B = \frac{\Phi_0}{N} \quad (7.4)$$

The time development of the density after the trapping potential is switched off is determined by the solution of equation (3.3) with $\Xi(\mathbf{r}) = 0$ and the initial condition of eqs (7.2) - (7.4).

The effective single particle potential $V_{eff}(\mathbf{r}, t)$ in eq (3.3) is equal to the ground state energy per atom at the local density $\rho_0(\mathbf{r}, t)$ [6]. It is a well known result [27] that with sufficiently weak interactions the ground state energy is proportional to the density. Hence it follows from eq (3.2) that with weak interactions $V_{eff}(\mathbf{r}) \propto |\eta(\mathbf{r})|^2$. Eq. (3.3) then reduces to the Gross-Pitaevski equation [27]. Previously published [28,29] numerical solutions of the Gross-Pitaevski equation, with the initial conditions of eqs (7.2)-(7.4) predict density oscillations with detailed characteristics in good agreement with those observed. Hence eq (3.3) supplies a straightforward quantitative explanation from first principles of density oscillations in overlapping ultra-cold gases at $T = 0$.

7b Finite Temperature

It follows from section 6a that the density is the sum of independent contributions from the delocalized and localized components of the wave function.

$$\rho(\mathbf{r}) = w_D(T)\rho_D(\mathbf{r}) + w_L(T)\rho_L(\mathbf{r}) \quad (7.5)$$

Only the delocalized component $\rho_D(\mathbf{r})$ displays MSPQB. Hence only this component contributes to macroscopic density oscillations. Eq (5.2) implies that the form of the oscillations in $\rho_D(\mathbf{r})$ is

independent of temperature and identical to that at $T = 0$. The localized component $\rho_L(\mathbf{r})$ does not display MSPQB and hence behaves “normally” with no density oscillations. It therefore follows from eq (7.5) that as T is raised and w_D decreases, the visibility of oscillations will also decrease. The oscillations will vanish at $T = T_C$.

Note that the superfluid fraction w_D rather than the condensate fraction f determines the visibility of density oscillations. As eq (6.28) demonstrates, f is always less than w_D . In principle these predictions could be tested in ultra-cold gases by measuring the superfluid fraction before the trapping potential is switched off and then measuring the visibility of the oscillations when the clouds are allowed to overlap.

8. Discussion and Summary

It was shown in section 4 that as the temperature is raised in the presence of BEC, the wave functions of occupied N particle states must change from delocalized functions as $T \rightarrow 0$ to localized functions as $T \rightarrow T_C$. The obvious question which arises is whether this transition could occur in any other way than that postulated in eq (5.1). Another possibility for example is that is that the range of delocalization of the wave function gradually reduces from $\sim V^{1/3}$ as $T \rightarrow 0$ to $(V/N)^{1/3}$ as $T \rightarrow T_C$. This can be ruled out as it is not consistent with experiments on superfluid ^4He or with existing theory. These clearly show that MSPQB and hence a component which is delocalized over length scales $\sim V^{1/3}$ is always present if $T < T_C$. Arguably the most convincing demonstration of this is given by experiments on persistent superfluid flow in liquid ^4He [30], which occurs at all temperatures $T < T_C$.

The subsidiary postulate (5.2), that the delocalized component is identical to the ground state, seems more uncertain. Experiment demonstrates that the entropy of the superfluid component in

liquid ${}^4\text{He}$ is zero. This implies that $\Psi_D(\mathbf{r},\mathbf{s})$ must be the same unique function for all states i occupied at a given T . The obvious choice for this function is the unique ground state wave function $\Psi_0(\mathbf{r},\mathbf{s})$, but the possibility that Ψ_D changes with temperature cannot be conclusively ruled out. However it was shown in refs [20,21,23,24] that available experimental data on the superfluid fraction, the condensate fraction, the static and dynamic structure factors and the thermal expansion of superfluid ${}^4\text{He}$ are all consistent with eq (5.2). These measurements demonstrate that to within $\sim 1\%$ in liquid ${}^4\text{He}$ the delocalized component of the wave function is identical to the ground state wave function.

It is interesting to note that the arguments in section 6f imply that in liquid ${}^4\text{He}$ the delocalized and localized components of the wave functions give different contributions to the static structure factor. This implies that configurations \mathbf{r},\mathbf{s} of the N atoms for which Ψ_D has significant amplitude must be significantly different to those for which Ψ_L has significant amplitude. It could be the case that $\Psi_L(\mathbf{r},\mathbf{s})$ is zero for \mathbf{s} where $\Psi_D(\mathbf{r},\mathbf{s})$ is non-zero and vice versa. This would imply that all the results of sections 6 and 7 are exact. Hence the results obtained in sections 6 and 7 are accurate to at worst $\sim 1/\sqrt{N}$.

To summarize it has been shown that a wide range of uniquely anomalous experimental phenomena in Bose-Einstein condensed liquids and gases at finite temperature can be quantitatively explained by two simply stated postulates. These are; (1) that the N particle wave functions of occupied states can be written as the sum of components which are localized and delocalized in coordinate space and (2) that the delocalized component is identical to the ground state wave function. It has been argued that these postulates are in fact forced by basic quantum mechanics, existing theoretical treatments of BEC and extensive experimental data on liquid ${}^4\text{He}$.

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