PHYSICAL REVIEW A **78**, 033618 (2008)

Origin of macroscopic single-particle quantum behavior in Bose-Einstein-condensed systems

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(Received 21 May 2008; published 26 September 2008)

It is shown that any Bose-Einstein-condensed fluid in its ground state will exhibit macroscopic single-particle quantum behavior (MSPQB). That is, (1) the many-particle wave function $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_n)$ factors into a single-particle product $\Pi_n\eta(\mathbf{r}_n)$; (2) the function $\eta(\mathbf{r})$ extends over macroscopic length scales and obeys the usual quantum equations for particle flux in a single-particle system; and (3) $\eta(\mathbf{r})$ obeys a nonlinear single-particle Schrödinger equation. The latter equation reduces to the Gross-Pitaevskii equation when interactions are weak and determines the density distribution of the fluid and the time development of this distribution. The arguments used rely only on elementary concepts of probability theory and many-particle wave mechanics and are valid even in strongly interacting fluids such as superfluid ^{4}He. It is shown that Bose-Einstein condensation implies that the N-particle wave function Ψ is delocalized. That is, if one considers a single-particle coordinate $\mathbf{r}$, then for all values that occur of the other $N-1$ coordinates, Ψ is a nonzero function of $\mathbf{r}$ over a region of space proportional to V, where V is the total volume within which the fluid is contained. MSPQB is a consequence of this delocalization and the absence of long-range correlations between particle positions in fluids. The results are accurate provided that only averages over regions of space containing many particles are considered. For averages over volumes of space containing N_Ω particles, inaccuracies due to quantum fluctuations are $\sim 1/\sqrt{N_\Omega}$.

DOI: 10.1103/PhysRevA.78.033618 PACS number(s): 03.75.Hh, 67.25.D−

I. INTRODUCTION

Arguably the most important property possessed by Bose-Einstein-condensed systems is macroscopic single-particle quantum behavior (MSPQB)—that is, every particle appears to occupy the same single-particle quantum state, with a wave function that extends over macroscopic length scales. There is clear experimental evidence for MSPQB in Bose-Einstein-condensed systems, such as superfluidity and quantized vortices in liquid ^{4}He and quantized vortices and interference effects observed in overlapping clouds of ultracold Bose-Einstein-condensed gases [1]. However, there is no generally applicable theoretical proof from first principles that Bose-Einstein condensation (BEC) implies MSPQB. This paper supplies such a proof.

Interest in the microscopic origin of MSPQB has been stimulated by the many new experimental results obtained in gases of Bose-Einstein-condensed ultracold atoms [1–3]. It has been recently shown [4–6] that MSPQB occurs in the ground state of weakly interacting Bose-Einstein-condensed systems and that the single-particle wave function obeys the Gross-Pitaevskii (GP) equation. However, the origin of MSPQB in strongly interacting systems such as liquid ^{4}He is still unclear. If all particles occupy the same single-particle state with wave function $\eta(\mathbf{r})$, the many-particle wave function $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ can be expressed as the product

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=\prod_{n=1}^{N}\eta(\mathbf{r}_n). \tag{1.1}$$

Equation (1.1) is exactly true only when there are no interactions between particles. One would expect that it remains approximately true when interactions are sufficiently weak, but it is not clear how it can be even approximately true in strongly interacting systems such as liquid ^{4}He.

It is argued here that the link between BEC and MSPQB can be understood rather simply, for any strength of particle interaction, using only elementary concepts of probability theory and many-particle wave mechanics. It is shown that MSPQB is a consequence of two properties of Bose-Einstein-condensed fluids. (1) Correlations between atomic positions do not extend further than a few atomic spacings. This is true basically by definition in any fluid. (2) The many-particle wave function is delocalized in the sense defined in the Abstract and in more detail in Sec. IV. Most fluids do not have a delocalized wave function and hence do not display MSPQB. However, it will be shown that delocalization of the wave function and hence MSPQB are a necessary consequence of BEC.

Section II contains definitions and specifies the notation used. Section III reviews the properties of a well-known model of the ground-state wave function of a Bose-Einstein-condensed system. It is shown that the model wave function possesses certain properties and it is argued in Secs. IV and V that these properties are possessed by the ground-state wave function of any Bose-Einstein-condensed fluid. In Secs. VI–VIII it is shown that these properties imply MSPQB. The nonlinear Schrödinger equation obeyed by the wave function $\eta(\mathbf{r})$ of the single-particle state is derived in Sec. VII. Section VIII derives the equation determining the time evolution of the density of a Bose-Einstein-condensed gas in its ground state, when its confining potential is switched off and the gas is allowed to expand. In Sec. IX it is shown that, in the limit of weak interactions, the single-particle equations derived in Secs. VII and VIII reduce to the time-dependent and time-independent Gross-Pitaevskii equations. Section X discusses the limits of validity of the results. Section XI contains a summary and conclusions.

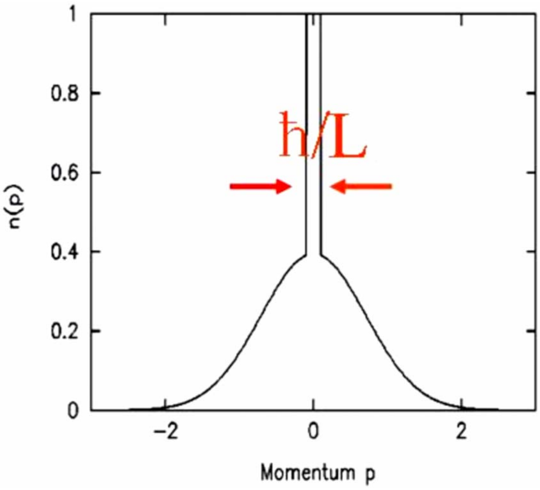

FIG. 1. (Color online) Bose-Einstein condensation. The atomic momentum distribution $n(p)$ contains a condensate peak of weight f and width $\hbar/L$, where L is the linear dimension of the system.

II. DEFINITIONS AND NOTATION

We take as the definition of Bose-Einstein condensation that the single-particle momentum distribution $n(\mathbf{p})$ contains a peak of fractional weight f, centered at zero momentum, and of width $\sim\hbar/L$, where L is the linear dimension of the entire system (see Fig. 1). The "condensate fraction" f is independent of the number of particles N when N is very large.

This is not the most general definition of BEC [7], but all other definitions imply that this is true in the ground state of any Bose-Einstein-condensed system. The presence of a condensate peak in $n(\mathbf{p})$ is actually the accepted experimental proof of BEC. Such peaks have been observed by neutron scattering from superfluid helium [8] and light scattering from ultracold clouds of atoms [1–3]. In ultracold gases it has been shown experimentally [9] that the width of the condensate peak in momentum space is $\sim\hbar/L$, in agreement with the definition used here. In superfluid helium, where samples are truly macroscopic, the width is too small to measure.

We consider the ground-state wave function $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ of a system of N particles, contained at uniform density within a volume $V\sim L^3$, with periodic boundary conditions. The wave function is normalized.

$$\int|\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2 d\mathbf{r}_1\cdots d\mathbf{r}_N=1. \tag{2.1}$$

We denote the coordinate of one of the particles as $\mathbf{r}$ and the coordinates of the other $N-1$ particles as $\mathbf{s}$. Which coordinate is singled out in this way is immaterial due to the Bose symmetry of $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ under particle interchange, but for definiteness $\mathbf{r}_1$ is denoted as $\mathbf{r}$ and $\mathbf{r}_2,\ldots,\mathbf{r}_N$ as $\mathbf{s}$ throughout.

The standard physical interpretation of the wave function is that $|\Psi(\mathbf{r},\mathbf{s})|^2$ is the probability distribution function (PDF) for the positions $\mathbf{r},\mathbf{s}$ of the N particles. We define the function

$$P(\mathbf{s})=\int|\Psi(\mathbf{r},\mathbf{s})|^2 d\mathbf{r}. \tag{2.2}$$

It follows from the above interpretation of $|\Psi(\mathbf{r},\mathbf{s})|^2$ that $P(\mathbf{s})$ is the PDF of the positions $\mathbf{s}$ of $N-1$ particles. Equations (2.1) and (2.2) imply that, as is consistent with this interpretation,

$$\int P(\mathbf{s})d\mathbf{s}=1. \tag{2.3}$$

We define the function

$$\psi_{\mathbf{s}}(\mathbf{r})=\Psi(\mathbf{r},\mathbf{s})/\sqrt{P(\mathbf{s})}. \tag{2.4}$$

$\psi_{\mathbf{s}}(\mathbf{r})$ is written with $\mathbf{s}$ as a subscript to emphasize that, wherever it is used, we consider the dependence on one coordinate $\mathbf{r}$ for a given value of $\mathbf{s}$. However, it should be stressed that to within a constant factor $\psi_{\mathbf{s}}(\mathbf{r})$ simply describes the dependence of the many-particle wave function $\Psi(\mathbf{r},\mathbf{s})$ on a single coordinate $\mathbf{r}$, given the values $\mathbf{s}$ of the other $N-1$ coordinates. $\psi_{\mathbf{s}}(\mathbf{r})$ is a convenient function to deal with as it can be treated in many ways as the "conditional wave function" [10–15] of a single particle, given the positions $\mathbf{s}$ of all other particles.

For example, it follows from the probability interpretation of $|\Psi(\mathbf{r},\mathbf{s})|^2$ that $|\psi_{\mathbf{s}}(\mathbf{r})|^2$ is the conditional PDF for the coordinate $\mathbf{r}$, given $\mathbf{s}$. It follows from Eqs. (2.1)–(2.4) that, as is consistent with this interpretation, $\psi_{\mathbf{S}}(\mathbf{r})$ is a normalized function of $\mathbf{r}$:

$$\int|\psi_{\mathbf{s}}(\mathbf{r})|^2 d\mathbf{r}=1. \tag{2.5}$$

The overall probability that particle 1 is at $\mathbf{r}$ is found by averaging $|\psi_{\mathbf{s}}(\mathbf{r})|^2$ over the probability distribution for different $\mathbf{s}$:

$$\rho(\mathbf{r})=\int|\Psi(\mathbf{r},\mathbf{s})|^2 d\mathbf{s}=\int P(\mathbf{s})|\psi_{\mathbf{s}}(\mathbf{r})|^2 d\mathbf{s}. \tag{2.6}$$

Since all particles are equivalent, the average number of particles per unit volume at $\mathbf{r}$ is $N\rho(\mathbf{r})$.

The conditional probability of momentum $\mathbf{p}$ given $\mathbf{s}$ also has a form analogous to the single-particle case [11],

$$n_{\mathbf{s}}(\mathbf{p})=\frac{1}{\hbar^3}\left|\int\psi_{\mathbf{s}}(\mathbf{r})\exp(i\mathbf{p}\cdot\mathbf{r}/\hbar^3)d\mathbf{r}\right|^2. \tag{2.7}$$

The measurable single-particle momentum distribution is again given by the weighted average over $\mathbf{s}$,

$$n(\mathbf{p})=\int P(\mathbf{s})n_{\mathbf{s}}(\mathbf{p})d\mathbf{s}. \tag{2.8}$$

The condensate fraction is the fraction of particles in the zero-momentum state,

$$f=\int P(\mathbf{s})f_{\mathbf{s}}d\mathbf{s}, \tag{2.9}$$

where $f_{\mathbf{s}}$ is a dimensionless number,

$$f_s = \frac{n_s(0)}{V} = \frac{1}{V}\left|\int \psi_s(\mathbf{r})d\mathbf{r}\right|^2. \tag{2.10}$$

With periodic boundary conditions in a cube of side L, particles in the condensate peak are equally likely to have any momentum within a cube of side $\hbar/L$, centered at $\mathbf{p}=\mathbf{0}$. With other boundary conditions and in systems where the density is not uniform, the shape of the condensate peak is modified (see Appendix B), but its width is still $\sim\hbar/L$, where L is the linear dimension of the system.

It should be stressed that Eqs. (2.6)–(2.10) are essentially just a formal rewriting in different notation of standard rigorous results from N-particle wave mechanics. However, when written in this form they can be given a new physical interpretation. Many observable physical properties are determined by some quantity Q_s, which is an integral over $\mathbf{r}$ of a functional of $\psi_s(\mathbf{r})$. To obtain the observable property, an average of Q_s over $\mathbf{s}$ is performed, weighted by the probability $P(\mathbf{s})$ that $\mathbf{s}$ will occur. Examples are the density, momentum distribution, condensate fraction, total kinetic and potential energy, and fluid flow—see Eqs. (2.6), (2.8), (2.9), (5.15), and (8.1).

III. FEYNMAN-PENROSE-ONSAGER MODEL OF THE GROUND STATE OF ^{4}He

Penrose and Onsager [16] used a simple model suggested by Feynman [17] to give the first realistic estimate of the condensate fraction in the ground state of liquid ^{4}He. The ground-state wave function was assumed to be zero if the hard cores of any two atoms overlap and to have the same value C for all other configurations of atoms. That is,

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \begin{cases} 0 & \text{if } |\mathbf{r}_n-\mathbf{r}_m| < a \text{ for any } n,m,\ n\neq m, \\ C & \text{otherwise.}\end{cases} \tag{3.1}$$

a is the hard-core diameter of a helium atom and the constant C is determined by the normalization condition on Ψ in Eq. (2.1). At densities equal to those in the ground state of liquid helium, the Feynman-Penrose-Onsager (FPO) model gives $f\sim 8\%$ [16], very close to the value of $(7\pm 1)\%$ observed in state of the art measurements [8].

It has previously been shown numerically [10,11] that the FPO model of ^{4}He implies that values of f_s cluster about the mean value $f\sim 0.08$, with a distribution that has a closely Gaussian form with standard deviation $\sim f/\sqrt{N}$ [18]. That is,

$$f_s = f(1\pm \sim 1/\sqrt{N}). \tag{3.2}$$

This is illustrated in Fig. 2 for $N=192$ atoms. Some non-Gaussian behavior is present in Fig. 2, but as N increases calculations show [11] that the distribution of f_s values becomes steadily more Gaussian. This implies that in a large system all $\mathbf{s}$ that occur give almost the same value for f_s. For example, with $N=10^{22}$, the probability of f_s differing from f by more than one part in 10^9 is $\sim\exp(-10\,000)$. Clearly such $\mathbf{s}$ will never occur [19]—that is (effectively), $P(\mathbf{s})=0$ for such $\mathbf{s}$. The FPO model implies that $\psi_s(\mathbf{r})$ has the $\mathbf{r}$ dependence,

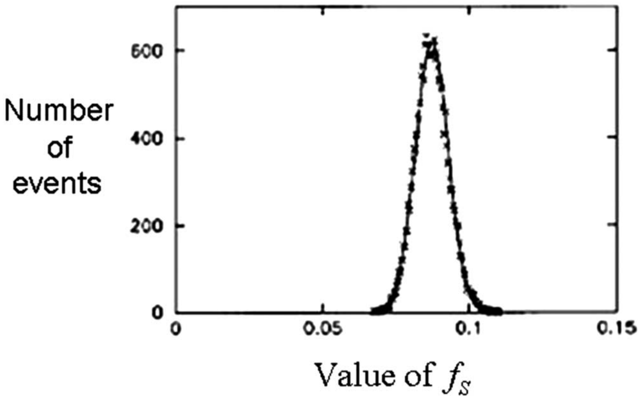

FIG. 2. Distribution of f_s values obtained in a numerical calculation [11] using the FPO model at the packing density and hard-core diameter of liquid ^{4}He at zero temperature. f_s was calculated for 20 000 configurations $\mathbf{s}$, obtained by use of a random number generator and the values binned. The solid line is a Gaussian function with the same mean and standard deviation as the points.

$$\psi_s(\mathbf{r}) = \begin{cases} 0 & \text{if for any } m\neq 1\ |\mathbf{r}-\mathbf{r}_m| < a, \\ c & \text{otherwise.}\end{cases} \tag{3.3}$$

The constant c is determined by the normalization condition in Eq. (2.5).

The form of $\psi_s(\mathbf{r})$ in the FPO model is illustrated in two dimensions in Fig. 3. $\psi_s(\mathbf{r})$ is nonzero only at points at least a distance a from the center of any black circle (the white regions in Fig. 3). This has a simple physical interpretation. In the FPO model $\psi_s(\mathbf{r})$ is nonzero only at points where the center of an impenetrable sphere could be inserted, without overlap with any of the $N-1$ impenetrable spheres, centered at positions $\mathbf{s}=\mathbf{r}_2,\ldots,\mathbf{r}_N$.

IV. DELOCALIZATION

It is a simple mathematical consequence of the form of $\psi_s(\mathbf{r})$ in Eq. (3.3) that $\psi_s(\mathbf{r})$ is nonzero within exactly a frac-

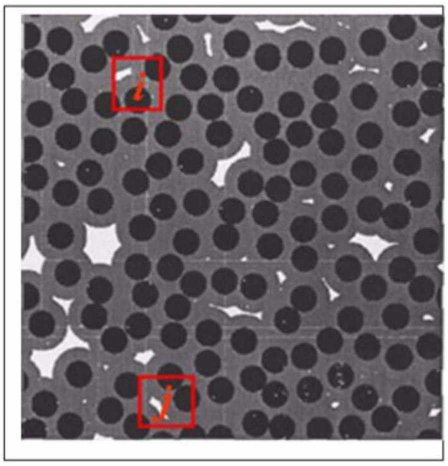

FIG. 3. (Color online) Two-dimensional illustration of the form of $\psi_s(\mathbf{r})$ for the FPO model. $\psi_s(\mathbf{r})$ is nonzero only within the white regions. The black circles represent $N-1$ hard-core atoms of diameter a at positions $\mathbf{s}=\mathbf{r}_2,\ldots,\mathbf{r}_n$. The two cells referred to in Sec. V are also shown.

tion $f_\mathbf{s}$ of the total volume V [20]. Hence the FPO model implies that $\psi_\mathbf{s}(\mathbf{r})$ is a "delocalized" function of $\mathbf{r}$. The term "delocalized" as used in this paper means that the function $\psi_\mathbf{s}(\mathbf{r})$, defined in Eq. (2.4), is a nonzero function of $\mathbf{r}$ within a volume proportional to the total volume of the fluid. This is ~8% of the total volume of the fluid in the FPO model. The origin of delocalization is obvious in the FPO model (see Fig. 3). $\psi_\mathbf{s}(\mathbf{r})$ is nonzero in any space in the fluid large enough to accommodate another particle without hard-core overlap. Clearly the total volume of these spaces is proportional to the size of the system. It also follows from Eq. (3.2) and the distribution illustrated in Fig. 2 that in the FPO model $\psi_\mathbf{s}(\mathbf{r})$ is delocalized within ~8% of the total fluid volume for *every* $\mathbf{s}$ that occurs.

The basic premise of this paper is that $\psi_\mathbf{s}(\mathbf{r})$ is a delocalized function of $\mathbf{r}$ for every $\mathbf{s}$ that occurs in the ground state of *any* Bose-Einstein-condensed system. The necessity for delocalization of $\psi_\mathbf{s}(\mathbf{r})$ can be understood from the definition of BEC in Sec. II and elementary Fourier transform theory. If $n_\mathbf{s}(\mathbf{p})$ in Eq. (2.7) contains a peak of width $\sim\hbar/L$, then $\psi_\mathbf{s}(\mathbf{r})$ must be a nonzero function of $\mathbf{r}$ over length scales $\sim L$. This inverse relation between widths in $\mathbf{r}$ and $\mathbf{p}$ space is well known. For example, it is used in standard derivations of the uncertainty principle and to interpret the widths of peaks in diffraction data.

The FPO model actually gives the minimum delocalization for a given value of $f_\mathbf{s}$. It has been shown more generally [11] that $\psi_\mathbf{s}(\mathbf{r})$ must be a nonzero function of $\mathbf{r}$ within a volume $\geqslant f_\mathbf{s}V$. Hence, it is true in any system that, if $f_\mathbf{s}\neq 0$, $\psi_\mathbf{s}(\mathbf{r})$ must be delocalized. For reasons discussed at the end of the following section it is assumed that in the presence of BEC *all* particle configurations $\mathbf{s}$ that occur give $f_\mathbf{s}\neq 0$, and hence that $\psi_\mathbf{s}(\mathbf{r})$ is delocalized for all $\mathbf{s}$ that occur when BEC is present.

V. FLUCTUATIONS IN THE GROUND STATE

The results of this section follow from three properties of a Bose-Einstein-condensed fluid.

(1) The function $\psi_\mathbf{s}(\mathbf{r})$ is a delocalized function of $\mathbf{r}$. This is true in the presence of BEC, but not usually true when BEC is absent.

(2) Correlations between particle positions extend only over distances $d\sim(V/N)^{1/3}$, the average spacing between atoms—this is essentially the definition of a fluid.

(3) Interactions between particles also extend only over distances $\sim d$. This assumption is implicit in assumption 2.

The key to understanding MSPQB is that these three properties imply that integrals over $\mathbf{r}$ of functionals of $\psi_\mathbf{s}(\mathbf{r})$ are almost the same for all $\mathbf{s}$ that occur, provided the integration volume is sufficiently large. In order to demonstrate this we first consider the simplest such integral

$$I_\mathbf{s}=\int_V \psi_\mathbf{s}(\mathbf{r})d\mathbf{r}, \tag{5.1}$$

where the integral is taken over the entire volume of the system. It is a well-known result of quantum mechanics that the ground-state wave function of any Bose system can be chosen as real and positive [21]. Hence both $\psi_\mathbf{s}(\mathbf{r})$ and $I_\mathbf{s}$ are real and positive. The variation in $I_\mathbf{s}$ with $\mathbf{s}$ can be characterized in terms of its deviation from the mean value $\bar{I}$, where

$$\bar{I}=\int P(\mathbf{s})I_\mathbf{s}d\mathbf{s}. \tag{5.2}$$

The fluctuation in $I_\mathbf{s}$ is defined as

$$\Delta I_\mathbf{s}=I_\mathbf{s}-\bar{I}. \tag{5.3}$$

In the rest of the paper the term "fluctuation" is used in this sense—that is, the deviation from the mean as $\mathbf{s}$ is varied. Clearly these are quantum fluctuations, associated with the fact that $\Psi(\mathbf{r},\mathbf{s})$ determines only probability distributions for physical properties other than the ground-state energy.

We first consider a fluid of uniform density and divide the total volume V into N equal microscopic cells, each containing on average a single particle. The contribution of cell i to the integral $I_\mathbf{s}$ is defined as the integral of $\psi_\mathbf{s}(\mathbf{r})$ over $\mathbf{r}$ within cell i,

$$g_{i\mathbf{s}}=\int_i \psi_\mathbf{s}(\mathbf{r})d\mathbf{r}. \tag{5.4}$$

$I_\mathbf{s}$ can then be formally written as the sum of contributions from different cells,

$$I_\mathbf{s}=\sum_{i=1}^{N} g_{i\mathbf{s}}. \tag{5.5}$$

In a system of uniform density, where all cells are equivalent, every cell makes the same contribution to $\bar{I}$. Hence the average over $\mathbf{s}$ of $g_{i\mathbf{s}}$ has the same value for every cell [22],

$$\bar{g}_i=\int P(\mathbf{s})g_{i\mathbf{s}}d\mathbf{s}=\bar{g}=\bar{I}/N. \tag{5.6}$$

The cell fluctuation from this average is

$$\Delta g_{i\mathbf{s}}=g_{i\mathbf{s}}-\bar{g}. \tag{5.7}$$

It follows from Eqs. (5.3)–(5.7) that $\Delta I_\mathbf{s}$ is the sum of cell fluctuations,

$$\Delta I_\mathbf{s}=\sum_{i=1}^{N} \Delta g_{i\mathbf{s}}. \tag{5.8}$$

We consider two cells i,j separated by many atomic spacings d, as illustrated in Fig. 3. Property 2 implies that the arrangement of atoms near (that is, within $\sim d$ of) cell i is uncorrelated with that near cell j. Property 3 implies that $\psi_\mathbf{s}(\mathbf{r})$ within a cell is determined by the arrangement of atoms only near the cell. Hence the microscopic form of $\psi_\mathbf{s}(\mathbf{r})$ within cell i must be uncorrelated with that in cell j. It follows that fluctuations in the integrals of $\psi_\mathbf{s}(\mathbf{r})$ over cells i and j are also uncorrelated. In other words the signs of the fluctuations $\Delta g_{i\mathbf{s}},\Delta g_{j\mathbf{s}}$ are uncorrelated, provided the cells i, j are sufficiently widely separated.

The magnitude of the cell fluctuations is determined by the strength of particle interactions. At the packing density and atomic size in liquid ^{4}He, the hard-core diameter a comparable to the size of a cell. It is obvious that in this case $g_{i\mathbf{s}}$ will depend strongly upon $\mathbf{s}$. For example $g_{i\mathbf{s}}$ will be significantly different for $\mathbf{s}$ giving one atom within cell i than for $\mathbf{s}$ giving no (or two) atoms within the cell (see Fig. 3). It follows that in liquid ^{4}He cell fluctuations are $\sim\bar{g}$. That is,

$$g_{i\mathbf{s}} = \bar{g} \pm \sim \bar{g}. \tag{5.9}$$

With weaker interactions, such as those in dilute gases, fluctuations are smaller and the results that will be derived are more accurate, but for purposes of discussion we assume the worst case estimate given by Eq. (5.9).

It follows from Eqs. (5.8) and (5.9) that the fluctuation $\Delta I_\mathbf{s}$ is the sum of N terms with uncorrelated signs and of modulus $\sim\bar{g}$. This is equivalent to a random walk in one dimension with step lengths $\sim\bar{g}$. For large N, values of $\Delta I_\mathbf{s}$ will therefore be distributed about zero according to a Gaussian distribution of standard deviation,

$$\sim \bar{g}\sqrt{N} = \bar{I}/\sqrt{N}. \tag{5.10}$$

It follows that values of $I_\mathbf{s}$ are distributed about $\bar{I}$, according to a Gaussian distribution of width $\sim\bar{I}/\sqrt{N}$,

$$I_\mathbf{s} = \bar{I}(1 \pm \sim 1/\sqrt{N}). \tag{5.11}$$

It follows from the definitions of $f_\mathbf{s}$ and $I_\mathbf{s}$ that $f_\mathbf{s}=V|I_\mathbf{s}|^2$. Hence this argument explains Eq. (3.2) and the Gaussian shape of the distribution shown in Fig. 2 for the FPO model. However, the arguments are valid not just for the FPO model, but for any fluid satisfying conditions 1–3 above. In particular they are valid for any Bose-Einstein-condensed fluid in its ground state.

Furthermore, although the derivation above was given for a system of uniform density, fluctuations in $I_\mathbf{s}$ are also proportional to $1/\sqrt{N}$ in systems where the density is not uniform. In any fluid with the properties listed at the start of this section $I_\mathbf{s}$ can be expressed as a sum of N cell contributions $g_{i\mathbf{s}}$, which each fluctuate independently about a mean value $\bar{g}_i$. If the density is nonuniform, $\bar{g}_i$ will be different in different cells. However, it still follows from the central limit theorem [23] that values of $I_\mathbf{s}$ are distributed about their mean value $\bar{I}=\Sigma\bar{g}_i$, according to a Gaussian distribution of width proportional to $1/\sqrt{N}$. This is true provided the following conditions are satisfied.

(a) Fluctuations $\Delta g_{i\mathbf{s}}$ in different cells are uncorrelated—this is true in a fluid, but not a crystalline system.

(b) N is sufficiently large—$\psi_\mathbf{s}(\mathbf{r})$ must be delocalized for this to be true. This is not usually true in the absence of BEC, but is implied by the presence of BEC.

(c) The PDF describing the distribution of $g_{i\mathbf{s}}$ values in any cell i has a finite variance [23]. This is clearly always the case since the cell size is finite.

The same arguments can be applied to other quantities Q that can be expressed in the form

$$Q = N\int P(\mathbf{s})Q_\mathbf{s}d\mathbf{s}, \tag{5.12}$$

where

$$Q_\mathbf{s} = \int F[\psi_\mathbf{s}(\mathbf{r})]d\mathbf{r} \tag{5.13}$$

and F is a functional of $\psi_\mathbf{s}(\mathbf{r})$. For example, the total potential energy of the system is

$$V' = \int \sum_n \sum_{m\neq n} v(\mathbf{r}_n - \mathbf{r}_m)|\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2 d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N. \tag{5.14}$$

The Bose symmetry of the wave function implies that all terms in the sum over n make the same contribution to V'. Hence, using the definition of $\psi_\mathbf{s}(\mathbf{r})$, V' can be expressed as

$$V' = N\int P(\mathbf{s})v_\mathbf{s}d\mathbf{s}, \tag{5.15}$$

where

$$v_\mathbf{s} = \int \sum_{m\neq 1} v(\mathbf{r}-\mathbf{r}_m)|\psi_\mathbf{s}(\mathbf{r})|^2 d\mathbf{r}. \tag{5.16}$$

Like the integral $I_\mathbf{s}$, $v_\mathbf{s}$ can be divided into the sum of N cell contributions which each fluctuate independently about a mean value as $\mathbf{s}$ varies. Hence the same arguments used to justify Eq. (5.11) imply that in a large system $v_\mathbf{S}$ is almost the same for all $\mathbf{s}$ that occur,

$$v_\mathbf{s} = v(1 \pm \sim 1/\sqrt{N}), \tag{5.17}$$

where $v=V'/N$ is the average single-particle potential energy.

Similarly the total kinetic energy of the fluid can be expressed as [11]

$$K = N\int P(\mathbf{s})\kappa_\mathbf{s}d\mathbf{s}, \tag{5.18}$$

where

$$\kappa_\mathbf{s} = \int_V \psi_\mathbf{s}^*(\mathbf{r})\frac{-\hbar^2}{2m}\frac{\partial^2\psi_\mathbf{s}(\mathbf{r})}{\partial\mathbf{r}^2}d\mathbf{r}. \tag{5.19}$$

By the same arguments $\kappa_\mathbf{s}$ is almost the same for all $\mathbf{s}$ that occur in a large system,

$$\kappa_\mathbf{s} = \kappa(1 \pm \sim 1/\sqrt{N}), \tag{5.20}$$

where κ is the mean kinetic energy per particle.

To conclude this section we return to the assumption given in Sec. IV that $\psi_\mathbf{s}(\mathbf{r})$ is a delocalized function of $\mathbf{r}$ for *all* $\mathbf{s}$ that occur. We first note the obvious fact that in the presence of BEC $f_\mathbf{s}$ must be nonzero for some $\mathbf{s}$ and that $\psi_\mathbf{s}(\mathbf{r})$ must therefore also be delocalized for some $\mathbf{s}$. Furthermore, it has just been shown that if $\psi_\mathbf{s}(\mathbf{r})$ is delocalized, then to within terms $\sim 1/\sqrt{N}$, $f_\mathbf{s}=f$. It follows that only $\mathbf{s}$ for which $f_\mathbf{s}\sim f$ or $f_\mathbf{s}\sim 0$ can occur in the presence of BEC. Clearly, particle configurations $\mathbf{s}$ giving $f_\mathbf{s}\sim f$ will give a significantly lower value for $\kappa_\mathbf{s}$ than those for which $f_\mathbf{s}\sim 0$. However, in the ground state, it follows from the definition of $\psi_\mathbf{s}(\mathbf{r})$ and the fact that $\Psi(\mathbf{r},\mathbf{s})$ is an eigenstate of energy that $\kappa_\mathbf{s}$ and $v_\mathbf{s}$ are linked by the relation

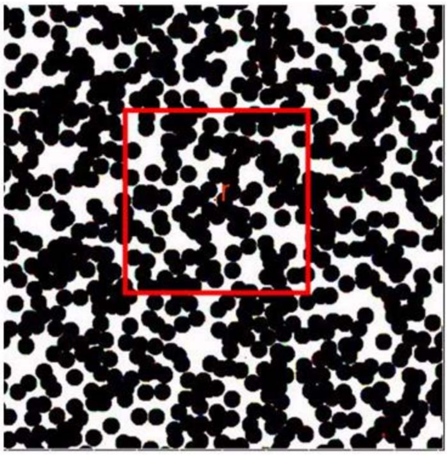

FIG. 4. (Color online) The square illustrates a particular element, centered at $\mathbf{r}$ and of volume Ω.

$$\kappa_{\mathbf{s}} + v_{\mathbf{s}} = E/N, \tag{5.21}$$

where E is the total ground-state energy. Hence $\mathbf{s}$ for which $f_{\mathbf{S}} \sim 0$ can also occur only if the increase in $\kappa_{\mathbf{s}}$ is exactly compensated by a decrease in $v_{\mathbf{s}}$. This is mathematically possible, but physically seems extremely unlikely.

Furthermore, if $\mathbf{s}$ for which $f_{\mathbf{s}} \sim f$ and $f_{\mathbf{s}} \sim 0$ both occur, this would imply fluctuations ~ 1 in the condensate fraction and hence the Bose order parameter (see Appendix C). Both are thermodynamic properties of a macroscopic system and would be expected to have fluctuations $\sim 1/\sqrt{N}$. According to Eq. (3.2) this is true if all $\mathbf{s}$ that occur give $f_{\mathbf{s}} \sim f$, but not if $\mathbf{s}$ giving $f_{\mathbf{s}} \sim 0$ also occur. Fluctuations in the total kinetic energy K of the fluid would also be ~ 1. The fluctuation in K is

$$\Delta K^2 = N \int P(\mathbf{s})(\kappa_{\mathbf{s}} - \kappa)^2 d\mathbf{s}. \tag{5.22}$$

Clearly, $\mathbf{s}$ for which $f_{\mathbf{s}} \sim f$ will give $\kappa_{\mathbf{s}}$ lower by $\sim \kappa$ than $\mathbf{s}$ for which $f_{\mathbf{s}} \sim 0$. Thus if both occurred with appreciable probability this would imply $\Delta K \sim K$. However, K is an additive property (that is, proportional to N) of a macroscopic body and it is a very general result of statistical physics [24] that fluctuations in such quantities are $\sim 1/\sqrt{N}$. This again implies that in the presence of BEC all $\mathbf{s}$ that occur give $f_{\mathbf{s}} \sim f$.

VI. COARSE-GRAINED AVERAGES

We next consider an element of volume Ω, centered at the point $\mathbf{r}$ as illustrated in Fig. 4. We assume that Ω is small compared to the total volume V, but that the element contains many atoms. Provided $\psi_{\mathbf{s}}(\mathbf{r})$ is delocalized, the argument applied to the whole volume V in the previous section can be applied to the element. If the element contains on average N_Ω atoms, fluctuations in integrals of functionals of $\psi_{\mathbf{s}}(\mathbf{r})$ over the element, such as (5.1), (5.16), and (5.19), will be $\sim 1/\sqrt{N_\Omega}$ [25].

We define the "coarse-grained average" (CGA) of $\psi_{\mathbf{s}}(\mathbf{r})$ as the average over such a volume Ω centered at $\mathbf{r}$,

$$\overline{\psi_{\mathbf{s}}(\mathbf{r})} = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} \psi_{\mathbf{s}}(\mathbf{r}') d\mathbf{r}'. \tag{6.1}$$

The CGA is a smoothing operation which removes structure on length scales $\sim d$, leaving only structure varying over length scales $\Omega^{1/3} \gg d$. In the rest of the paper a bar over an expression denotes the CGA. It follows from the previous discussion that $\overline{\psi_{\mathbf{s}}(\mathbf{r})}$ is the same to $\sim 1/\sqrt{N_\Omega}$ for all $\mathbf{s}$ that occur,

$$\overline{\psi_{\mathbf{s}}(\mathbf{r})} = \bar{\psi}(\mathbf{r})[1 \pm \sim 1/\sqrt{N_\Omega}]. \tag{6.2}$$

The symbol $\cong$ is henceforward used to denote equality to within terms $\sim 1/\sqrt{N_\Omega}$. That is, Eq. (6.2) is equivalent to

$$\overline{\psi_{\mathbf{s}}(\mathbf{r})} \cong \bar{\psi}(\mathbf{r}). \tag{6.3}$$

It is shown in Appendix C that $\bar{\psi}(\mathbf{r})$ can be identified as the thermodynamic order parameter of the system.

By the same arguments the CGA of $|\psi_{\mathbf{s}}(\mathbf{r})|^2$ is also the same for all $\mathbf{s}$ that occur to within terms $\sim 1/\sqrt{N_\Omega}$,

$$\overline{|\psi_{\mathbf{s}}(\mathbf{r})|^2} = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} |\psi_{\mathbf{s}}(\mathbf{r}')|^2 d\mathbf{r}' \cong \bar{\rho}(\mathbf{r}). \tag{6.4}$$

It follows from Eqs. (2.6) and (2.3) that $\bar{\rho}(\mathbf{r})$ is the coarse-grained average of the particle density $\rho(\mathbf{r})$,

$$\bar{\rho}(\mathbf{r}) = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} \rho(\mathbf{r}') d\mathbf{r}'. \tag{6.5}$$

It is clear that $\bar{\rho}(\mathbf{r})$ is just the macroscopic thermodynamic particle density in the fluid.

A visual understanding of Eqs. (6.3) and (6.4) can be obtained from the FPO model, for which the CGAs $\overline{\psi_{\mathbf{s}}(\mathbf{r})}$ and $\overline{|\psi_{\mathbf{s}}(\mathbf{r})|^2}$ are both proportional to the total volume within the element $\Omega(\mathbf{r})$, where $\psi_{\mathbf{s}}(\mathbf{r})$ is nonzero (the white regions in Fig. 4). The total volume of these regions lying within $\Omega(\mathbf{r})$ is the same to within $\sim 1/\sqrt{N_\Omega}$ for all particle arrangements $\mathbf{s}$ that occur. This is true for basically the same physical reason that the total number of particles within $\Omega(\mathbf{r})$ is the same to within $\sim 1/\sqrt{N_\Omega}$ for all particle arrangements that occur.

The CGA over N coordinates of $|\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2$ is similarly defined as

$$\overline{|\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2} = \frac{1}{\Omega^N} \int_{\Omega(\mathbf{r}_1)} d\mathbf{r}_1' \int_{\Omega(\mathbf{r}_2)} d\mathbf{r}_2' \cdots \times \int_{\Omega(\mathbf{r}_N')} d\mathbf{r}_N' |\Psi(\mathbf{r}_1',\mathbf{r}_2',\ldots,\mathbf{r}_N')|^2. \tag{6.6}$$

In this case the CGA smooths the structure in all coordinates. It follows from the definition of $\psi_{\mathbf{s}}(\mathbf{r})$ and Eq. (6.4) that

$$\overline{|\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2} \cong \bar{P}(\mathbf{r}_2,\ldots,\mathbf{r}_N)\bar{\rho}(\mathbf{r}_1), \tag{6.7}$$

where $\bar{P}(\mathbf{r}_2,\ldots,\mathbf{r}_N)$ is the CGA of $P(\mathbf{r}_2,\ldots,\mathbf{r}_N)$ over $N-1$ coordinates,

$$\bar{P}(\mathbf{r}_2,\ldots,\mathbf{r}_N)=\frac{1}{\Omega^{N-1}}\int_{\Omega(\mathbf{r}_1)}d\mathbf{r}_2'\cdots\int_{\Omega(\mathbf{r}_N)}d\mathbf{r}_N'P(\mathbf{r}_2',\ldots,\mathbf{r}_N'). \tag{6.8}$$

Due to the Bose symmetry of the wave function, Eq. (6.7) could equally well be written in any of the forms

$$\begin{aligned}\overline{|\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2}&\cong\bar{P}(\mathbf{r}_1,\mathbf{r}_3,\ldots,\mathbf{r}_N)\bar{\rho}(\mathbf{r}_2)\\&\cong\bar{P}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_4,\ldots,\mathbf{r}_N)\bar{\rho}(\mathbf{r}_3),\quad\text{etc.}\end{aligned} \tag{6.9}$$

Since the functions $\overline{|\Psi|^2}$, $\bar{P}$, and $\bar{\rho}$ are all well-defined mathematical functions, Eq. (6.9) can be satisfied only if

$$\overline{|\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2}\cong\prod_{n=1}^{N}\bar{\rho}(\mathbf{r}_n). \tag{6.10}$$

Equation (6.10) also implies that

$$\bar{P}(\mathbf{r}_2,\ldots,\mathbf{r}_N)\cong\prod_{n=2}^{N}\bar{\rho}(\mathbf{r}_n). \tag{6.11}$$

VII. CGA OF THE SCHRÖDINGER EQUATION

We next multiply the N-body Schrödinger equation by Ψ^* and perform a CGA of each side over N coordinates,

$$\begin{aligned}&\overline{\Psi^*\sum_{n=1}^{N}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial\mathbf{r}_n^2}+\Xi(\mathbf{r}_n)\Psi+\sum_{m\neq n}v(\mathbf{r}_n-\mathbf{r}_m)\Psi\right)}\\&\quad=-i\hbar\overline{\Psi^*\frac{\partial\Psi}{dt}}.\end{aligned} \tag{7.1}$$

$\Xi(\mathbf{r}_n)$ is the applied potential and $2v(\mathbf{r}_n-\mathbf{r}_m)$ is the potential energy of interaction between particles n and m. Considering first the term associated with the potential energy of interaction between particles,

$$\begin{aligned}\overline{\sum_n\sum_{m\neq n}v(\mathbf{r}_n-\mathbf{r}_m)|\Psi|^2}&=\frac{1}{\Omega^N}\int_{\Omega(\mathbf{r}_1)}d\mathbf{r}_1'\int_{\Omega(\mathbf{r}_2)}d\mathbf{r}_2'\cdots\\&\quad\times\int_{\Omega(\mathbf{r}_N)}d\mathbf{r}_N'\sum_{n=1}^{N}\sum_{m\neq n}v(\mathbf{r}_n'-\mathbf{r}_m')|\Psi|^2.\end{aligned} \tag{7.2}$$

It follows from the definition of $\psi_{\mathbf{s}}(\mathbf{r})$ that the term $n=1$ can be written as

$$\begin{aligned}\overline{\sum_{m\neq1}v(\mathbf{r}_1-\mathbf{r}_m)|\Psi|^2}&=\frac{1}{\Omega^{N-1}}\int_{\Omega(\mathbf{r}_2)}d\mathbf{r}_2'\cdots\\&\quad\times\int_{\Omega(\mathbf{r}_N)}d\mathbf{r}_N'P(\mathbf{r}_2',\ldots,\mathbf{r}_N')\frac{1}{\Omega}\\&\quad\times\int_{\Omega(\mathbf{r}_1)}\sum_{m\neq1}v(\mathbf{r}_1'-\mathbf{r}_m')|\psi_{\mathbf{s}}(\mathbf{r}_1')|^2d\mathbf{r}_1'.\end{aligned} \tag{7.3}$$

By the arguments of Secs. V and VI the integral over $\mathbf{r}_1'$ in Eq. (7.3) is the same for all $\mathbf{s}$ that occur to within terms $\sim1/\sqrt{N_\Omega}$. Hence it is determined only by $\mathbf{r}_1$ and can be expressed in the form

$$\int_{\Omega(\mathbf{r}_1)}\sum_{m\neq1}^{N}v(\mathbf{r}_1'-\mathbf{r}_m)|\psi_{\mathbf{s}}(\mathbf{r}_1')|^2d\mathbf{r}_1'\cong\Omega\bar{\rho}(\mathbf{r}_1)\bar{v}(\mathbf{r}_1). \tag{7.4}$$

It is shown in Sec. IX that $\bar{v}(\mathbf{r})$ is the average potential energy per particle within the element $\Omega(\mathbf{r})$.

It follows from Eqs. (7.4) and (7.3) that

$$\begin{aligned}\overline{\sum_{m\neq1}v(\mathbf{r}_1-\mathbf{r}_m)|\Psi|^2}&\cong\bar{P}(\mathbf{r}_2,\ldots,\mathbf{r}_N)\bar{v}(\mathbf{r}_1)\bar{\rho}(\mathbf{r}_1)\\&\cong\prod_{m\neq1}^{N}\bar{\rho}(\mathbf{r}_m)\bar{v}(\mathbf{r}_1)\bar{\rho}(\mathbf{r}_1),\end{aligned} \tag{7.5}$$

where Eqs. (6.8) and (6.11) have been used. All other terms in the sum over n can be treated in an identical fashion. Thus Eq. (7.2) reduces to

$$\overline{\sum_n\sum_{m\neq n}v(\mathbf{r}_n-\mathbf{r}_m)|\Psi|^2}\cong\sum_{n=1}^{N}\prod_{m\neq n}\bar{\rho}(\mathbf{r}_m)\eta^*(\mathbf{r}_n)\bar{v}(\mathbf{r}_n)\eta(\mathbf{r}_n), \tag{7.6}$$

where $\eta(\mathbf{r})$ is defined as

$$\eta(\mathbf{r})=\sqrt{\bar{\rho}(\mathbf{r})}. \tag{7.7}$$

The kinetic energy term can be treated similarly. It is shown in Appendix A that, provided the density and hence $\eta(\mathbf{r})$ vary slowly with $\mathbf{r}$,

$$\begin{aligned}&\frac{1}{\Omega}\int_{\Omega(\mathbf{r})}\psi_{\mathbf{s}}^*(\mathbf{r}')\frac{-\hbar^2}{2m}\frac{\partial^2\psi_{\mathbf{s}}(\mathbf{r}')}{\partial\mathbf{r}^2}d\mathbf{r}'\\&\quad\cong\frac{-\hbar^2}{2m}\eta^*(\mathbf{r})\frac{\partial^2\eta(\mathbf{r})}{\partial\mathbf{r}^2}+\bar{\rho}(\mathbf{r})\bar{\kappa}(\mathbf{r}).\end{aligned} \tag{7.8}$$

The first term on the left in Eq. (7.8) is the contribution made to the kinetic energy by the slow variation of $\eta(\mathbf{r})$ over macroscopic length scales and is the kinetic energy associated with the net momentum of particles in the element $\Omega(\mathbf{r})$. $\bar{\kappa}(\mathbf{r})$ is the average kinetic energy per particle within $\Omega(\mathbf{r})$ after subtraction of the "center of mass" kinetic energy associated with the first term.

It follows from Eq. (7.8), by a similar argument to that used in the derivation of Eq. (7.6), that

$$\begin{aligned}\overline{\sum_n-\frac{\hbar^2}{2m}\Psi^*\frac{\partial^2\Psi}{\partial\mathbf{r}_n^2}}&\cong\sum_{n=1}^{N}\prod_{m\neq n}\bar{\rho}(\mathbf{r}_m)\eta^*(\mathbf{r}_n)\left(-\frac{\hbar^2}{2m}\frac{\partial^2\eta(\mathbf{r}_n)}{\partial\mathbf{r}_n^2}\right.\\&\quad\left.+\bar{\kappa}(\mathbf{r}_n)\eta(\mathbf{r}_n)\right).\end{aligned} \tag{7.9}$$

It follows by use of Eqs. (6.10) and (7.7) that, provided that the variation of $\Xi(\mathbf{r})$ over the volume Ω is negligible, the term involving the external potential can be written as

$$\overline{\sum_{n=1}^{N}\Xi(\mathbf{r}_n)|\Psi|^2} \cong \sum_{n=1}^{N}\prod_{m\neq n}\bar{\rho}(\mathbf{r}_m)\,\eta^*(\mathbf{r}_n)\Xi(\mathbf{r}_n)\,\eta(\mathbf{r}_n). \tag{7.10}$$

Adding Eqs. (7.6), (7.9), and (7.10), it follows that to within terms $\sim 1/\sqrt{N_\Omega}$ the left-hand side of Eq. (7.1) reduces to

$$\sum_{n=1}^{N}\prod_{m\neq n}\bar{\rho}(\mathbf{r}_m)\,\eta^*(\mathbf{r}_n)\left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}_n^2}+V_{\text{eff}}(\mathbf{r}_n)+\Xi(\mathbf{r}_n)\right)\eta(\mathbf{r}_n), \tag{7.11}$$

where

$$V_{\text{eff}}(\mathbf{r}_n)=\bar{\kappa}(\mathbf{r}_n)+\bar{v}(\mathbf{r}_n). \tag{7.12}$$

It follows by use of Eqs. (7.7) and (6.10) that the right-hand side of Eq. (7.1) can be written in the form

$$-i\hbar\overline{\Psi^*\frac{\partial\Psi}{dt}}=E\overline{|\Psi|^2}\cong\sum_{n=1}^{N}\prod_{m\neq n}\bar{\rho}(\mathbf{r}_m)\,\eta^*(\mathbf{r}_n)\varepsilon\,\eta(\mathbf{r}_n). \tag{7.13}$$

E is the total ground-state energy and $\varepsilon = E/N$ is the average energy per particle. Equating Eqs. (7.11) and (7.13), it follows that to within terms $\sim 1/\sqrt{N_\Omega}$ the particle n obeys the equation

$$\frac{\hbar^2}{2m}\frac{\partial^2\eta(\mathbf{r}_n)}{\partial\mathbf{r}_n^2}+[V_{\text{eff}}(\mathbf{r}_n)+\Xi(\mathbf{r}_n)]\eta(\mathbf{r}_n)\cong\varepsilon\,\eta(\mathbf{r}_n). \tag{7.14}$$

It follows that for averages over macroscopic regions of space, the system behaves as if every particle occupies the same single-particle state with a wave function $\eta(\mathbf{r})$ satisfying Eq. (7.14).

VIII. TIME DEVELOPMENT OF THE WAVE FUNCTION

In experiments on trapped Bose gases, measurements of the atomic momentum distribution are made by switching off the confining potential and measuring the expansion of the cloud over time. Once the potential is switched off, the system is no longer in its ground state and the wave function can develop a phase that depends upon the coordinates **r**, **s**. The variation of density with time also implies that a nonzero flow of particles must develop within the fluid.

It is assumed that the wave function remains delocalized after the potential is switched off. It seems clear on physical ground that this must be the case, since any localization would require a macroscopic amount of energy. For example, if $\psi_{\mathbf{s}}(\mathbf{r})$ becomes localized within a volume Δr^3, the condensate peak will be broadened by $\sim\hbar/\Delta r$ (see Appendix B). Hence the kinetic energy of atoms in the condensate would change from the ground-state value of $Nf(\hbar/L)^2/2m$ to $Nf(\hbar/\Delta r)^2/2m$—a macroscopic change if N is macroscopic. Any phase variation over length scales $\sim\Delta r$ would give a similar increase in the kinetic energy of the fluid. Hence it is also assumed that any phase that develops has an insignificant variation over the averaging volume Ω. For simplicity of exposition, the wave function is still denoted as $\Psi(\mathbf{r},\mathbf{s})$ although Ψ is no longer strictly the ground-state wave function.

It has been shown previously [11] that in any Bose system of identical particles, described by a wave function $\Psi(\mathbf{r},\mathbf{s})$, the particle flux at **r** can be expressed in the form

$$\mathbf{F}(\mathbf{r})=N\int P(\mathbf{s})\mathbf{F}_{\mathbf{s}}(\mathbf{r})d\mathbf{s}, \tag{8.1}$$

where

$$\mathbf{F}_{\mathbf{s}}(\mathbf{r})=\frac{\hbar}{m}|\psi_{\mathbf{s}}(\mathbf{r})|^2\,\boldsymbol{\nabla}\,\theta_{\mathbf{s}}(\mathbf{r}) \tag{8.2}$$

and $\theta_{\mathbf{s}}(\mathbf{r})$ is the phase of $\psi_{\mathbf{s}}(\mathbf{r})$.

Since Eqs. (8.1) and (8.2) are of the form given in Eqs. (5.12) and (5.13), it follows that the CGA of $\mathbf{F}_{\mathbf{s}}(\mathbf{r})$ is the same to within terms $\sim 1/\sqrt{N_\Omega}$ for all **s** that occur,

$$\frac{1}{\Omega}\int_{\Omega(\mathbf{r})}\mathbf{F}_{\mathbf{s}}(\mathbf{r}')d\mathbf{r}'\cong\mathbf{F}(\mathbf{r}). \tag{8.3}$$

Writing $\mathbf{F}(\mathbf{r})$ in the form

$$\mathbf{F}(\mathbf{r})\cong\bar{\rho}(\mathbf{r})\frac{\hbar}{m}\,\boldsymbol{\nabla}\,\bar{\theta}(\mathbf{r}) \tag{8.4}$$

implies that $(\hbar/m)\boldsymbol{\nabla}\,\bar{\theta}(\mathbf{r})$ can be interpreted as the velocity of an element $\Omega(\mathbf{r})$ of density $\bar{\rho}(\mathbf{r})$. It follows from Eq. (8.2) and the definition of $\bar{\rho}(\mathbf{r})$ in Eq. (6.4) that $\boldsymbol{\nabla}\bar{\theta}(\mathbf{r})$ is the average of $\boldsymbol{\nabla}\theta_{\mathbf{s}}$ over $\Omega(\mathbf{r})$, weighted by the probability distribution $|\psi_{\mathbf{s}}(\mathbf{r})|^2$,

$$\boldsymbol{\nabla}\,\bar{\theta}(\mathbf{r})=\int_{\Omega(\mathbf{r})}|\psi_{\mathbf{s}}(\mathbf{r}')|^2\,\boldsymbol{\nabla}\,\theta_{\mathbf{s}}(\mathbf{r}')d\mathbf{r}'\bigg/\int_{\Omega(\mathbf{r})}|\psi_{\mathbf{s}}(\mathbf{r}')|^2d\mathbf{r}'. \tag{8.5}$$

Note that Eqs. (8.1) and (8.2) are valid in any Bose system of identical particles, but that Eqs. (8.3)–(8.5) are valid only if $\psi_{\mathbf{s}}(\mathbf{r})$ is delocalized.

The presence of a slowly varying average phase $\bar{\theta}(\mathbf{r})$ can be incorporated by generalizing Eq. (7.7) to

$$\eta(\mathbf{r})=\sqrt{\bar{\rho}(\mathbf{r})}\,\exp[i\bar{\theta}(\mathbf{r})]. \tag{8.6}$$

It is shown in Appendix A that Eq. (7.9) is still valid with $\eta(\mathbf{r})$ given by Eq. (8.6), provided that $\psi_{\mathbf{s}}(\mathbf{r})$ is delocalized and both $\bar{\rho}(\mathbf{r})$ and $\bar{\theta}(\mathbf{r})$ vary slowly with **r**, as assumed. The derivation of Eqs. (7.6) and (7.10) is unaffected by the presence of a phase factor in $\eta(\mathbf{r})$. Hence the left-hand side of Eq. (7.1) still reduces to the form given by Eq. (7.11).

With the substitution of Ψ by Eq. (1.1) the right-hand side of Eq. (7.1) reduces to

$$i\hbar\overline{\Psi^*\frac{\partial\Psi}{dt}}\cong\left(\sum_{n=1}^{N}\prod_{m\neq n}\bar{\rho}(\mathbf{r}_m)\,\eta^*(\mathbf{r}_n)\right)i\hbar\frac{\partial}{\partial t}\eta(\mathbf{r}_n). \tag{8.7}$$

Equating (8.7) and (7.11), it follows that, to within terms $\sim 1/\sqrt{N_\Omega}$, Eq. (7.1) is satisfied by substitution in Eq. (1.1), provided that each particle coordinate satisfies

$$\frac{\hbar^2}{2m}\frac{\partial^2 \eta(\mathbf{r}_n)}{\partial \mathbf{r}_n^2} + V_{\mathrm{eff}}(\mathbf{r}_n)\,\eta(\mathbf{r}_n) + \Xi(\mathbf{r}_n)\,\eta(\mathbf{r}_n) \cong i\hbar\frac{\partial}{\partial t}\eta(\mathbf{r}_n). \tag{8.8}$$

To within terms $\sim 1/\sqrt{N_\Omega}$, the fluid therefore again behaves as if every particle occupies the same single-particle state, with a wave function $\eta(\mathbf{r})$ satisfying a single-particle Schrödinger equation.

IX. THE GROSS-PITAEVSKII EQUATIONS

According to Eq. (7.12) the effective single-particle potential $V_{\mathrm{eff}}(\mathbf{r})$ in Eqs. (7.14) and (8.8) is the sum of $\bar{\kappa}(\mathbf{r})$, defined in Eq. (7.8), and $\bar{v}(\mathbf{r})$, defined in Eq. (7.4). $\bar{v}(\mathbf{r})$ is the contribution made by the element $\Omega(\mathbf{r})$ to the potential energy integral in Eq. (5.16). It follows by use of Eq. (5.15) that, to within terms $\sim 1/\sqrt{N_\Omega}$, $N\Omega\bar{\rho}(\mathbf{r})\bar{v}(\mathbf{r})$ is the total potential energy of particles within $\Omega(\mathbf{r})$. Since the element contains $\cong N\Omega\bar{\rho}(\mathbf{r})$ atoms, $\bar{v}(\mathbf{r})$ is the average potential energy per particle within the element. It is shown in Appendix A that $\bar{\kappa}(\mathbf{r})$ is the average kinetic energy per particle within $\Omega(\mathbf{r})$, after subtraction of the kinetic energy associated with the net momentum of the element.

Hence the effective single particle potential is

$$V_{\mathrm{eff}}(\mathbf{r}) = \varepsilon[\rho(\mathbf{r})], \tag{9.1}$$

where ε is the average energy per particle within an element $\Omega(\mathbf{r})$ with zero net momentum. The density within the element can be taken as constant and equal to the value $\rho(\mathbf{r})$ at the center of the element. In the ground state the total energy has its minimum value and this will be obtained when atoms within each element have minimum energy. Hence ε is the ground-state energy per particle at the local density.

It follows from the definition of $\eta(\mathbf{r})$ in Eqs. (7.7) and (8.6) that Eqs. (7.14) and (8.8) are nonlinear equations for $\eta(\mathbf{r})$. Furthermore, it is a standard result of calculations on the dilute Bose gas that ε is proportional to ρ at low density. Hence, with weak interactions, $V_{\mathrm{eff}}(\mathbf{r}) \propto |\eta(\mathbf{r})|^2$ and Eqs. (7.14) and (8.8) reduce to the time-independent and time-dependent GP equations. However, with $V_{\mathrm{eff}}(\mathbf{r})$ given by Eq. (9.1), Eqs. (7.14) and (8.8) are valid for any strength of particle interaction. Any nonlinearity in the relation $\varepsilon(\rho)$ will lead to deviations from the predictions of the GP equation. The dependence of ε upon the density can be calculated by a variety of methods, even with strong interactions. Hence corrections to the GP equation could also be calculated and, if sufficiently accurate measurements could be made, the accuracy of Eqs. (7.14) and (8.8) could be experimentally tested.

X. LIMITS OF VALIDITY

It should first be stressed that the arguments of Secs. V–IX are valid only if the wave function is delocalized. A physical example of a system that does not have a delocalized wave function is a close-packed fluid (see Fig. 5).

If particle configurations $\mathbf{r}_1, \ldots, \mathbf{r}_N$ that occur in the ground state contain no space large enough to accommodate another particle, then configurations $\mathbf{s}$ of $N-1$ particles that occur will contain only a single space. Loosely speaking, if a particle is removed it can be replaced only in the space left by its removal. Hence, in a sufficiently close-packed fluid, $\psi_{\mathbf{s}}(\mathbf{r})$ is localized within a single space of dimension $\sim d$.

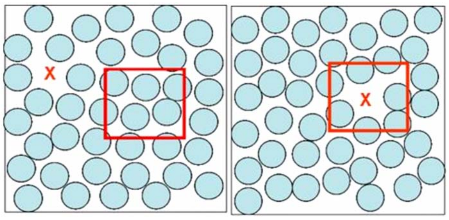

FIG. 5. (Color online) Two different possible configurations $\mathbf{s}$ of $N-1$ hard-sphere particles in a close-packed system. $\psi_{\mathbf{s}}(\mathbf{r})$ is localized within a single space of dimension $\sim d$ surrounding the cross in the figures. A particular element Ω is also illustrated. In the left-hand figure $\psi_{\mathbf{s}}(\mathbf{r})$ is localized outside the element and CGAs over the element are zero. In the right-hand figure $\psi_{\mathbf{s}}(\mathbf{r})$ is localized inside the element and CGA's over the element are nonzero.

The arguments given in Secs. V–VIII fail in a number of ways in this case. Integrals such as (5.1), (5.16), and (5.19) cannot be expressed as the sum of many cell contributions, since only ~ 1 cell will give a nonzero contribution. The CGA is not a useful operation, since there can be no long-range averaged structure in expressions containing $\psi_{\mathbf{s}}(\mathbf{r})$. Furthermore, coarse-grained averages are not even approximately independent of $\mathbf{s}$. For example, if $\mathbf{s}$ is such that $\psi_{\mathbf{s}}(\mathbf{r})$ is localized within the element $\Omega(\mathbf{r})$, as is the case on the right in Fig. 5, CGAs over the element are nonzero. For $\mathbf{s}$ where $\psi_{\mathbf{s}}(\mathbf{r})$ is localized outside $\Omega(\mathbf{r})$, as on the left in Fig. 5, they are zero. Hence, if $\psi_{\mathbf{s}}(\mathbf{r})$ is localized, none of the arguments in Secs. IV–VIII are valid and the single-particle equations (7.14) and (8.8) are not even approximately accurate.

Localization of $\psi_{\mathbf{s}}(\mathbf{r})$ to within distances $\sim d$ also implies that BEC is not present, since it follows from standard Fourier transform theory that any peak in $n_{\mathbf{s}}(\mathbf{r})$ must then have a minimum width of $\sim\hbar/d$. Delocalization of $\psi_{\mathbf{s}}(\mathbf{r})$ and hence MSPQB are usually present only in the presence of BEC. It is worth noting, however, that BEC is not strictly necessary for MSPQB to occur. BEC implies that the wave function is delocalized over a distance comparable to the macroscopic dimension $\sim L$ of the entire sample. All that is required for MSPQB to occur is that the wave function is delocalized over distances much greater than a typical interatomic spacing.

It should also be stressed that the results are accurate only when behavior over macroscopic length scales is considered. For example, they do not accurately describe measurements that resolve spatial structure on very short length scales. The uncertainties are $\sim 1/\sqrt{N_\Omega}$, where N_Ω is the number of atoms within the averaging or resolution volume. This failure is due to the probabilistic nature of the many-particle wave function and appears to be an unavoidable consequence of quantum fluctuations. These dominate over length scales $\sim d$, the average spacing between atoms. In particular, this implies that the results are valid only if the macroscopic density $\bar{\rho}(\mathbf{r})$, flow velocity $(\hbar/m)\boldsymbol{\nabla}\bar{\theta}(\mathbf{r})$, and external potential $\Xi(\mathbf{r})$ vary negligibly over length scales comparable to the interatomic spacing.

This is not a serious limitation for describing macroscopic behavior, since similar constraints apply to all macroscopic thermodynamic variables. These are defined as averages over volumes containing many atoms and are always uncertain to within terms $\sim 1/\sqrt{N_\Omega}$, where N_Ω is the number of atoms within the volume over which the macroscopic average is taken. Hence Eqs. (7.14) and (8.8) describe macroscopic thermodynamic behavior to the same degree of accuracy that thermodynamic variables can be defined. Note that the derivation of the GP equation in Sec. IX is similarly valid only to within terms $\sim 1/\sqrt{N_\Omega}$. This is consistent with the generally accepted view that the GP equations is not accurate over length scales $\sim d$.

XI. SUMMARY AND CONCLUSIONS

It has been shown that macroscopic single-particle quantum behavior will occur in the ground state of any Bose-Einstein-condensed system, irrespective of the strength of interactions between particles. This is essentially a consequence of two properties of Bose condensed fluids. (1) The ground state wave function is delocalized in the sense discussed in Sec. IV. (2) In any fluid there are no correlations between the positions of atoms separated by distances much greater than a typical interatomic spacing.

The conclusions are valid provided that only macroscopic properties are considered—that is, averages over regions of space containing many atoms. Inaccuracies due to quantum fluctuations are $\sim 1/\sqrt{N_\Omega}$, where N_Ω is the number of particles within the volume over which the average is taken. To within terms $\sim 1/\sqrt{N_\Omega}$, the averaged many-particle wave function can be factorized into a product of single-particle wave functions $\eta(\mathbf{r})$ as in Eq. (1.1). The function $\eta(\mathbf{r})$ satisfies the usual considerations of particle flux given in Eq. (8.4) and obeys the single-particle Schrödinger equations given in Eqs. (7.14) and (8.8). Equation (7.14) determines the macroscopic particle density in the ground state of Bose-Einstein-condensed systems. Equation (8.8) gives the time evolution of this density when a gas in its ground state is released from a trap. These equations reduce to the time-dependent and time-independent Gross-Pitaevskii equations when interactions are weak, but are valid for any strength of interaction between particles. Observed deviations from the predictions of the GP equation could be used to experimentally test the validity of Eqs. (7.14) and (8.8).

All the results derived are valid only if $\psi_{\mathrm{s}}(\mathbf{r})$ is a delocalized function of $\mathbf{r}$. In Bose-Einstein-condensed systems $\psi_{\mathrm{s}}(\mathbf{r})$ must be delocalized over length scales comparable to the system size, that is, $\sim L$. In the absence of BEC $\psi_{\mathrm{s}}(\mathbf{r})$ is usually localized within a region of dimension comparable to the interatomic spacing and MSPQB does not occur. Hence Bose-Einstein-condensed fluids exhibit macroscopic single-particle quantum behavior, whereas most other fluids do not.

APPENDIX A: KINETIC ENERGY

The total kinetic energy is given by Eqs. (5.18) and (5.19). The CGA of the integrand in (5.19) is

$$\kappa_{\mathrm{s}}(\mathbf{r}) = \int_{\Omega(\mathbf{r})} \psi^*{}_{\mathrm{s}}(\mathbf{r}') \frac{-\hbar^2}{2m} \frac{\partial^2 \psi_{\mathrm{s}}(\mathbf{r}')}{\partial \mathbf{r}'^2} d\mathbf{r}'. \tag{A1}$$

We define the function

$$\chi_{\mathrm{s}}(\mathbf{r}) = \psi_{\mathrm{s}}(\mathbf{r})/\eta(\mathbf{r}). \tag{A2}$$

$\eta(\mathbf{r})$ is defined by Eq. (7.7) in the ground state and Eq. (8.6) in the time-dependent case. It follows from the definition of $\chi_{\mathrm{s}}(\mathbf{r})$ and Eq. (6.4) that

$$\int_{\Omega(\mathbf{r})} |\chi_{\mathrm{s}}(\mathbf{r}')|^2 d\mathbf{r}' \cong 1. \tag{A3}$$

The phase of $\chi_{\mathrm{s}}(\mathbf{r})$ is

$$\theta'_{\mathrm{s}}(\mathbf{r}) = \theta_{\mathrm{s}}(\mathbf{r}) - \bar{\theta}(\mathbf{r}), \tag{A4}$$

where $\bar{\theta}(\mathbf{r})$ is defined in Eq. (8.5) and $\theta_{\mathrm{s}}(\mathbf{r})$ is the phase of $\psi_{\mathrm{s}}(\mathbf{r})$. It follows from Eq. (8.5) that the average value of $\boldsymbol{\nabla}\theta'_{\mathrm{s}}(\mathbf{r})$ over the element $\Omega(\mathbf{r})$ is zero. Hence $\chi_{\mathrm{s}}(\mathbf{r})$ can be regarded as the conditional wave function of a system at constant density and with zero net flow.

We assume that $\eta(\mathbf{r})$ varies sufficiently slowly with $\mathbf{r}$ that $\bar{\eta}(\mathbf{r})$ and its first and second derivatives can be approximated by their values at the center of the element. Then these functions can be taken outside the integral over $\Omega(\mathbf{r})$ and

$$\begin{aligned}\kappa_{\mathrm{s}}(\mathbf{r}) \approx{}& |\bar{\eta}(\mathbf{r})|^2 \int_{\Omega(\mathbf{r})} \chi_{\mathrm{s}}^*(\mathbf{r}') \frac{-\hbar^2}{2m} \frac{\partial^2 \chi_{\mathrm{s}}(\mathbf{r}')}{\partial \mathbf{r}'^2} d\mathbf{r}' \\ &+ \bar{\eta}^*(\mathbf{r}) \frac{\partial \bar{\eta}(\mathbf{r})}{\partial \mathbf{r}} \int_{\Omega(\mathbf{r})} \chi_{\mathrm{s}}^*(\mathbf{r}') \frac{-\hbar^2}{2m} \frac{\partial \chi_{\mathrm{s}}(\mathbf{r}')}{\partial \mathbf{r}'} d\mathbf{r}' \\ &+ \bar{\eta}^*(\mathbf{r}) \frac{-\hbar^2}{2m} \frac{\partial^2 \bar{\eta}(\mathbf{r})}{\partial \mathbf{r}^2} \int_{\Omega(\mathbf{r})} |\chi_{\mathrm{s}}(\mathbf{r}')|^2 d\mathbf{r}'.\end{aligned} \tag{A5}$$

Physically, the transformation in Eq. (A2) separates long-range-averaged structure in the particle density and flow from the random structure on length scales $\sim d$. The microscopic momentum density is

$$\mathbf{p}(\mathbf{r}) = (\hbar/i)\chi_{\mathrm{s}}^* \partial \chi_{\mathrm{s}}/\partial \mathbf{r} \tag{A6}$$

and it has a sign that varies randomly over length scales $\sim d$. The long-range-averaged momentum density is

$$\mathbf{P}(\mathbf{r}) = (\hbar/i)\partial \bar{\eta}/d\mathbf{r} \tag{A7}$$

and it has an almost constant value $\mathbf{P}$ within an element.

Dividing the element $\Omega(\mathbf{r})$ into microscopic cells, each of size d^3, where d is the average distance between atoms, the integral in Eq. (A1) can be expressed as the sum over N_Ω cell contributions. The transformation (A2) subtracts $\mathbf{P}$ from the momentum $\mathbf{p}_n$ of each cell. Hence the kinetic energy is

$$\sum_{n=1}^{N_\Omega} \frac{(\mathbf{p}_n - \mathbf{P})^2}{2M} = \sum_{n=1}^{N_\Omega} \left(\frac{\mathbf{p}_n{}^2 - 2\mathbf{p}_n \cdot \mathbf{P} + \mathbf{P}^2}{2M} \right). \tag{A8}$$

The three terms in (A8) correspond to the three terms in (A5). Physically the first term in each equation is the kinetic energy due to the random motion on length scales $\sim d$. By the arguments of Sec. VI this is independent of **s** to within terms $\sim 1/\sqrt{N_\Omega}$,

$$\frac{-\hbar^2}{2m}\int_{\Omega(\mathbf{r})}\chi_{\mathbf{s}}(\mathbf{r}')\frac{\partial^2\chi_{\mathbf{s}}(\mathbf{r}')}{\partial\mathbf{r}'^2}d\mathbf{r}' \cong \bar{\kappa}(\mathbf{r}). \tag{A9}$$

The third term is the kinetic energy due to the net momentum of the element. The second term in Eqs. (A8) and (A5) averages to zero to within terms $\sim 1/\sqrt{N_\Omega}$, due to the random variation in the direction of the $\mathbf{p}_n$. Hence, to within terms $\sim 1/\sqrt{N_\Omega}$ and using Eqs. (A3) and (A9) Eq. (A1) reduces to

$$\kappa_{\mathbf{s}}(\mathbf{r}) \cong \bar{\eta}^*(\mathbf{r})\frac{-\hbar^2}{2m}\frac{\partial^2\bar{\eta}(\mathbf{r})}{\partial\mathbf{r}^2} + |\bar{\eta}(\mathbf{r})|^2\bar{\kappa}(\mathbf{r}). \tag{A10}$$

APPENDIX B: MOMENTUM DISTRIBUTION OF ATOMS IN THE CONDENSATE

In systems where the particle density varies with position, it follows from Eq. (A2) that $\psi_{\mathbf{s}}(\mathbf{r})$ can be regarded as the product of $\chi_{\mathbf{s}}(\mathbf{r})$ with an "envelope" function $\eta(\mathbf{r})$. It follows from the convolution theorem that the Fourier transform of $\psi_{\mathbf{s}}(\mathbf{r})$ is

$$\tilde{\psi}_{\mathbf{s}}(\mathbf{p}) = \tilde{\eta}(\mathbf{p}) \otimes \tilde{\chi}_{\mathbf{s}}(\mathbf{p}), \tag{B1}$$

where

$$\tilde{\psi}_{\mathbf{s}}(\mathbf{p}) = \int \psi_{\mathbf{s}}(\mathbf{r})\exp(i\mathbf{p}\cdot\mathbf{r})d\mathbf{r}, \tag{B2}$$

with similar expressions for $\tilde{\eta}(\mathbf{p})$ and $\tilde{\chi}_{\mathbf{s}}(\mathbf{p})$.

In the presence of BEC, $\chi_{\mathbf{s}}(\mathbf{r})$ can be regarded as a function that is nonzero as $\mathbf{r}\to\infty$ and $\tilde{\chi}_{\mathbf{s}}(\mathbf{p})$ therefore contains a δ function peak $\delta(\mathbf{p})$. However, since $\eta(\mathbf{r})$ is nonzero only over a finite region of dimension $\sim L$, $\tilde{\eta}(\mathbf{p})$ has a minimum width $\sim\hbar/L$. After convolution with the δ function in $\tilde{\chi}_{\mathbf{s}}(\mathbf{p})$, this gives a condensate peak with width $\sim\hbar/L$ and a distribution of momenta $|\tilde{\eta}(\mathbf{p})|^2$. For example, with a density distribution $\rho(\mathbf{r})\propto\exp[-r^2/(2\sigma^2)]$, the momentum distribution of atoms in the condensate peak is a Gaussian of standard deviation $\frac{1}{2}\hbar/\sigma$.

APPENDIX C: THE ORDER PARAMETER

The single-particle density matrix is defined in terms of the wave function as

$$\rho_1(\mathbf{r},\mathbf{r}') = \int \Psi^*(\mathbf{r},\mathbf{s})\Psi(\mathbf{r}',\mathbf{s})d\mathbf{s} = \int P(\mathbf{s})\psi^*_{\mathbf{s}}(\mathbf{r})\psi_{\mathbf{s}}(\mathbf{r}')d\mathbf{s}, \tag{C1}$$

where the definition of $\psi_{\mathbf{s}}(\mathbf{r})$ in Sec. II has been used. The CGA of $\rho_1(\mathbf{r},\mathbf{r}')$ over the two coordinates $\mathbf{r}$, $\mathbf{r}'$ can be defined in a similar way to Eq. (6.6):

$$\begin{aligned}\bar{\rho}_1(\mathbf{r},\mathbf{r}') &= \frac{1}{\Omega^2}\int_{\Omega(\mathbf{r})}\int_{\Omega(\mathbf{r}')}\rho_1(\mathbf{r}'',\mathbf{r}''')d\mathbf{r}''d\mathbf{r}''' \\ &= \int P(\mathbf{s})\overline{\psi^*_{\mathbf{s}}(\mathbf{r})\psi_{\mathbf{s}}(\mathbf{r}')}d\mathbf{s}.\end{aligned} \tag{C2}$$

It follows by use of Eqs. (6.3) and (2.3) that

$$\bar{\rho}_1(\mathbf{r},\mathbf{r}') \cong \bar{\psi}^*(\mathbf{r})\bar{\psi}(\mathbf{r}'). \tag{C3}$$

This should be compared with the standard [16] criterion for the presence of BEC,

$$\rho_1(\mathbf{r},\mathbf{r}') \to \langle\hat{\psi}(\mathbf{r})\rangle\langle\hat{\psi}^*(\mathbf{r}')\rangle \quad \text{for } |\mathbf{r}-\mathbf{r}'| \gg d. \tag{C4}$$

Note that the condition $|\mathbf{r}-\mathbf{r}'|\gg d$ does not appear in Eq. (C3). The nonconstant part of $\rho_1(\mathbf{r},\mathbf{r}')$ generally decays to zero for $|\mathbf{r}-\mathbf{r}'|>\sim d$. Hence the contribution to $\bar{\rho}_1(\mathbf{r},\mathbf{r}')$ of the region excluded in Eq. (C4) is $\sim 1/N_\Omega$ and the CGA of Eq. (C4) is satisfied to within terms $\sim 1/N_\Omega$ even when $\mathbf{r}=\mathbf{r}'$.

$\langle\hat{\psi}(\mathbf{r})\rangle$ in Eq. (C4) is generally identified with the order parameter, a new thermodynamic variable created when the BEC forms. It follows by comparison between Eqs. (C3) and (C4) that the order parameter can also be identified as $\bar{\psi}(\mathbf{r})$. The inexact equality in Eq. (C3) reflects the fact that, as defined in Eqs. (6.1) and (6.2), $\bar{\psi}(\mathbf{r})$ has fluctuations $\sim 1/\sqrt{N_\Omega}$. This is consistent with the status of the order parameter as a macroscopic thermodynamic variable. It is easily shown that, if $\psi_{\mathbf{s}}(\mathbf{r})$ is localized within a region $\sim d^3$, $\bar{\psi}(\mathbf{r})$ is zero to within terms $\sim 1/\sqrt{N_\Omega}$. Again this is consistent with the interpretation of $\bar{\psi}(\mathbf{r})$ as the order parameter.

It is also worth noting that this definition of the order parameter is compatible with that given previously [11],

$$\langle\psi(\mathbf{r})\rangle = \int P(\mathbf{s})\psi_{\mathbf{s}}(\mathbf{r})d\mathbf{r}. \tag{C5}$$

It follows from Eqs. (6.2) and (2.3) that the CGA of Eq. (C5) is

$$\overline{\langle\psi(\mathbf{r})\rangle} \cong \overline{\psi(\mathbf{r})}. \tag{C6}$$

Hence, provided only averages over regions of space containing many atoms are considered, the two definitions are equivalent.

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[18] This is true providing $N > \sim 100$. At small N the distribution appears more like a Poisson distribution.

[19] With smaller systems, deviations can be significant. For example, $N=10^5$ gives deviations of $\sim 1\%$ with significant probability.

[20] Assume $\psi_{\mathbf{S}}(\mathbf{r})$ is nonzero only within a volume V_f. Then it follows from Eq. (2.5) that $c=1/\sqrt{V_f}$ and from Eq. (2.10) that $f_{\mathbf{S}}=V_f/V$.

[21] See, for example, K. Huang, *Statistical Mechanics*, 2nd ed. (Wiley, New York, 1987), Appendix III A.

[22] Similar comments apply to other physical quantities that can be expressed in terms of $\psi_{\mathbf{S}}(\mathbf{r})$ and which have no $\mathbf{r}$ dependence. A trivial example is the particle density $\bar{\rho}(\mathbf{r})$. If this is constant, it follows from the definition in Eq. (2.6) that the average of $|\psi_{\mathbf{S}}(\mathbf{r})|^2$ over $\mathbf{s}$ is independent of $\mathbf{r}$. Hence every cell makes the same contribution to the integral of the density over V. Other examples are the integrands in Eqs. (5.16), (5.18), and (8.1).

[23] See, for example, E. W. Weistein, http://mathworld.wolfram.com/CentralLimitTheorem.html

[24] L. Landau and E. M. Lifshitz, *Statistical Physics*, 3rd ed. (Pergamon, New York, 1978), Sec. II.

[25] There is a slight complication, in that the number of atoms within the total volume V is fixed whereas the number of atoms within an element is not. However, it follows from a similar argument to that used to derive Eq. (5.11), or indeed from the standard theory of fluids (Ref. [24] Sec. 118), that the fluctuation in the number of particles within an element is $\Delta N_\Omega / N_\Omega \sim 1/\sqrt{N_\Omega}$. Fluctuations in N_Ω will add to fluctuations at fixed N_Ω, but total fluctuations will still be $\sim 1/\sqrt{N_\Omega}$.