Fragmented Condensate Ground State of Trapped Weakly Interacting Bosons in Two Dimensions

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The ground state and its structure for a rotating, harmonically trapped N-boson system with a weak repulsive contact interaction are studied as the angular momentum L increases up to $3N$. We show that the ground state is generally a fragmented condensate due to angular momentum conservation. In response to an (arbitrarily weak) asymmetric perturbation of the trap, however, the fragmented ground state can be transformed into a single condensate state. We manifest this intrinsic instability by calculating the conditional probability distributions, which show patterns analogous to the boson density distributions predicted by mean-field theory.

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Following the experimental realization of a dilute atomic Bose-Einstein condensate (BEC), the formation and properties of vortices in an atomic BEC have caused considerable interest both experimentally [1] and theoretically [2–9] in the past few years. Although the recent demonstrations of vortex states by several different groups are in the Thomas-Fermi limit of strong interatomic interaction, a great deal of attention has also been attached to the nonvanishing angular momentum (AM) states of weakly interacting N-boson systems in harmonic traps. In Ref. [3], Wilkin *et al.* considered the case of an attractive interaction and showed that the ground state is *uncondensed* and is an example of the *fragmented* condensate discussed by Nozières and Saint James [10]. Mottelson [4], Bertsch, and Papenbrock [5] considered the lowest energy quantum states of a repulsively interacting Bose gas when $L \leqslant N$. Wilkin *et al.* have employed a composite boson/fermion picture to describe configurations beyond the one-vortex state [6]. A more tractable mean-field calculation performed by Butts and Rokhsar revealed a succession of transitions between stable vortex patterns of differing symmetries in the high AM regime [7]. The connection between the mean-field theory (MFT) and exact diagonalization scheme has been studied by Jackson *et al.* for a special case of $L = 2N$ [8]. Finally, some analytical results have also been reported for the lowest energy states [9].

In this Letter, we address the question of whether the ground state of a weakly interacting N-boson system with a given AM is what one would normally expect, i.e., a state with a single coherent Bose condensate, in which a mean-field approximation is valid. We propose that this is not the case and the ground state is generally a *fragmented* condensate in the presence of the weakly repulsive interatomic interaction except $L/N = 0$ or 1 in the thermodynamic limit. By evaluating the macroscopic eigenvalues of the single-particle (SP) density matrix, we determine the degree of condensation. The origin of fragmentation turns out to be a requirement of the conservation of AM. As a result, by turning on an (arbitrarily weak) asymmetric perturbation of the trap, the fragmented ground state can be easily deformed to a single condensate state [11]. This intrinsic instability can be manifested by the conditional probability distributions (CPDs) calculated for the ground state, which show patterns analogous to boson density distributions predicted by MFT. Note that the weakly interacting N-boson system considered here is quite similar to the spin-1 Bose gas studied by Ho and Yip [12], in which the fragmentation originates from the spin conservation.

We start from the model Hamiltonian describing N bosons in a two-dimensional harmonic trap interacting via a weak contact interaction. The SP spectrum is usually expressed in terms of the AM quantum number m and the radial quantum number n_r, by $E_{n_r,m} = (2n_r + |m| + 1)\hbar\omega$. In the ground state of the system, all the bosons are in states with $n_r = 0$, and with m being zero or having the same sign as the total AM. In the second quantized form, the Hamiltonian reads

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V},$$
$$\mathcal{H}_0 = \hbar\omega \sum_j (j + 1)\hat{a}_j^+ \hat{a}_j, \tag{1}$$
$$\mathcal{V} = \frac{1}{2} g \sum_{i,j,k,l} V_{ijkl}\hat{a}_i^+ \hat{a}_j^+ \hat{a}_k \hat{a}_l,$$

where $\mathcal{H}_0$ is the SP oscillator Hamiltonian and $\mathcal{V}$ is the two-body interaction between bosons. In the perturbative regime of weak interactions, $Ng \ll \hbar\omega$. The operator $\hat{a}_j$ and $\hat{a}_j^+$ annihilate and create one boson in the SP oscillator state $|j\rangle$ with energy $(j + 1)\hbar\omega$ and AM $j\hbar$, respectively, and obey the bosonic commutation rules. The contact interaction elements are given by $V_{ijkl} = \delta_{i+j,k+l}2^{-(i+j)}(i + j)!/(i!j!k!l!)^{1/2}$ [9], and most of them are actually vanishing. For a given total AM L and number of bosons N, we consider the Fock space spanned by states $|\alpha\rangle = |n_0, n_1, \ldots, n_k\rangle$ with $\sum_j n_j = N$ and $\sum_j jn_j = L$. Here, n_j denotes the occupation of the jth SP oscillator state $|j\rangle$. There is a huge degeneracy corresponding to many different ways of distributing L quanta of AM among N atoms. Here, we restrict ourselves in a *truncated* Fock space of $0 \leqslant j \leqslant j_{\max} = 6$ [8,13]. To obtain the energy spectra and the corresponding eigenstates, we set up the matrix elements in the Fock space basis, and subsequently diagonalize the matrix by using the Davidson algorithm [14].

A fragmented ground state.—First, consider the SP density matrix in the form of

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{ij} \psi_i^*(\mathbf{r}) \rho_{ij} \psi_j(\mathbf{r}'), \tag{2}$$

with $\psi_m(\mathbf{r}) = \langle \mathbf{r} \,|\, m \rangle$. In Ref. [15], Yang showed that the appearance of condensation is associated with the single macroscopic eigenvalue (i.e., of order N) of the density matrix $\rho(\mathbf{r}, \mathbf{r}')$ with the "condensate wave function" being the associated eigenvector, while the case of more than one macroscopic eigenvalue has been referred to as a "fragmented" condensate [10]. The most important difference between the single and fragmented condensate is the lack of phase coherence of the latter. To find the eigenvalues of the SP density matrix, we write [15]

$$\rho_{ij} = \mathrm{Sp} \hat{a}_i \rho \hat{a}_j^+, \tag{3}$$

where the trace runs over all the $N - 1$ boson states, and the density matrix $\rho = |\Psi_{\mathrm{GS}}\rangle\langle\Psi_{\mathrm{GS}}|$. It is readily seen that the eigenvalues are nothing but the occupation numbers of the SP oscillator state due to the conservation of the total AM, namely, $\rho_{ij} = \delta_{ij} n_j$. It is difficult to give an explicit expression for the occupation numbers n_j. In the case of $L = N$, Wilkin *et al.* find that, in the limit of $N \rightarrow \infty$, to the order $O(1/N)$ [3],

$$n_0 = 1, \qquad n_1 = N - 2, \qquad \text{and} \qquad n_2 = 1. \tag{4}$$

They therefore conclude that the N-boson system is fully condensed into the one-vortex state in the thermodynamic limit. More detailed information can be obtained from the exact diagonalization calculations [5]. In Fig. 1, we show the L dependence of the occupation numbers n_j and their fluctuations $\Delta n_j = (\langle \hat{n}_j^2 \rangle - \langle \hat{n}_j \rangle^2)^{1/2}$ for $j = 0, 1, 2, 3, 4$ for a system of $N = 40$ bosons. When $L \leqslant N$, the occupation numbers evolve rather smoothly as the AM increases [5], while, for $L > N$, there are many kinks in the curves, reflecting the complexity of the ground states. The most prominent feature in the figure is that for a high AM there are generally at least two *significant* occupation numbers. For instance, at $L = 70$, the system has two large occupation numbers: $n_j \approx 9$ and 23 for $j = 0$ and 2, respectively. Evidently the case gives a fragmented condensate. Although the present calculation is performed in the case of $N = 40$, the conclusion that a fragmented condensate ground state exists universally applies to the trapped, weakly interacting and rotating N-boson systems with an arbitrary N including the thermodynamic limit $N \rightarrow \infty$ [7].

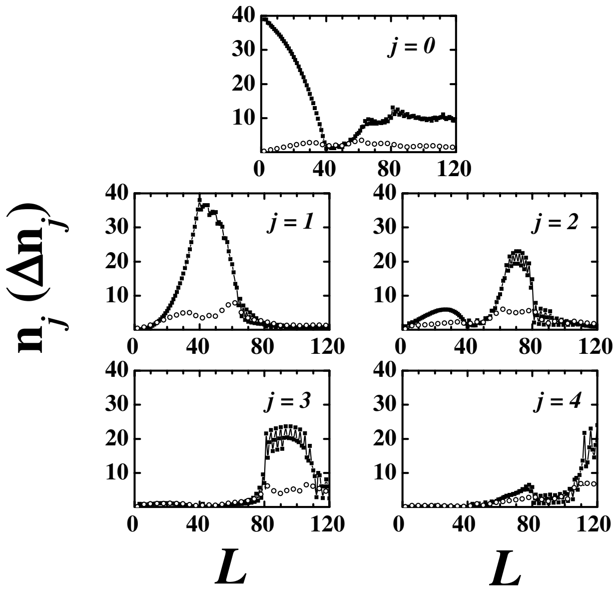

FIG. 1. Values of n_j (solid squares) and Δn_j (open circles) of five lowest SP oscillator states as a function of L for a system of $N = 40$ bosons with $j_{\max} = 6$. The cases of $j = 5$ and 6 are not shown due to their low occupancy.

To examine the validity of the above statement, we investigate the N dependence of the number of significantly occupied SP states by computing the inverse participation ratio [5,16]:

$$I_C = \sum_j (n_j/N)^2. \tag{5}$$

The I_C is the first nontrivial moment of the distribution of occupation numbers among the different SP states (note that $\sum_j n_j/N = 1$ by normalization). Its inverse $1/I_C$ qualitatively measures the number of significantly occupied SP states. Figure 2 shows a plot of $1/I_C$ as a function of AM L for a system of $N = 30$, 40, 50, and 60 bosons. It is easy to see that in the regime of $L/N < 1.6$ the value of $1/I_C$ varies smoothly as L/N increases and shows little dependence on N. In particular, the variation of the peak height at $L/N \approx 1.6$ is less than 3% as N increases from 30 to 60 (not shown in the figure). For $L/N > 1.6$, some irregular small oscillations appear in the curves. However, the overall profile of $1/I_C$ is still nearly independent of N. These small oscillations are purely due to the finite N effect [17] and decay gradually with increasing N. One may expect them to vanish in the limit of $N \rightarrow \infty$. Therefore, we conclude that $1/I_C$ can be further used to *qualitatively* measure the number of *macroscopically* occupied SP states in the thermodynamic limit, or, in other words, to determine whether the ground state is fragmented or not.

As shown in Fig. 2, there are two global minima ($\approx$1) at $L/N = 0$ and $L/N = 1$, which can be well interpreted as a signature of single condensates. For other values of L/N (especially in the high AM), however, $1/I_C$ is generally larger than 2. This clearly indicates the fragmented

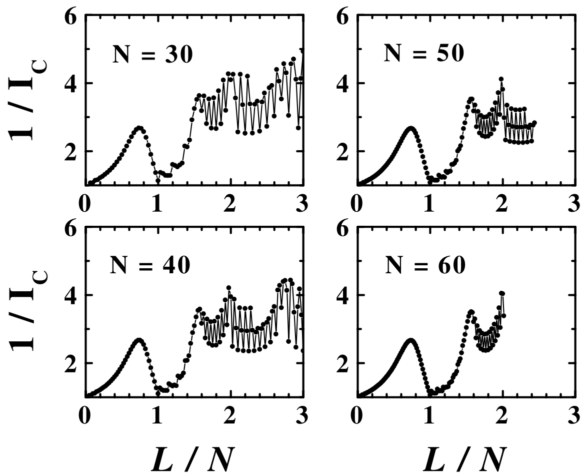

FIG. 2. $1/I_C$ versus L/N for a system of $N = 30$, 40, 50, and 60 bosons. Small oscillations at $L/N > 1.6$ are caused by the finite N effect. The overall profile of $1/I_C$ is nearly independent of N, thus $1/I_C$ can be used to qualitatively measure the number of macroscopic occupation numbers in the limit of $N \to \infty$.

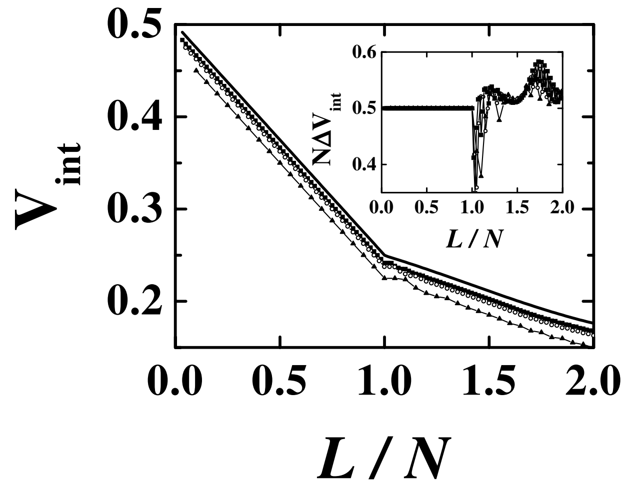

FIG. 3. $V_{\rm int}$ in units of gN^2 as a function of L/N for a system of $N = 20$ (solid triangles), 40 (open circles), and 60 (solid squares) bosons. For comparison, the $V_{\rm int}$ predicted by MFT is also depicted by the thick solid line. The inset shows the energy difference $\Delta V_{\rm int} = V_{\rm int}^{mf} - V_{\rm int}$ in units of gN. Note that all the $\Delta V_{\rm int}$ with different N are approximately located on a universal curve.

nature of the corresponding ground states. Another notable feature in Fig. 2 is that the overall profile of $1/I_C$ exhibits a valley around $L/N = 1.0$, 1.8, and 2.4. This is consistent with the broad peaks of n_j at $L \approx 40$, 70, and 90 for $j = 1$, 2, and 3, respectively, as shown in Fig. 1. The number fluctuations Δn_j are in the order of $O(n_j^{1/2})$ for these peaks, exhibiting a *local* characteristic of a single coherent condensate.

The intrinsic spontaneous symmetry breaking of a fragmented state.—Let us now consider the stability of such a fragmented ground state. In Refs. [11,12], the authors argued that the fragmented state is inherently unstable to the formation of a single condensate of a well-defined phase. The essential idea is that even a weak perturbation that breaks the conservation laws will rapidly generate phase coherence, modifying the density matrix deterministically to give a unique macroscopically occupied SP state. To support this point, we first show that the fragmented state and its corresponding single condensate state have the same energies in the limit of $N \to \infty$, up to the order of $O(gN)$. A similar conclusion has been reported by Jackson *et al.* for the special case of $L = 2N$ [8]. In Fig. 3, the interaction energy $V_{\rm int}$ in units of gN^2 is plotted as a function of L/N for a system of $N = 20$, 40, and 60 bosons. As N increases, $V_{\rm int}$ becomes closer in value to that of a single condensate $V_{\rm int}^{mf}$, as predicted by the MFT [7]. The inset shows the energy difference $\Delta V_{\rm int} = V_{\rm int}^{mf} - V_{\rm int}$ in units of gN. It is readily seen that all the $\Delta V_{\rm int}$ with different N are approximately located on a *universal* curve. This strongly suggests that $\Delta V_{\rm int}$ can be described by an approximate form:

$$\Delta V_{\rm int} = \alpha g N \ll \hbar\omega\,, \tag{6}$$

where in the thermodynamic limit the factor $\alpha \sim 1$ depends on L/N only and the inequality comes from our assumption of weak interaction. As a result, even a perturbation of order $O(1/N)$ can be enough to drive the fragmented state into a single condensate state. This fact clearly indicates that the fragmented state will spontaneously break whatever the fragmentation was permitted by cylindrical symmetry in the first place.

This result can be understood in another way by considering the CPDs [18] that give the density correlation among bosons. We define the CPD for finding one boson at $\mathbf{r}$ given another at $\mathbf{v}_0$ as

$$\mathcal{P}(\mathbf{r}\,|\,\mathbf{v}_0) = \frac{\langle\Psi_{\rm GS}|\sum_{i\neq j}\delta(\mathbf{r}-\mathbf{r}_i)\delta(\mathbf{v}_0-\mathbf{r}_j)|\Psi_{\rm GS}\rangle}{(N-1)\langle\Psi_{\rm GS}|\sum_j\delta(\mathbf{v}_0-\mathbf{r}_j)|\Psi_{\rm GS}\rangle}\,. \tag{7}$$

Unlike the usual density distribution that is cylindrically symmetric under rotational invariant confinement, the CPD is asymmetric and reflects an *intrinsic* density distribution [19].

What will an inherently unstable fragmented state evolve into if a weak perturbation is switched on? One may expect that the system will rapidly change into a state having the same intrinsic density distribution as the fragmented state, and simultaneously generate phase coherence [12]. In view of this, the CPD gives the tendency of a system's evolution and can be regarded as a measurement of the possible spontaneous symmetry breaking.

In Fig. 4, we show the L dependence of the CPDs for a system of $N = 40$ bosons. As expected, we observe the successive vortexlike patterns of differing symmetries, which are in good qualitative agreement with the mean-field calculations [7]. Both of them show a gradual transition for the formation of one- (Fig. 4a) and two-vortexlike (Fig. 4b) states in contrast to the rapid appearance of the three-vortexlike state (Fig. 4c) [7]. As mentioned above,

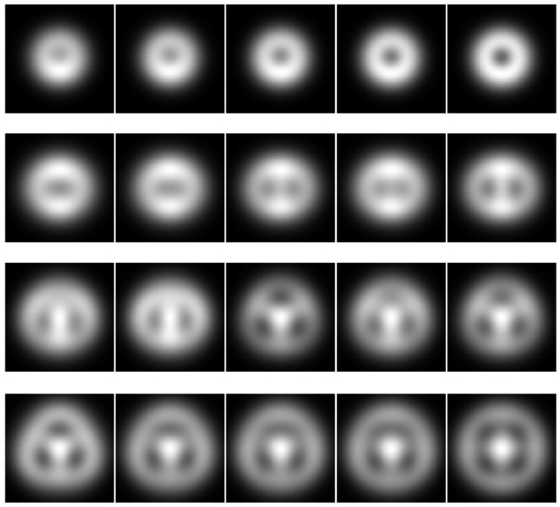

FIG. 4. Selected CPDs for a system of $N = 40$ bosons. (a), (b), (c), and (d) correspond to the emergence of vortexlike patterns with p-fold symmetry ($p = 1, 2, 3, 4$). In each panel, L increases in steps of one unit, and the starting value of L in (a), (b), (c), and (d) is 33, 62, 79, and 108, respectively. The values of x and y in each subplot range from -3.0 to $+3.0$. The given point $\mathbf{v}_0$ is $(0, 1.0)$. For large N, the CPD is nearly independent of $\mathbf{v}_0$.

we identify this similarity as a signal of spontaneous symmetry breaking of fragmented states.

On the other hand, one should not confuse CPDs with the "true" vortex patterns predicted by the MFT [7]. The latter has phase coherence, which is not just well defined in CPDs. Besides this, they have a different physical mechanism for the vortex emergence with the increasing L. For example, our results seem to show that the one and two vortex are produced at the center of the cloud of condensate, in apparent contradiction to the prediction of the MFT that the vortex enters the cloud from the low-density periphery. These differences may be resolved through the Josephson tunneling experiment suggested by Leggett and Sols [20]. Certainly, more accurate theoretical studies on the fragmented state are required.

In conclusion, we have studied the ground state of a weakly interacting N-boson system with a given AM. We propose that the ground state is generally a fragmented condensate state, which is rather fragile in response to a weak asymmetric perturbation. By calculating the corresponding CPDs, we manifest this intrinsic instability. A comparison with the mean-field results is also given.

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[17] As we shall see, the ground state has an *intrinsic* vortexlike density distribution, which has a twofold and threefold symmetry for $2.0 > L/N > 1.6$ and $2.8 > L/N > 2.0$, respectively. A naive interpretation of *certain* stable ground states with p-fold symmetry is that some bosons possess p quanta of AM and others have zero AM [6]. In these ground states, when L is increased by one unit, the system will be puzzled as to how to distribute the extra AM, until additional $p - 1$ units are supplied. This causes an oscillation of the occupation numbers for a finite N, as shown in Fig. 1, and in turn yields the oscillatory behavior of the inverse participation ratio. Note that the period of oscillation is p, as one may expect.

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[19] The difference between CPD and the usual boson density can be interpreted as follows: The CPD describes bosons in their *intrinsic* (*body-fixed*) frame of reference, while the density distribution describes bosons in the laboratory frame of reference where the rotational and center-of-mass displacements are superimposed upon the intrinsic probability density. Note that the CPD can be rewritten as $\mathcal{P}(\mathbf{r} \,|\, \mathbf{v}_0) = \rho(\mathbf{r}) g^{(2)}(\mathbf{r}, \mathbf{v}_0)$, where $\rho(\mathbf{r})$ and $g^{(2)}(\mathbf{r}, \mathbf{v}_0)$ are the density distribution and normalized second-order correlation function, respectively. For a single condensate, $g^{(2)}(\mathbf{r}, \mathbf{v}_0) = 1$, and the CPD is simply reduced to the boson density, i.e., $\mathcal{P}(\mathbf{r} \,|\, \mathbf{v}_0) = \rho(\mathbf{r})$.

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