Symmetry breaking in small rotating cloud of trapped ultracold Bose atoms

D. Dagnino\textsuperscript{1}, N. Barberán\textsuperscript{1}, M. Lewenstein\textsuperscript{2,3}, K. Osterloh\textsuperscript{3}, and A. Riera\textsuperscript{1}

\textsuperscript{1}Dept. ECM, Facultat de Física, U. de Barcelona, E-08028 Barcelona, Spain
\textsuperscript{2}ICREA and IFCO İnstitut de Ciències Fotòniques, Av. del Canal Olímpico s/n, 08860 Castelldefels, Barcelona, Spain and
\textsuperscript{3}Institute for Theoretical Physics, University of Hannover, Appelstrasse 2, 30167 Hannover, Germany

We study the signatures of rotational and phase symmetry breaking in small rotating clouds of trapped ultracold Bose atoms by looking at rigorously defined condensate wave function. Rotational symmetry breaking occurs in narrow frequency windows, where the ground state of the system has degenerated with respect to the total angular momentum, and it leads to a complex wave function that exhibits vortices clearly seen as holes in the density, as well as characteristic vorticity. Phase symmetry (or gauge symmetry) breaking, on the other hand, is clearly manifested in the interference of two independent rotating clouds.

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Symmetry breaking in finite systems has been a subject of intensive debate in physics, in general (cf. the Ref.\textsuperscript{1}), and in physics of ultracold gases in particular over the years. For Bose-Einstein condensates (BEC) two symmetries play a particular role: $U(1)$ phase symmetry and $SU(2)$ (or $SO(3)$) rotational symmetry. In the large $N$ limit, one breaks these symmetries by hand, as proposed originally by Bogoliubov\textsuperscript{2}. Thus, the accurate way to deal with macroscopic Bose Einstein condensates (BEC’s) is by the use of a classical field, also called an order parameter, or the wave function (WF) of the condensate. This function is a single particle (SP) wave function, which is the solution of the Gross Pitaevskii (GP) equation within the mean field approximation, that characterizes the system in a proper way.\textsuperscript{3} It has an arbitrary, but fixed phase, and for rotating systems with more than one vortex it exhibits arbitrarily places, but fixed vortex array.\textsuperscript{3} For dilute ultracold Bose gases (i.e. when $n|a|^3 << 1$\textsuperscript{4} where $n$ is the density and $a$ is the s-wave scattering length) mean field, or Bogoliubov approach is capable to reproduce very well the main properties, despite the fact for finite, fixed $N$ and total angular momentum $L$, which are both constants of the motions, mean field theory cannot be exact. This observation has stimulated a lot of discussion about the nature of the phase of BEC\textsuperscript{2,5,6}, and particle-conserving Bogoliubov approach\textsuperscript{5}. The modern point of view (for a recent discussion see\textsuperscript{7}) implies that two BEC’s with fixed $N$ each one, will produce a well defined interference pattern of fringes as a result of the measurement in only one shot (comparable with the calculated n-correlation function) in contrast with the density, which would be obtained as a mean image of random interference patterns from several shots. The position of fringes in the given measurement are determined by subsequent localization of atoms arriving at detectors: the first atom is completely random, second is correlated, third even more correlated etc.\textsuperscript{6} Thus the information about the pattern is obtained from the many-body wave function by looking at pair, triple, ... correlations. The breaking of rotational symmetry should occur in large rotating clouds in the similar way, and a pure L-state would show, in a time-of-flight experiment, a definite interference pattern accurately represented by n-correlation functions, different from a circular symmetric profile of the single particle density. It would be a test of the meaning assigned to the measurement. Unfortunately, for large N-systems, the total angular momentum of the stationary states is not well defined and there is no qualitative difference between density and n-correlation function, usually showing in both cases vortex arrays. For small rotating clouds the situation is, however, different, as we have shown in Ref.\textsuperscript{6}. Typically, the GS’s are pure-L states for most of the values of $\Omega$. Only, in the very narrow window of frequencies, where the ground states is degenerated with respect to $L$, vortex arrays can be obtained, arbitrary small symmetry breaking deformation of the trap potential leads to the appearance of symmetry breaking vortex arrays both in density and pair-correlations. Namely, in the regime of pure L-GS small systems would provide a suitable test for the meaning of the measurement distinguishing between the density or the pair-correlation output.

In this Letter we study the effects of symmetry breaking in small rotating clouds of trapped ultracold Bose atoms in more depth, by introducing the rigorous definition of the condensate wave function, defined as an eigenvector of the one body density matrix operator (OBDM), corresponding to the largest eigenvalue. Such definition of the order parameter has been introduced in classical papers on off-diagonal long range order\textsuperscript{10}. It has, however, rarely been used since its application requires the knowledge of the full many-body wave function, or at least of the exact OBDM. Since for quantum gases exact analytic solutions are either not known (2D and 3D), or very difficult to handle (1D), so far this definition has been only applied to the case of model system with harmonic forces. Here we apply for the first time to the rotating gas, using exact numerically calculated OBDM for few atom systems. We identify in this way possible states with vortices, and obtain phase characteristics of the wave function (reflecting quantized circulation of vortices), and provide unambiguous definition of the
degree of condensation. With such calculated order parameter we then reproduce the density and interference patterns for two condensed clouds, and shed new light on the discussion of the origins of symmetry breaking in finite mesoscopic systems.

We consider a two-dimensional system of few Bose atoms trapped in a parabolic rotating trap around the \( z \)-axis. The rotating frequency \( \Omega \) is strong enough to consider the Lowest Landau Level regime with atoms interacting via contact forces. Our main goal is the description of the stationary states for different values of \( \Omega \), analyzed from the rotating frame of reference, unless otherwise stated. Our analysis is performed using the exact diagonalization formalism, valid for arbitrary interactions and densities. However, in contrast to the mean field approach, this method deals with multi-particle wavefunctions and loses the intuitive picture provided by the mean field order parameter. Our goal is to obtain in a precise way a complex scalar field that models efficiently the system, and to reproduce the density and interference patterns for two condensed clouds, and shed new light on the discussion of the origins of symmetry breaking in finite mesoscopic systems.

In our numerical simulations to represent both the field operator and the multiparticle GS wave function. The same SP basis is used in our numerical simulations to represent both the field operator and the multiparticle GS wave function.

\[
\hat{a}_l = \int d\vec{r} \psi_l^*(\vec{r}) \hat{\Psi}(\vec{r}),
\]

and \( \hat{a}_l \) being the hermitian conjugate of \( \hat{a}_l^\dagger \). The Hilbert space attain then a tensor structure with respect to the modes \( \hat{a}_l \), and the new Fock (occupation number) many body basis \( |n_1\rangle \otimes |n_2\rangle \otimes \cdots \) \( m \)-body basis is determined by the functions \( \psi_l \). The same SP basis is used in our numerical simulations to represent both the field operator and the multiparticle GS wave function. The same SP basis is used in our numerical simulations to represent both the field operator and the multiparticle GS wave function.

In what follows, we show some results that confirm the expectations usually used in literature. However, at certain values of \( \Omega \) where degeneracy takes place and vortex states and some vortices appear distributed in an ordered arrays, this scalar field plays the role of a genuine order parameter. On the other hand, it loses its capability to represent the system as \( \Omega \) approaches the melting point, and the rest of the modes (that could be regarded as phonon modes, quasi-particles) will tend to reduce the fluctuations of the phase. A natural consequence of this observation is to expect that a very fine approximation of the GS is given by the coherent state \( |\alpha_1\rangle \), such that \( \hat{a}_l |\alpha_1\rangle = \sqrt{n_1} \psi_l e^{i\phi_1} |\alpha_1\rangle \). If \( n_1 \) for \( l = 2, 3, \ldots \) are very small we may neglect them, and approximate the many body wave function by \( |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\alpha_3\rangle \otimes \cdots \). In a more precise description, we should rather approximate the GS by \( |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\alpha_3\rangle \otimes \cdots \), where \( \hat{a}_l |\alpha_1\rangle = \sqrt{n_1} \psi_l e^{i\phi_1} |\alpha_1\rangle \) where the phases \( \phi_l \) are arbitrary; one should, however, choose them to be random in order to reproduce (on average) the same OBDM as the one obtained by exact numerical diagonalization.

This representation implies that the next simplifying step would be the representation of the GS by a classical field entering the GP equation, and containing all the involved coherent states \( |\alpha_k\rangle \), \( k = 1, \ldots, m + 1 \) as, \( \Psi(\vec{r}) = \sum_{k=1}^{m+1} \sqrt{n_k} \psi_k e^{i\phi_k} \) with random phases. Calculation of quantum mechanical averages would then in principle require averaging over random phases, which makes this approach technically difficult.

As long as the exact GS is a state with well defined angular momentum, (a pure \( L \)-state) not degenerated with other lowest energy states in different \( L \)-subspaces, it is easy to demonstrate that the FD functions are the eigenstates of Eq.(1) and the eigenvalues \( n_l \) are the occupations usually used in literature. However, at certain values of \( \Omega \) where degeneracy takes place and vortex states without circular symmetry (except the case of only one centered vortex) are possible, the eigenfunctions of Eq.(1) are linear combinations of the FD functions and the macro-occupied function \( \psi_1 \) that represents the vortex state has expected SP angular momentum given by \( \hbar l = \sum_j |l_j| |\beta_{l_j}|^2 \hbar l_j \) where \( l_j \) are integers.

A convenient definition of the degree of condensation which senses the loss of macro-occupation is given by

\[
c = \frac{n_1 - \bar{n}}{N}
\]

where \( N \) is the total number of atoms and \( \bar{n} \) is the mean occupation calculated without the first value \( n_1 \).

In what follows, we show some results that confirm the convenience to represent the whole system by \( \psi_1 \) at certain values of \( \Omega \). As a general result, for vortex states, \( n_1 \)
is always larger than the occupation of the most important FD state within the exact GS. In addition, $\psi_1$ provides a non-ambiguous way to characterize vortices, not only showing dimples in the density profile, but also indicating the position of each one by the change on multiples of $2\pi$ of the phase $S(\vec{r})$ in $|\psi_1(\vec{r})| \propto e^{iS(\vec{r})}$ when moving around each vortex. In Fig.1 for $N = 6$ atoms, we show for three different values of $\Omega$ where degeneracy takes place, the comparison between the contour plots of the density of the exact GS and the density of $\psi_1$, as well as the map of the phase $S(\vec{r})$ of $\psi_1$. In the first case (a) the GS contains two vortices that appear in a clearer way in the order parameter, as it excludes the non condensed part that smears the structure of the GS. The same picture is shown in (b) where four vortices become visible. In the second case, the map of the phase not only localizes vortices with one unit of quantized circulation, but also indicates that incipient vortices are growing at the edge of the system. In the last case (c), a six-fold symmetry is obtained not attached in this case to vortices, but to a mixed structure of dimples and bumps, a precursor of the Wigner type structure observed for few atoms in the Laughlin state at an angular momentum of $L = 30$. The degree of condensation as defined in Eq.(5) decreases as $0.343, 0.192$ and $0.015$ from (a) to (c). The order in vortices and disorder in atoms evolves to order in atoms. As $\Omega$ approaches the frequency of the trap, the occupations tend to equalize and in the Laughlin state, where $n_L$ are the FD occupations (since it is a pure L-state), and the degree of condensation tends to zero.

Some excited states with large L can also be analyzed. For $N = 3$ and $L = 9$ we obtain a large vortex state with three units of circulation. Such state has been predicted in previous theoretical studies as a possible giant vortex GS (with all vorticity confined to the center of the condensate), in the presence of a small quartic potential added to the parabolic trap. In such a case stationary states for $\Omega > \omega_\perp$ are possible. In our calculations the giant vortex appears as an excited state, anticipating this possibility. So far there is no experimental evidence of giant vortex structures in bosonic systems, but they have been reported in superconductive disks.

Finally we show the interference pattern produced by the overlap of two initially independent condensates represented by $\psi_1$ functions. This study is motivated by an increasing amount of recent work revealing the possibility of obtaining very detailed experimental information on the interference pattern produced not only during the overlap of two, or more independent condensates, but also within a unique condensate.

The idea underlying our assumption is the following: we represent the two independent condensates which we call $a$ and $b$ by their macroscopic occupied function $\psi_a$ and $\psi_b$ respectively. By this we mean that the condensates are in two unknown coherent states $|\alpha_a\rangle$ and $|\alpha_b\rangle$ from which we know their order parameter except for their constant phases $\phi_a$ and $\phi_b$ (see Eq.(3)). At time $t = 0$ s the condensates are separated by a distance $d$ and the traps are switched off. The time evolution of the system is obtained (once the transformation to the laboratory frame of reference is performed, multiplying the functions by $\exp(-i\Omega L_z)$ in three steps: First, the Fourier transform of the total order parameter (the sum of the two contributions) is performed. Then, the time evolution of the Fourier components by multiplying them by exponentials of the type $\exp(i\hbar k^2t/2m)$ is realised; this step is done under the assumption that during the time-of-flight the interactions are irrelevant. Finally, in the third step, inverse Fourier transformation is performed. The results are shown in Fig.2 where three different times are considered. Fortunately, the uncertain about the phase relation $\phi = \phi_a - \phi_b$ is not important in the case considered, as only two terms are involved and a change on the relative phase would only produce a global shift of the interference pattern.

We conclude that, we have demonstrated that the use of the eigenfunctions of the OBDM operator provides a useful and precise tool to analyze the exact GS obtained from exact diagonalization and specially the vortex states. These eigenfunctions localize and quantize the vortices and reproduce the time evolution of the interference pattern of two overlapping condensates. We want to point out that our results imply an alternative interpretation about a subject that has attracted much attention.
FIG. 2: Time evolution of the interference pattern during the overlap of two released condensates initially separated by a distance \(d = 15\lambda\). Initially each condensate contains \(N = 6\) atoms and their GS are characterized by \(L = 6\) at \(\Omega = 0.019\) and by a mixture of \(L = 6, 8\) and \(10\) at \(\Omega = 0.0847\) respectively (all quantities are in units of \(\lambda\) and \(u\)).

recently related with the interference pattern formation. One possibility suggested by Mullin and collaborators is that the experimental measurement projects the initial condensates in Fock states into phase states, the atom distribution between the two components become uncertain and the pattern formation is possible. The other possibility discussed by Cederbaum et al., is that the interference pattern appears if one includes interaction during the time-of-flight even for states that initially are Fock states. In our case, the real initial states are Fock states and no interaction is included during the time-of-flight. However, we assume that the degree of condensation of the initial states is large enough to be properly represented by an order parameter (condensate wave function). Fluctuations of the number of condensed atoms reduce the phase fluctuations and determine the order parameter phase. In effect, exact ground state manifest themselves as phase states even for small number of particles, and in this way the interference pattern is produced. Note, however, that in our picture the process of determination of phase is itself random, and various phases \(\phi_k\) are expected to show up from shot to shot.

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