Fragility of fragmentation in Bose-Einstein condensates

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A Bose-Einstein condensate produced by a Hamiltonian which is rotationally or translationally symmetric may be fragmented as a direct result of these symmetries. A corresponding mean-field unfragmented state, with an identical energy to leading order in the number of particles, can generally be constructed. As a consequence, vanishingly weak symmetry-breaking perturbations destabilize the fragmented state, which would thus be extremely difficult to realize experimentally and lead to an unfragmented condensate.

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I. INTRODUCTION

One of the most fundamental issues in the problem of Bose-Einstein condensation is that of fragmentation. Years after the prediction of this phase transition by Bose and Einstein, Penrose and Onsager [1] provided a rigorous criterion for the existence of a Bose-Einstein condensate. Starting from the N-particle wave function of a system, one determines the eigenvalues of the (Hermitian) one-body density matrix,

$$\rho(\mathbf{r}_1',\mathbf{r}_1) = N \int d\mathbf{r}_2 \cdots d\mathbf{r}_N \Psi^*(\mathbf{r}_1',\mathbf{r}_2, \ldots \mathbf{r}_N)\Psi(\mathbf{r}_1,\mathbf{r}_2, \ldots ,\mathbf{r}_N). \tag{1}$$

If at least one eigenvalue is of order N, the system is Bose-Einstein condensed; otherwise, it is not. A single eigenvalue of order N indicates simple condensation; when more than one of the eigenvalues are of order N, the condensate is said to be fragmented [2].

Years after this definition was introduced, Noziéres and Saint James [3] argued that, in a Hartree-Fock approximation, the Fock term makes it energetically favorable for the system to fragment if the effective interaction between the bosons is attractive. The question of condensate fragmentation remained academic, since homogeneous systems with an effective attractive interaction are unstable against collapse. Modern techniques for dealing with trapped cold atoms have rekindled interest in this question since these gases can be metastable if the effective interaction is attractive, and it may thus be possible to realize a fragmented state. This issue has been the subject of a number of studies over the last decade; see, e.g., Refs. [4–14].

In the present study we consider the problem of fragmentation for an effective attractive interaction between the atoms. As two characteristic examples we consider bosonic atoms at zero temperature that are confined in toroidal and in harmonic traps. We will argue that the issue of fragmentation is subtle. For any fragmented state, it is always possible to construct a mean-field, nonfragmented product state that has the same energy to leading and often subleading order in N as the fragmented state, which is the first main result of the present study. In these representative problems and in any case where the Hamiltonian is rotationally or translationally invariant, the single-particle density matrix is diagonal and its eigenvalues are the occupation numbers of the corresponding single-particle states. The system is fragmented merely as a consequence of the symmetry of the Hamiltonian. Due to the low excitation energies of states of well-defined (angular) momentum [i.e., characteristically $O(1/N)$], such states are fragile and virtually impossible to realize in practice. We shall show that small symmetry-breaking terms in the Hamiltonian that vanish in the limit $N\to\infty$ can materially alter wave functions and can reconstruct an unfragmented condensate. The fragmentation of condensates due to the assumed symmetry of the Hamiltonian, as well as the fragility of fragmented condensates due to weak perturbations and their instability against a nonfragmented state, is the second main result of our study.

Specific examples of this fragility have also been discussed in previous studies [5,6,12–14]. Rokhsar [5] has shown that a fragmented condensate is inherently unstable to the formation of a conventional Bose-Einstein condensate. Ueda and Leggett [6] have also shown that any deviation from an exactly axisymmetric Hamiltonian stabilizes a single coherent Bose-Einstein condensate relative to a fragmented condensate. Similar conclusions have been also derived in more recent studies by Ho and Yip [12], Liu *et al.* [13], and Alon *et al.* [14]. The present study provides a general picture of the problem of fragmentation and places it within a broader framework.

II. BOSONS IN A TOROIDAL TRAP WITH AN EFFECTIVE ATTRACTIVE INTERACTION

Consider a tight toroidal trap where the interaction energy between the atoms is much smaller than the excitation energy in the transverse direction. The Hamiltonian of this system reduces to [15,16]

$$H = \sum_{i=1}^{N} - \frac{\partial^2}{\partial \theta_i^2} + V(\theta_i) - \frac{1}{2}|U| \sum_{i\neq j=1}^{N} \delta(\theta_i - \theta_j), \tag{2}$$

where θ is the angle in cylindrical polar coordinates, $V(\theta)$ is the potential that acts along the toroidal trap, and U describes the coupling and is proportional to the scattering length for elastic atom-atom collisions. The dimensionless parameter $\gamma=-(N-1)|U|/(2\pi)$ gives the ratio between the interaction and the kinetic energy. As shown in Refs. [15,16], the gas becomes unstable against the formation of a localized blob—i.e., a bright solitary wave—when $\gamma < \gamma_c = -1/2$.

It is convenient to expand the eigenfunctions of this Hamiltonian in the basis of states $\exp(iq\theta)/\sqrt{2\pi}$, with $q = 0, \pm 1, \pm 2 \ldots$, which are eigenstates of the angular momentum operator $\hat{L} = -i\partial/\partial\theta$, with eigenvalues q. For clarity, we truncate the space and consider only single-particle states with $q=-1$, 0, and 1. We also use the notation for the corresponding Fock states:

$$|m\rangle = |(-1)^m, 0^{N-2m-L}, (+1)^{m+L}\rangle, \tag{3}$$

where m, $N-2m-L$ and $m+L$ are the occupancies of the single-particle states with $q=-1$, 0, and 1, respectively. Clearly, the above states are eigenfunctions of the angular momentum operator $\hat{L}$ and of the number operator $\hat{N}$.

The Hamiltonian of Eq. (2) commutes with $\hat{N}$. If $V(\theta)$ is zero or constant, it also commutes with $\hat{L}$. For a specific N and L, the eigenstates $|\psi_L\rangle$ of this Hamiltonian can be expanded in the basis of the states $|m\rangle$:

$$|\psi_L\rangle = \sum_m d_m^L |(-1)^m, 0^{N-2m-L}, (+1)^{m+L}\rangle. \tag{4}$$

The eigenvalue equation $H|\psi_L\rangle = E(L)|\psi_L\rangle$, where $E(L)$ is the eigenenergy, has the form [17]

$$H_{m,m} d_m^L + H_{m,m-1} d_{m-1}^L + H_{m,m+1} d_{m+1}^L = E(L) d_m^L, \tag{5}$$

where $H_{n,m} = \langle n|H|m\rangle$ are the matrix elements of the Hamiltonian between the states $|n\rangle$ and $|m\rangle$. In the specific truncated space, only the matrix elements $H_{m,m}$ and $H_{m,m\pm 1}$ are nonzero. In the limit $N \to \infty$, numerical solution to this equation yields

$$E(L) = -\frac{9N}{14} + 0.488 + \frac{3}{2}\frac{L^2}{N} + O(1/N). \tag{6}$$

For large N, it is convenient to regard m as a continuous variable. Assuming that d_m^L is a differentiable function of m up to any order,

$$d_{m\pm 1}^L \approx d_m^L \pm \partial_m d_m^L + (1/2)\partial_m^2 d_m^L, \tag{7}$$

and the matrix eigenvalue equation can be written as a familiar harmonic oscillator problem:

$$-\frac{1}{2\mu}\partial_m^2 d_m^L + \left[E_0^L + \frac{\lambda}{2}(m - m_0^L)^2\right] d_m^L = E(L) d_m^L. \tag{8}$$

The solution of this equation, with the boundary condition that d_m^L vanish as $m \to \pm\infty$, has the expected Gaussian form

$$d_m^L \propto \exp[-\sqrt{\lambda\mu}(m - m_0^L)^2/2]. \tag{9}$$

For the specific value of $\gamma=-1$ we find that $m_0^L = 0.1429N - L/2$, $\lambda = 14/N$, and $1/\mu = 0.2057N$. The root-mean-square deviation of m from m_0^L scales like $\sqrt{N}$. The number of states participating actively in Eq. (4) is $O(\sqrt{N})$, and the approximation of Eq. (8) is justified in the large-N limit. Similarly, we find $E_0^L \approx -9N/14 - 0.357 + (3/2)L^2/N$. Our approximation to the energy, $E(L) = E_0^L + (1/2)\sqrt{\lambda/\mu}$, thus agrees with the exact result of Eq. (6) for all terms shown. The error in energies obtained with this smooth approximation is $O(1/N)$ for all $|L| < O(\sqrt{N})$, to be considered below.

The one-body density matrix corresponding to the state $|\psi_L\rangle$ described by Eqs. (4) and (9) is diagonal in the basis of angular momentum eigenstates. This is a direct consequence of the fact that the states $|\psi_L\rangle$ are eigenfunctions of the total angular momentum. The diagonal elements are the occupancies of the three single-particle states with $q=-1$, 0, and 1. Since the average value of $m = m_0$ is of order N (but not equal to N), all three eigenvalues are of order N. The condensate is fragmented.

We now consider the effect of a very weak inhomogeneous potential $V(\theta)$ on the eigenvalues of the single-particle density matrix. (This point has also been addressed in Ref. [9].) As we will see, the state is no longer fragmented in the presence of such an inhomogeneity. We choose $V(\theta) \propto \delta \cos\theta$, with $\delta \ll 1$. This potential connects single-particle states with $\Delta q = \pm 1$:

$$V(\theta) = \delta(a_0 a_1^\dagger + a_1 a_0^\dagger + a_0 a_{-1}^\dagger + a_{-1} a_0^\dagger), \tag{10}$$

with a_q and $a_q^\dagger$ the usual annihilation and creation operators of particles with angular momentum q. For sufficiently weak $V(\theta)$, the resulting eigenstates $|\psi\rangle$ of the Hamiltonian, Eq. (2), can be expressed as a linear superposition of the states $|\psi_L\rangle$:

$$|\psi\rangle = \sum_{m,L} d_m^L |(-1)^m, 0^{N-2m-L}, (+1)^{m+L}\rangle. \tag{11}$$

Given the form of $V(\theta)$, it can connect the state $|(-1)^m, 0^{N-2m-L}, (+1)^{m+L}\rangle$ to the four states

$$|1\rangle = |(-1)^{m-1}, 0^{N-2m-L+1}, (+1)^{m+L}\rangle,$$

$$|2\rangle = |(-1)^{m+1}, 0^{N-2m-L-1}, (+1)^{m+L}\rangle,$$

$$|3\rangle = |(-1)^{m}, 0^{N-2m-L-1}, (+1)^{m+L+1}\rangle,$$

$$|4\rangle = |(-1)^{m}, 0^{N-2m-L+1}, (+1)^{m+L-1}\rangle. \tag{12}$$

Thus, Eq. (5) assumes the form

$$H_{m,m} d_m^L + H_{m,m-1} d_{m-1}^L + H_{m,m+1} d_{m+1}^L + \delta\sqrt{\bar{m}_0(N - 2\bar{m}_0)} \times (d_m^{L+1} + d_m^{L-1} + d_{m+1}^{L-1} + d_{m-1}^{L+1}) = E d_m^L. \tag{13}$$

Here, $\sqrt{\bar{m}_0(N-2\bar{m}_0)}$ approximates the value of this prefactor with its value at the minimum—i.e., $\bar{m}_0 = m_0^{L=0} = 0.143153N$.

Converting this matrix eigenvalue equation into a differential equation as above, we find

$$-\frac{1}{2\mu}\partial_m^2 d_m^L + \left[E_0^L + \frac{\lambda}{2}(m - m_0^L)^2\right] d_m^L + \delta\sqrt{\bar{m}_0(N - 2\bar{m}_0)} \times (4d_m^L + 2\partial_{LL} d_m^L + \partial_{mm} d_m^L - 2\partial_L \partial_m d_m^L) = E d_m^L. \tag{14}$$

The solution of this differential equation has the form

$$d_m^L \propto \exp[-a_1(m + L/2 - \bar{m}_0)^2 - a_2 L^2], \tag{15}$$

with a_1 and a_2 positive, since this function vanishes as m and L tend to infinity in any direction. Numerical calculations with a symmetry-breaking term $V(\theta)$ of the form

$\delta=-(1/100)(100/N)^{1.15}$ verify that the coefficients d_m^L are indeed Gaussian distributed as a function of m and L.

Direct calculation reveals that the one-body density matrix now has only one eigenvalue of order N. [The next-largest eigenvalue is $\mathcal{O}(N^{0.576})$.] This result is readily understood as a consequence of the Gaussian support of the d_m^L. If the symmetry-breaking potential $V(\theta)$ is sufficiently strong that the root-mean-square variations in m and L grow with N, but small enough that $\Delta m/\langle m\rangle$ and $\Delta L/\langle L\rangle$ vanish as $N\to\infty$, the matrix elements of the one-body density matrix, $\rho_{ij}=\langle a_i^\dagger a_j\rangle$, are $\sqrt{n_i n_j}$, with n_i the occupation number of single-particle state i. The one-body density matrix is thus rank 1 separable. It has one nonzero eigenvalue of $\Sigma_j n_j=N$; the elements of the corresponding eigenvector are proportional to $\sqrt{n_j}$. All other eigenvalues are zero, and the condensate is unfragmented.

The symmetry-breaking potential $V(\theta)$ must be sufficiently strong if it is to yield the desired mixing of the states $|\psi_L\rangle$. According to Eq. (6), the states with $L\neq 0$ are separated from the $L=0$ ground state by a term that scales as L^2/N. Since the contribution of $V(\theta)$ to the energy is of order $N\delta$, δ must vanish less rapidly than $1/N^2$. In addition, low-lying excited states (for each L) are separated by an energy of $\mathcal{O}(N^0)$ from the lowest-energy state. Validity of the truncation to the states $|\psi_L\rangle$ requires that δ vanish more rapidly than $1/N$. Clearly, the second condition is dictated by approximations made in this calculation and not with the absence of fragmentation. In short, even symmetry-breaking potentials which vanish in the large-N limit are sufficient to ensure that the condensate is not fragmented.

III. BOSONS IN A HARMONIC TRAP WITH AN EFFECTIVE ATTRACTIVE INTERACTION

We now turn to two additional systems which have been considered as examples of condensate fragmentation. First, consider rotating bosonic atoms confined in a two-dimensional harmonic trap and subject to the Hamiltonian [4]. In cylindrical polar coordinates,

$$H=\sum_{i=1}^{N}-\frac{1}{2}\nabla_i^2+\frac{1}{2}\rho_i^2-\frac{1}{2}|\eta|\sum_{i\neq j=1}^{N}\delta(\mathbf{r}_i-\mathbf{r}_j). \tag{16}$$

Here η, which describes the atom-atom interaction, is proportional to the s-wave scattering length. If the coupling is weak, $|\eta|\ll 1$, this Hamiltonian can be truncated to include only states in the lowest Landau level with zero radial nodes and m quanta of angular momentum, $\phi_m=z^m e^{-|z|^2/2}/\sqrt{\pi m!}$, with $z=x+iy$, where x and y are Cartesian coordinates. In this case, as shown by Wilkin, Gunn, and Smith [4] and by Mottelson [18], the interaction energy of the lowest-energy state for any given angular momentum is the same as that of the nonrotating system:

$$E(L)=-\frac{|\eta|}{2}N(N-1)\int|\phi_0|^4 d^2\rho=-\frac{|\eta|}{4\pi}N(N-1). \tag{17}$$

The full energy of these states contains an additional contribution of $|L|+1$ from the confining potential. The corresponding exact many-body eigenstate describes a center-of-mass excitation with

$$\Psi_{\rm ex}^L(z_1,z_2,\ldots,z_N)=\mathcal{N}_L Z^L\sum_{i=1}^{N}\exp(-|z_i|^2/2). \tag{18}$$

Here, $\mathcal{N}_L=1/\sqrt{\pi^N N^L L!}$ and Z is the center-of-mass coordinate—i.e., $Z=\Sigma_{i=1}^N z_i$.

The eigenvalues of the single-particle density matrix are $\rho_m=(N-1)^{L-m}L!/[N^{L-1}(L-m)!m!]$ [4]. Due to the axial symmetry of the Hamiltonian, this density matrix is diagonal and its eigenvalues are simply the occupation numbers $N|c_m|^2$, of the single-particle states. The energy is minimized when all c_m have the same phase, which can be taken as positive without loss of generality. In the limit of infinite N and L with $l=L/N$ finite, we see that [19] $|c_m|^2(l)=l^m\exp(-l)/m!$. According to the usual criterion, this is a fragmented state.

It is possible, however, to construct a mean-field, product wave function which has the same interaction energy and which is necessarily unfragmented. Consider the simple form

$$\Psi_{\rm MF}^l(z_1,z_2,\ldots,z_N)=\prod_{i=1}^{N}\sum_{m=0}^{\infty}c_m\phi_m(z_i), \tag{19}$$

with the coefficients $c_m=\sqrt{l^m/m!}\exp(-l/2)$. This state is normalized, and the expectation value of the angular momentum per particle is $l=L/N$. The interaction energy of this state can be calculated analytically:

$$\begin{aligned}E_{\rm MF}^l&=-\frac{|\eta|}{2}N(N-1)\int\left|\sum_{m=0}^{\infty}c_m\phi_m(z)\right|^4dxdy\\&=-\frac{|\eta|}{4\pi}N(N-1)e^{-2l}\sum_{m=0}^{\infty}\frac{1}{m!}\left(\frac{l}{2}\right)^m\sum_{k,j=0}^{m}\binom{m}{k}\binom{m}{j}\\&=-\frac{|\eta|}{4\pi}N(N-1)e^{-2l}\sum_{m=0}^{\infty}\frac{1}{m!}\left(\frac{l}{2}\right)^m4^m\\&=-\frac{|\eta|}{4\pi}N(N-1),\end{aligned} \tag{20}$$

which is identical to the energy given by Eq. (17). The overlap between the states $\Psi_{\rm ex}^L$ and $\Psi_{\rm MF}^l$ can also be calculated analytically as

$$\langle\Psi_{\rm ex}^L|\Psi_{\rm MF}^l\rangle=\left(\frac{L}{Ne}\right)^{L/2}\frac{\pi^{N/2}N^L}{\sqrt{\pi^N N^L L!}}\approx\frac{1}{\sqrt{2\pi L}}. \tag{21}$$

This overlap vanishes in the thermodynamic limit $L\to\infty$. This comes as no surprise, since $\Psi_{\rm ex}^L$ describes a state that is spread uniformly around the center of the trap, while $\Psi_{\rm MF}^l$ describes precisely the nonrotating "clump" of matter displaced from the center of the trap and rotating around it.

The existence of a mean-field state with an energy close to the exact eigenvalue is a relatively general consequence of rotational or translational invariance. Given a Hamiltonian which is axially or translationally invariant, the one-body density matrix is diagonal with eigenvalues equal to the occupation numbers of the corresponding single-particle states. From these occupancies, it is possible to construct a mean-field wave function with the same energy as the exact solution to leading and often subleading order in the number of particles, N. The same conclusion applies to the argument of Nozieres and Saint James: The exchange interaction does not necessarily favor fragmentation since there exists a nonfragmented mean-field product state with the same energy in the $N\to\infty$ limit. As seen in the case of toroidal confinement, the question of whether the system is better described by a wave function which is an eigenfunction of the total momentum or angular momentum (and thus fragmented) or is better described by a mean-field wave function (and thus not fragmented) must depend on the response of the system to vanishingly small symmetry-breaking terms.

This issue can be investigated with arguments and conclusions identical to those above. A one-body symmetry-breaking term $V(z)=\delta(z+z^*)$ is introduced, where again $z=x+iy$. The basis of states is truncated to include only the lowest-energy states Ψ_{ex}^L. Evidently, $V(z)$ can only connect the state L with the states $L\pm 1$. The corresponding matrix elements are, e.g.,

$$\langle \Psi_{\text{ex}}^{L+1}|V|\Psi_{\text{ex}}^{L}\rangle = \delta\sqrt{N(L+1)} \quad \text{for } L \geqslant 0. \tag{22}$$

If δ vanishes with increasing N, this truncation of states is legitimate. If it vanishes more slowly than $1/\sqrt{N}$, there will be significant mixing of the states Ψ_{ex}^L. As in the case of toroidal confinement, the wave function will have localized (i.e., Gaussian) support in the space of single-particle states. Precisely as before, only one eigenvalue of the one-body density matrix is of order N and the condensate is not fragmented.

Identical arguments can be applied to the related but simpler two-state model of Ref. [7]. There, the condensate is fragmented due to a "parity" symmetry. This is reflected in the fact that eigenstates contain, e.g., only an even (or odd) number of particles in one of the states. The energy difference between the lowest-energy even and odd states vanishes exponentially with N. Once again, a vanishingly small one-body symmetry-breaking term, proportional to $(a_0^\dagger a_1 + a_1^\dagger a_0)$, is sufficient to reconstruct an unfragmented condensate. These two examples will be described in greater detail elsewhere. Finally, similar arguments apply to the studies of Refs. [12,13], where a state fragmented by some symmetry of the Hamiltonian can be restored to a simple unfragmented condensate by very weak symmetry-breaking perturbations.

IV. GENERAL CONCLUSIONS

For many systems of a large but finite number of bosons with attractive interactions, mean-field theory provides a good description of the ground-state energy and leads to the unambiguous prediction of an unfragmented condensate. The imposition of general constraints, such as conserved total momentum or angular momentum, characteristically produces minimal changes in the ground-state energy and frequently indicates condensate fragmentation. This apparent contradiction has led some authors to suggest modified criteria for condensate fragmentation. We have offered an alternate resolution. The various examples considered here all suggest that the small excitation energies of excited states in these systems can render them sensitive to vanishingly small symmetry-breaking perturbations. The resulting localized (i.e., often Gaussian) support of the wave function then leads to a one-body density matrix, approximately given as $\rho_{ij}=\sqrt{n_i n_j}$, which is rank 1 separable with one eigenvalue of $O(N)$ in the $N\to\infty$ limit. The unfragmented condensate, deconstructed by rigorous symmetries, can be reconstructed by small symmetry-breaking perturbations. Such perturbations can be difficult to eliminate experimentally. (Such antagonism between the mean-field approximation and symmetries is well known. For example, insistence on maintaining translational invariance in fermion systems leads inevitably to a trivial Hartree-Fock wave function of plane-wave states and a poor description of both the ground-state energy and wave function.) While the present results in no sense rule out the possibility of condensate fragmentation in systems of bosonic atoms, they do suggest that it is important to demonstrate that theoretical indicators of fragmentation are robust with respect to small symmetry-breaking perturbations.

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