Spatial fragmentation of a Bose-Einstein condensate in a double-well potential

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We present a theoretical study of the ground state of a Bose-Einstein condensate with repulsive inter-particle interactions in a double-well potential, using a restricted variational principle. Within such an approach, there is a transition from a single condensate to a fragmented condensate as the strength of the central barrier of the potential is increased. We determine the nature of this transition through approximate analytic as well as numerical solutions of our model, in the regime where the inter-particle interactions can be treated perturbatively. The degree of fragmentation of the condensate is characterized by the degrees of first-order and second-order spatial coherence across the barrier.

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I. INTRODUCTION

The recent experimental demonstration of interference phenomena in Bose-condensed atomic gases [1], motivates a study of the spatial coherence of a condensate in a double-well potential. In particular, we are interested in the loss of spatial coherence that can occur at zero temperature due to fragmentation of the condensate. A fragmented condensate is one for which there is a macroscopic occupation of two or more orthogonal single-particle wavefunctions. If the occupied single-particle wavefunctions are spatially well separated, coherence over the spatial extent of the entire system will be lost, persisting only over the spatial extent of each fragment.

As Nozières [2] has pointed out, for repulsive inter-particle interactions it is the exchange energy that typically prevents fragmentation into a number of degenerate (or nearly degenerate) single-particle wavefunctions. However, this argument is inapplicable for bosons in an external potential with several local minima, since single-particle wavefunctions that are localized about these minima may have very little overlap with one another, thereby leading to a very small exchange energy. Moreover, since the self-interaction energy in such a fragmented condensate is smaller than that of a single condensate, it is possible for the total interaction energy to be smaller as well. Although every particle in the fragmented condensate will pay a price in kinetic energy to occupy localized wavefunctions, the overall energy may still be less than that of a single condensate. Indeed, it can be shown that in the limit of a symmetric double-well potential with an infinitely strong central barrier, one can always find a fragmented state that has a total energy lower than any single condensate [3].

Thus we have the following situation in a double-well potential: in the absence of any central barrier the ground state is well approximated by a single condensate, while in the presence of an infinitely strong barrier it is well approximated by a fragmented condensate. It is clear therefore that there must be a transition between these two extremes as one increases the strength of the barrier. The first goal of this paper is to propose a theoretical model for describing this transition. Specifically, we argue for an approximation of the fully interacting ground state that is more general than a Fock state, and that can be said to describe ‘partial fragmentation’ of the condensate. The equations that such a state must satisfy are derived within a variational approach. The second goal of the paper is to solve these equations in a regime where the inter-particle interactions can be treated perturbatively. Numerical solutions of the equations and analytic approximations to these solutions are obtained within this regime. It should be noted that this limit is inappropriate for the description of the MIT condensate interference experiment [1], and consequently, our results do not specify the nature of the transition for this experimental set-up. Nonetheless, we expect the generic features of the transition to persist in the experimentally relevant regime.

We pause to consider previous treatments of this topic and their relation to this work. Röhrle et al. [4] have provided a model of the MIT condensate interference experiment; however, it is a mean field analysis and therefore cannot describe fragmentation. Fragmentation in the case of attractive inter-particle interactions has been considered by Wilkin, Gunn and Smith [5], but this effect is qualitatively different from that of the repulsive case. Finally, Milburn et al. [6] have considered the energy eigenstates of a Bose-Einstein condensate in a double-well potential, and predict fragmentation when the inter-particle interactions are sufficiently strong. However, these authors consider only traps with weakly coupled wells, and therefore cannot determine the degree of fragmentation of the ground state in the regime of low barrier strengths where the coupling between the wells is strong. Moreover, this paper does not address the issue of the spatial coherence of the ground state. Since the presence of long-
range order is a defining characteristic of Bose-Einstein condensation, it is critical to understand the manners in which this spatial coherence can be lost.

There has also been theoretical work on the problem of Bose condensates containing atoms in two different internal states, which is analogous to the two well problem. Esry et al. consider the probability distributions and lifetimes of two interacting condensates in different internal states confined to the same trap, while Cirac et al. as well as Steel and Collett consider the ground states of such a system when the internal atomic states can be controlled by a Josephson-like laser coupling. In this case, the distinguishability of atoms in the two condensates is ensured by their internal state rather than their single-particle wavefunctions. However, the requirement of orthogonality in the spatial degrees of freedom is indispensable in a multiple well problem since it is precisely the shape of the single-particle wavefunctions that determines the degree of fragmentation in the system.

The remainder of the paper is organized as follows. In section II we present our model and define some useful measures of spatial coherence of the condensate. In section III we present approximate analytic solutions of our model in the regime of nearly non-interacting particles, and compare these to a numerical solution for a particular choice of the external potential. The experimental signature of fragmentation and finite temperature effects are discussed in section V, followed by our concluding remarks in section VI.

II. THE MODEL

A. The basic approach

Our system consists of an even number, $N$, of spinless bosons at zero temperature. We model the interactions by a two-particle pseudopotential in the shape-independent approximation, $V(r, r') = g\delta(r - r')$ with an interaction strength $g = 4\pi a_{sc}\hbar^2/m$, where $a_{sc}$ is the s-wave scattering length, and $m$ is the mass of the bosons. The Hamiltonian is given by

$$H = \int d^3r \left[ -\frac{\hbar^2}{2m} \nabla \hat{\Psi}^\dagger(r)\nabla \hat{\Psi}(r) + U(r)\hat{\Psi}^\dagger(r)\hat{\Psi}(r) \right],$$

where $\hat{\Psi}(r)$ is the quantum field operator, and $U(r)$ is the external potential. The external potential is taken to exhibit a single minimum along the $y$ and $z$ axes, and a double minimum along the $x$ axis. It is also taken to be symmetric about $x = 0$.

In order to capture the phenomenon of fragmentation in our model of the ground state, we must go beyond a mean field analysis. Specifically, we consider arbitrary superpositions of Fock states where up to two single-particle states are occupied. This corresponds to postulating a state vector of the form

$$|\psi\rangle = \sum_{N_1 = 0}^{N} C_{N_1} |N_1, N_2\rangle_{(\phi_1, \phi_2)},$$

where

$$|N_1, N_2\rangle_{(\phi_1, \phi_2)} = \frac{(a_1^\dagger)^{N_1} (a_2^\dagger)^{N_2}}{\sqrt{N_1!N_2!}} |vac\rangle$$

is the Fock state in which $N_1$ particles occupy the single-particle state $\phi_1(r) = \langle r | a_1^\dagger | vac \rangle$ and $N_2$ particles occupy $\phi_2(r) = \langle r | a_2^\dagger | vac \rangle$. The total number of particles is fixed, $N_2 \equiv N - N_1$, the vector consisting of the set of coefficients $C_{N_1}$ is normalized, and the single-particle wavefunctions $\phi_1$ and $\phi_2$ are both normalized and orthogonal to one another.

The state (2) is certainly not the most general state one can consider. Indeed, a state such as (2) would be a poor choice if one were interested in studying the depletion of a single condensate due to interactions, since one there expects a certain fraction of the particles to be distributed among a macroscopic number of single-particle states. However, in this paper we are interested in the possibility of the particles being redistributed into a few single-particle states that are each macroscopically occupied. We restrict ourselves to two single-particle states because the double-well geometry we are considering encourages fragmentation into two pieces. Although it may be energetically favorable to fragment into more than two pieces at very high particle densities, we defer consideration of this possibility to a later work.

Among the many-body states defined by (2), we consider only those which have the same symmetry as the Hamiltonian under reflections about $x = 0$. This implies that the single-particle wavefunctions are mirror images of one another across $x = 0$ within a phase factor, $\phi_1(-x, y, z) = e^{i\theta}\phi_2(x, y, z)$, and that the coefficients satisfy $C_{N_1} = C_{N - N_1}$. With this assumption, and choosing $\phi_1$ and $\phi_2$ to be real, the Hamiltonian takes the form

$$\hat{H}_2 = \epsilon_{11}\hat{N} + \left(\epsilon_{12} + gT_1(\hat{N} - 1)\right) \left(a_1^\dagger a_2 + a_1 a_2^\dagger\right)$$

$$+ \frac{gT_0}{2} \left(\hat{N}_1^2 + \hat{N}_2^2 - \hat{N}\right)$$

$$+ \frac{gT_2}{2} \left(a_1^\dagger a_1^\dagger a_2 a_2 + a_1 a_2^\dagger a_2^\dagger a_1 + 4\hat{N}_1\hat{N}_2\right),$$

where $\hat{N}_1 = a_1^\dagger a_1$, $\hat{N}_2 = a_2^\dagger a_2$, $\hat{N} = \hat{N}_1 + \hat{N}_2$, and where

$$\epsilon_{11} = \int d^3r \phi_1^2(r) \left(-\frac{\hbar^2}{2m} \nabla^2 + U(r)\right) \phi_1(r),$$

$$\epsilon_{12} = \int d^3r \phi_1^2(r) \left(-\frac{\hbar^2}{2m} \nabla^2 + U(r)\right) \phi_2(r),$$

$$T_0 = \int d^3r \phi_1^4(r),$$

$$T_1 = \int d^3r \phi_1^2(r) \phi_2^2(r).$$
\[ T_1 = \int d^3r \phi_1^2(\mathbf{r}) \phi_2(\mathbf{r}), \]
\[ T_2 = \int d^3r \phi_1^2(\mathbf{r}) \phi_2^2(\mathbf{r}). \]

These quantities have the following physical interpretation: \( \epsilon_{11} \) is the single-particle energy for the state \( \phi_1 \); \( \epsilon_{12} \) is proportional to the inversion frequency of a single particle in the external potential; finally, \( T_0 \) quantifies the self-interaction energy, while \( T_1 \) and \( T_2 \) both quantify the cross-interaction energy.

In order to facilitate comparison of our work with earlier studies \([4], [5]\), we re-express the Hamiltonian in terms of operators satisfying angular momentum commutation relations, rather than in terms of the creation and annihilation operators we have employed thus far. We introduce the operators
\[
\hat{J}_x = \frac{1}{2} (\hat{a}^\dagger_2 a_1 + a_1^\dagger a_2), \\
\hat{J}_y = \frac{i}{2} (\hat{a}^\dagger_1 a_2 - a_2^\dagger a_1), \\
\hat{J}_z = \frac{1}{2} (\hat{N}_2 - \hat{N}_1),
\]
which form an angular momentum algebra with total angular momentum \( j = N/2 \) \([6]\). In terms of these operators, the Hamiltonian can be rewritten as
\[
\hat{H}_2 = E_0 + 2 (\epsilon_{12} + gT_1(N-1)) \hat{J}_x + 2gT_2 \hat{J}_y^2 + g(T_0 - T_2) \hat{J}_z^2,
\]
where
\[
E_0 = \epsilon_{11} N + \frac{1}{8} N(N+2)(gT_0 + gT_2),
\]
and where we have used \( \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 = j(j+1) \) to eliminate \( \hat{J}_z^2 \) from the expression. The observable corresponding to \( \hat{J}_x \) is the particle number difference between the localized states \( \phi_1 \) and \( \phi_2 \). Defining the wavefunctions \( \phi_s = 2^{-1/2} (\phi_1 + \phi_2) \) and \( \phi_a = 2^{-1/2} (\phi_1 - \phi_2) \), which are respectively symmetric and antisymmetric about \( x = 0 \), one sees that \( \hat{J}_x \) can be rewritten as \( \frac{1}{2} (\hat{a}_s^\dagger \hat{a}_a - \hat{a}_a^\dagger \hat{a}_s) \), where \( \hat{a}_s^\dagger \) and \( \hat{a}_a^\dagger \) are the creation operators associated with \( \phi_s \) and \( \phi_a \) respectively. Thus, \( \hat{J}_x \) corresponds to the particle number difference between the symmetrized states \( \phi_s \) and \( \phi_a \). Finally, \( \hat{J}_y \) corresponds to the condensate momentum. Since we are considering the ground state it follows that \( \langle J_y \rangle = 0 \), and since the ground state is symmetric under reflections about \( x = 0 \) it follows that \( \langle J_x \rangle = 0 \).

### B. A restricted variational principle

We now turn to the problem of identifying the ground state of our model. This can be achieved by minimizing the expectation value of \( \hat{H}_2 \) with respect to variations in both the coefficients \( C_{N_1} \) and the single-particle wavefunction \( \phi_1 \), subject to the constraints that the set of coefficients is normalized, and \( \phi_1 \) is both normalized and orthogonal to \( \phi_2 \), its mirror image about \( x = 0 \). However, it is in fact more convenient to minimize the expectation value of \( \hat{H}_2 \) with respect to variations in \( \phi_s \) and \( \phi_a \) rather than \( \phi_1 \). The reason for this is that no constraint corresponding to orthogonality is required when working with \( \phi_s \) and \( \phi_a \), since they are orthogonal by construction; as a result the analysis is simplified.

We begin with the variation of \( \phi_s \) and \( \phi_a \), implementing the normalization constraints through Lagrange multipliers \( E_s \) and \( E_a \) respectively. This results in two coupled non-linear Schrödinger equations for \( \phi_s \) and \( \phi_a \)
\[
\left[ -\frac{\hbar^2 \nabla^2}{2m} + U(\mathbf{r}) + g\Gamma_\alpha^s \phi_\alpha^s(\mathbf{r}) + g\Gamma_\alpha^a \phi_\alpha^a(\mathbf{r}) \right] \phi_\alpha(\mathbf{r}) = E_\alpha \phi_\alpha(\mathbf{r}), \quad (5)
\]
where
\[
\Gamma_\alpha^s = \langle \phi_s^\dagger \phi_s^\dagger \phi_s - \phi_s^\dagger \phi_s \phi_s^\dagger \phi_s \rangle, \text{ and }
\Gamma_\alpha^a = \langle \phi_a^\dagger \phi_a^\dagger \phi_a - \phi_a^\dagger \phi_a \phi_a^\dagger \phi_a \rangle.
\]
and where the indices \((\alpha, \beta)\) take the values \((s, a)\) and \((a, s)\).

We now minimize the expectation value of \( \hat{H}_2 \) with respect to variations in the \( C_{N_1} \), and implement the normalization constraint on the \( C_{N_1} \) through a Lagrange multiplier \( E \). This results in a five-term recurrence relation for the coefficients
\[
\left[ N\epsilon_{11} + \frac{gT_0}{2} (N_1^2 + N_2^2 - N) + 2gT_2N_1N_2 - E \right] C_{N_1} + [\epsilon_{12} + gT_1(N-1)] \left[ \sqrt{N_1(N_2+1)} C_{N_1-1} \right] \nonumber \]
\[
+ [\epsilon_{12} + gT_1(N-1)] \left[ \sqrt{N_2(N_1+1)} C_{N_1+1} \right] = 0,
\]
for each value of \( N_1 \); \( E \) is immediately identified as the expectation value of \( \hat{H}_2 \). The latter set of equations forms a matrix eigenvalue equation for the \( N \)-element vector of coefficients \( C_{N_1} \). Given values for \( \epsilon_{11}, \epsilon_{12}, T_0, T_1 \) and \( T_2 \), we can solve this equation by diagonalizing a \( N \times N \) matrix with non-zero entries along five diagonals, a problem which is numerically tractable if the number of non-zero coefficients is not too large.

Since equations \((3)\) and \((5)\) form a coupled set of equations for \( \phi_s, \phi_a \) and the \( C_{N_1} \), we must in general solve these self-consistently. Of the many solutions thus obtained, the ground state is the one which minimizes the value of \( E \). However, it is not obvious that the solution that minimizes \( E_s \) and \( E_a \) also minimizes \( E \); thus it may be necessary to compare the energies of many solutions in order to find the ground state.
C. The regime of nearly non-interacting particles

The full problem outlined above is rather complex. In this paper, we consider only perturbative solutions of Eq. (4) in the nearly non-interacting regime, which we here define as the regime where the interaction energy is small compared to the difference between $\epsilon_{s}^{(1)}$, the energy of the first symmetric excited state of the external potential, and $\epsilon_{s}$, the energy of the ground state. This is ensured by the criterion

$$gNT_0 \ll \epsilon_{s}^{(1)} - \epsilon_s.$$  \hfill (8)

Since $T_0$ is on the order of the inverse of the volume of the trap, this criterion places an upper limit on the density of the condensate.

In this regime, we can treat the non-linear terms in Eq. (4) perturbatively. To obtain the expectation value of $\hat{H}_2$ to first order in the perturbation, we need only solve for the eigenfunctions of Eq. (5) to zeroth order. Thus, we need only solve the two linear Schrödinger equations

$$\left[ -\frac{\hbar^2 \nabla^2}{2m} + U(r) - \epsilon_{\alpha} \right] \phi_{\alpha}(r) = 0,$$  \hfill (9)

for $\alpha = s, a$. In this case, the wavefunctions $\phi_s$ and $\phi_a$ are simply the two lowest single-particle energy eigenfunctions of the external potential, and the assumption of a state of the form of Eq. (2) corresponds to a two mode approximation.

The solutions of Eq. (9) determine the magnitudes of $\epsilon_{11}, \epsilon_{12}, T_0, T_1$ and $T_2$, and these subsequently define the form of the recurrence relation that must be solved to obtain the coefficients $C_{N_1}$. Although the full results are presented in section III, it is illustrative to consider the ground state of $\hat{H}_2$ in two particularly simple limits: that of no barrier and that of an infinitely strong barrier.

In the absence of any barrier, $|\epsilon_{12}| \approx \epsilon_{s}^{(1)} - \epsilon_s$, and since $|T_1|$ and $T_2$ are on the order of $T_0$ or less, it follows from the criterion that $|\epsilon_{12}| \gg N \rho T_0, N \rho T_1, N g T_2$. If we provisionally assume that the ground state fulfills the conditions that $N \langle \hat{J}_z \rangle \gg \langle \hat{J}_z^2 \rangle, \langle \hat{J}_z \rangle$, then we are led to approximate the Hamiltonian by

$$\hat{H}_2 \simeq E_0 + 2\epsilon_{12} \hat{J}_z.$$  \hfill (10)

The ground state of Eq. (10) is simply the Fock state $|N\rangle_{\phi_s}$, which describes $N$ particles occupying the single-particle ground state $\phi_s$. Since this solution satisfies our provisional assumption, the approximation is consistent. Such a Fock state is of course what one would expect for the ground state of a single well in the limit of nearly non-interacting particles. When this state is written in the form of Eq. (2), that is, in the basis of $|N_1, N_2\rangle_{(\phi_1, \phi_2)}$ states, rather than the basis of $|N_s, N_a\rangle_{(\phi_s, \phi_a)}$ states, the coefficients $C_{N_1}$ form a binomial distribution over $N_1$, centered at $N/2$. It seems appropriate to refer to any state of the form $|N\rangle_{\phi_0}$ for macroscopic $N$ and arbitrary $\phi_0$, as a ‘single condensate’. In this paper, we are concerned only with single condensates wherein the single-particle wavefunction $\phi_0$ is symmetric about $x = 0$. We do not introduce any additional terminology to distinguish such a state from one with arbitrary $\phi_0$, since no confusion is likely to arise.

In the limit of infinite barrier strength, the amplitudes of $\phi_s$ and $\phi_a$ at $x = 0$ are necessarily zero, while $\phi_s$ and $\phi_a$ at $x \neq 0$ satisfy the same equation. Consequently, $\phi_s$ and $\phi_a$ differ only in their symmetry under reflection about $x = 0$, and $\epsilon_{12} = T_1 = T_2 = 0$. The Hamiltonian of Eq. (4) then reduces to

$$\hat{H}_2 = E_0 + gT_0 \hat{J}_z^2.$$  \hfill (11)

The ground state is $|N/2, N/2\rangle_{(\phi_1, \phi_2)}$, which describes two independent condensates, or in other words, a condensate which is fragmented into two pieces. Since we are considering a potential well that is symmetric about $x = 0$, the two fragments are equally populated. It seems appropriate to refer to any state of the form $|N_1, N_2\rangle_{(\phi_1, \phi_2)}$ where $N_1$ and $N_2$ are macroscopic and $\phi_1$ and $\phi_2$ are orthogonal, as a ‘dual condensate’. In this paper we will be concerned only with dual condensates wherein $N_1 = N_2 = N/2$, and $\phi_1$ and $\phi_2$ are mirror images of one another across $x = 0$.

The analysis above confirms, for the limit of nearly non-interacting particles, the results of an earlier study [12]: the ground state is well approximated by a single condensate at zero barrier strength, and a dual condensate at infinite barrier strength. At intermediate barrier strengths, we keep all the terms in $\hat{H}_2$ for our calculations. Although the cross-interaction terms are typically found to be small for generic shapes of the double-well potential, it is not obvious that these terms are negligible for an arbitrary potential, and thus we include them in our analytic results wherever possible.

D. Measures of the degree of fragmentation

Finally, in order to facilitate the interpretation of our results we highlight some observables that reveal the degree of spatial fragmentation of the condensate. The most useful observables for this purpose are those that probe the spatial coherence of the condensate across the barrier. In analogy to measures of optical coherence [13], we normalize the first-order correlation function, $\rho_1(\mathbf{r}, \mathbf{r'}) = \langle \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r'}) \rangle$, to obtain the degree of first-order spatial coherence between points $\mathbf{r}$ and $\mathbf{r'}$,

$$g^{(1)}(\mathbf{r}, \mathbf{r'}) = \frac{\rho_1(\mathbf{r}, \mathbf{r'})}{|\rho_1(\mathbf{r}, \mathbf{r})\rho_1(\mathbf{r'}, \mathbf{r'})|^2}.$$  \hfill (12)

Considering points $\mathbf{r} = (x, y, z)$ and $\mathbf{r'} = (-x, y, z)$ where $x$ is positive and chosen to be sufficiently large so that
straightforward to obtain the single particle ground state and to compare this solution to the analytic approximations. 

\[ C^{(1)} = \frac{\langle a_1^\dagger a_2 + a_2^\dagger a_1 \rangle}{N}. \]  

(13) 

We refer to \( C^{(1)} \) simply as the degree of first-order spatial coherence across the barrier. It is straightforward to verify that it attains its maximum value of 1 for a single condensate and a value of 0 for a dual condensate.

The second-order correlation function \( \rho_2(r, r') = \langle \hat{\Psi}(r) \hat{\Psi}(r') \hat{\Psi}(r') \hat{\Psi}(r) \rangle \), which is simply the normally ordered density-density correlation, can be normalized to obtain the degree of second-order spatial coherence between points \( r \) and \( r' \),

\[ g^{(2)}(r, r') = \frac{\rho_2(r, r')}{[\rho_2(r, r) \rho_2(r', r')]^{1/2}}. \]  

(14)

Defining \( C^{(2)} \) in a manner completely analogous to \( C^{(1)} \), we find

\[ C^{(2)} = \frac{1 - 4 \left( \frac{\Delta N_1}{\sqrt{N}} \right)^2}{\frac{\Delta N_1}{\sqrt{N}^2} + 4 \left( \frac{\Delta N_1}{\sqrt{N}} \right)^2}. \]  

(15)

where \( \Delta N_1 \equiv \left( \langle N_1^2 \rangle - \langle N_1 \rangle^2 \right)^{1/2} \) is the variance in the number of particles occupying the localized state \( \phi_1 \). We refer to \( C^{(2)} \) as the degree of second-order spatial coherence across the barrier. The variance in \( N_1 \) for a single condensate \( \langle N \rangle_{\phi_1} \) is that of a binomial distribution over \( N_1 \), namely \( \sqrt{N}/2 \). For a dual condensate the number of particles in a well is fixed, so that \( \Delta N_1 = 0 \). As a consequence, \( C^{(2)} - 1 = 0 \) for a single condensate \( \langle N \rangle_{\phi_1} \), and \( C^{(2)} - 1 = 2/N \) for a dual condensate. Since \( \Delta N_1 \) is sufficient to specify \( C^{(2)} \), while being simpler to interpret, we use \( \Delta N_1 \) together with \( C^{(1)} \) to characterize our results.

III. ANALYTIC APPROXIMATIONS AND NUMERICAL SOLUTIONS

For a given shape of the double-well potential, it is straightforward to obtain the single particle ground state and first excited state by solving the linear Schrödinger equation (12). The localized single-particle states \( \phi_1 \) and \( \phi_2 \) are simply the sum and difference of the single-particle ground and first excited states. Using these wavefunctions, the coefficients \( C_{N_1} \) can be obtained by solving the recurrence relation (8).

We here present approximate analytic solutions for the \( C_{N_1} \) given an arbitrary shape of the double-well potential. Subsequently, we consider a particular form of the external potential for which the single particle ground and first excited states are obtained numerically. This allows us to obtain a numerical solution for the \( C_{N_1} \) and to compare this solution to the analytic approximations.

A. Continuum approximation

Suppose the coefficients for the ground state satisfy the condition

\[ |C_{N_1+1} - C_{N_1}| \ll C_{N_1}. \]

It is then useful to construct a function \( C(u) \), defined over the real numbers, such that \( C(u) = C_{N_1} \) at the discrete points \( u = N^{-1} (N_1 - N/2) \), and such that \( C(u) \ll NC(u) \). Given this assumption of smoothness, a coefficient of the form \( C_{N_1+p} \), where \( p \) is a small integer, is well approximated by a Taylor expansion of \( C(u + p/N) \) to second order in \( p/N \). In this way, the recurrence relation (8) for the \( C_{N_1} \) can be recast as a second order differential equation for the function \( C(u) \). Moreover, any sum over \( N_1 \) can be approximated by an integral over \( u \). In particular, the constraint of normalization for the coefficients is replaced by the constraint that the integral of \( C^2(u) \) over all \( u \) is \( 1/N \). The assumption of smoothness is readily verified to be appropriate for a single condensate, and we therefore expect it to continue to hold for solutions over a range of small barrier heights.

We also make use of the fact that the coefficients \( C_{N_1} \) are significant only in the region where \( N_1 \lesssim \sqrt{N} \), or equivalently, that the function \( C(u) \) is significant only when \( u \lesssim \sqrt{1/N} \). This follows from the fact that any set of coefficients that has significant amplitude outside the range \( N_1 \lesssim \sqrt{N} \) also has an energy that is larger than a single condensate; the interaction energy is greater since it scales with \( \Delta N_1 \), and the single-particle energy is greater since it is a minimum for a single condensate. It is therefore appropriate to expand each of the \( N_1 \)-dependent terms as a power series in \( u \):

\[ \frac{2}{N} \sqrt{N_1(N_2+1)} = \sum_{n=0}^{\infty} I_n u^n, \]

\[ \frac{4}{N^2} \sqrt{(N_1-1)N_1(N_2+1)(N_2+2)} = \sum_{n=0}^{\infty} J_n u^n, \]

which implicitly defines the \( I_n \) and \( J_n \).

The second-order differential equation for \( C(u) \) we obtain is found to have a first-order term which can be eliminated by the substitution \( \hat{C}(u) = C(u) \exp(-\sum \phi_{2n} u^{2n}) \) with an appropriate choice of the constants \( \phi_{2n} \). It then follows that \( \hat{C}(u) \) satisfies a second-order differential equation identical to that of a particle with position \( u \) in a one-dimensional potential well of even powers of \( u \). Since the solution is only significant in the range \( u \lesssim \sqrt{1/N} \), we make the approximation that terms in the potential that are quartic or of higher order in \( u \) are small perturbations upon the quadratic term, and can be neglected. In this case, the function \( \hat{C}(u) = C(u) \exp(-\tau u^2/2) \) satisfies the equation for the modes of a simple harmonic oscillator:

\[ -\ddot{C}(u) + (\nu^2 + \tau^2) u^2 \dot{C}(u) = (\eta + \tau) \dot{C}(u), \]  

(16)
where, after expanding the $I_n$ and $J_n$ to leading order in $1/N$,
\[
\eta = 2N^2 \frac{E/N - (\epsilon_{11} + \epsilon_{12} + Ng\left(\frac{4}{7}T_0 + T_1 + \frac{4}{7}T_2\right))}{-\epsilon_{12} - Ng(T_1 + T_2)},
\]
\[
\nu^2 = \frac{2N^2}{-\epsilon_{12} - Ng(T_1 + T_2)} \times \left[ 2 \left(1 - \frac{\eta}{\nu}\right) \left(-\epsilon_{12} - NgT_1\right) + Ng \left(\frac{1}{4} \frac{7}{7} - 3\right) T_2 \right],
\]
\[
\tau = 2.
\]
(17)

Thus, the solution for $C(u)$ that minimizes $\eta$, thereby minimizing the energy $E$, is a Gaussian
\[
C(u) = \frac{1}{\sqrt{2\pi}^{\frac{1}{4}} N} e^{-\frac{u^2}{\sigma^2}},
\]
(18)
with width
\[
\sigma = \frac{1}{2\sqrt{2N}} \sqrt{1 - A + \sqrt{A^2 + B}},
\]
(19)
where
\[
A = \frac{3}{2N} - \epsilon_{12} - Ng(T_1 + \frac{4}{7}T_2),
\]
and
\[
B = \frac{-\epsilon_{12} - Ng(T_1 + \frac{4}{7}T_2)}{-\epsilon_{12} - Ng(T_1 + T_2)},
\]
and with energy
\[
E = N \left[ \frac{-\epsilon_{12} - Ng(T_1 + T_2)}{4N^2g^2T_0 + T_1 + 3T_2} \right].
\]
(20)
The variance in $N_1$ for this solution is simply $N\sigma$, while the degree of first-order spatial coherence is given by
\[
C^{(1)} = e^{-\frac{1}{4(N^2\sigma^2)} (1 + \frac{1}{N} - 2\sigma^2)}.
\]
(21)

In the absence of any barrier, $|\epsilon_{12}| \gg NgT_0, Ng T_1, Ng T_2$, and it can be verified that eq. (19) predicts the appropriate value for this limit, namely $\Delta N_1 \approx 1/2\sqrt{N}$, the value for a single condensate. As the barrier strength is increased, the magnitudes of $\epsilon_{12}$, $T_1$ and $T_2$ decrease while the magnitude of $T_0$ does not vary significantly; it therefore follows from (13) that $\Delta N_1$ will decrease with barrier strength. When $\Delta N_1$ falls below 1, the assumption of smoothness breaks down. Thus the range of validity of the continuum approximation is $\Delta N_1 \gtrsim 1$, or equivalently, $C^{(1)} \gtrsim 0.88$.

If the potential is such that $Ng T_1, Ng T_2 \ll |\epsilon_{12}|$ continues to hold as the barrier strength is raised from zero, then to leading order in $1/N$ the expression for $\sigma$ simplifies to
\[
\sigma = \frac{1}{\sqrt{2\sqrt{N} \sqrt{1 + \frac{2}{7} \frac{7}{7} - \epsilon_{12}}}},
\]
depending only on the ratio of the interaction energy to the splitting between the symmetric and antisymmetric levels of the trap.

### B. Two-coefficient approximation

At large barrier strengths, we make use of the following conditions:
\[
|\gamma| \ll 1, \text{ where } \gamma = \frac{\sqrt{\frac{N}{2} \left(\frac{N}{2} + 1\right)}(-\epsilon_{12} - g(N - 1)T_1)}{gT_0},
\]
(22)
and
\[
|\zeta| \ll 1, \text{ where } \zeta = \frac{N^2gT_2}{\sqrt{\frac{N}{2} \left(\frac{N}{2} + 1\right)}(-\epsilon_{12} - g(N - 1)T_1)}.
\]
(23)
The first of these conditions is always satisfied for sufficiently strong barriers since in the limit of an infinitely strong barrier, $\epsilon_{12} = T_1 = 0$, while $T_0$ is finite. Moreover, we have numerically verified that the second condition holds at sufficiently large barrier strengths for a variety of external potentials. Within the domain of applicability of these conditions, we seek coefficients $C_N$, that satisfy the recurrence relation (13) to first order in $\gamma$ and $\zeta$. Dividing the recurrence relation by $gT_0$, one finds that all terms involving $N^2gT_2$ have a magnitude on the order of $\zeta$ and can therefore be neglected. In this limit, the following set of coefficients are a solution:
\[
C_{N_1} = \sqrt{1 - 2\gamma^2} \text{ for } N_1 = \frac{N}{2} + 1, \frac{N}{2} - 1
\]
\[
= \gamma \text{ for } N_1 = \frac{N}{2}, \frac{N}{2} - 1
\]
\[
= 0 \text{ otherwise.}
\]
(24)
The energy in this case is
\[
E = N\epsilon_{11} + \left(\frac{N(N - 2)}{4} - 2\gamma^2\right)gT_0.
\]
(25)
We refer to this approximation as the two-coefficient approximation, and we dub any state of the form of (24) a perturbed dual condensate. For such a state, $C^{(1)}$ and $\Delta N_1$ are given by
\[
C^{(1)} = 2\gamma \sqrt{1 - 2\gamma^2} \sqrt{1 + \frac{2}{7}}, \text{ and } \Delta N_1 = \sqrt{2}\gamma.
\]
(26)
(27)
Keeping terms to first order in $\gamma$, and to leading order in powers of $1/N$, we have $C^{(1)} = 2\gamma$. The range of validity of the two-coefficient approximation is the range of barrier strengths for which $C^{(1)} \ll 1$ and $\Delta N_1 \ll 1$.

An alternative manner of deriving this solution that is perhaps more physically intuitive, is to begin by assuming a state of the form of (24) and showing that the value of $\gamma$ that minimizes the energy is indeed the value given in (22). We begin by recalling the form of $H_2$, exhibited in (3). Assuming that $|\zeta| \ll 1$, the $T_2$ term in $H_2$ can safely be neglected. If we introduce the operators

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6
\[ \hat{n}_1 = \hat{N}_1 - \frac{N}{2} \quad \text{and} \quad \hat{n}_2 = \hat{N}_2 - \frac{N}{2}, \]

then we find that

\[ \langle \hat{H}_2 \rangle = E_{\text{dual}} + (\epsilon_{12} + gT_1(N - 1)) \langle a_1^\dagger a_2 + a_2^\dagger a_1 \rangle + \frac{1}{2}gT_0(\langle \hat{n}_1^2 \rangle + \langle \hat{n}_2^2 \rangle), \]

where \( E_{\text{dual}} \) is the energy of the dual condensate. Since the magnitude of the cross-interaction term involving \( T_1 \) only depends on the many-body state through expectation values of bilinear operators, this term together with the \( \epsilon_{12} \) term can be considered as an effective single-particle energy. To first order in \( \gamma \) and to leading order in \( 1/N \), the perturbed dual condensate has

\[ \langle a_1^\dagger a_2 + a_2^\dagger a_1 \rangle = 2\gamma N \]

and consequently it has an effective single-particle energy benefit over the dual condensate of \( 2\gamma N(\epsilon_{12} - gNT_1) \) (this quantity is positive at the barrier strengths of interest, since \( \epsilon_{12} < 0 \) and typically \( T_1 < 0 \)). On the other hand, \( \langle \hat{n}_1^2 \rangle = \langle \hat{n}_2^2 \rangle = 2\gamma^2 \) for such a state, corresponding to a self-interaction energy cost of \( 2\gamma^2 gT_0 \). Thus, the effective single-particle energy of the perturbed dual condensate decreases linearly with \( \gamma \), while the self-interaction energy increases quadratically with this parameter. The minimum occurs precisely when \( \gamma \) has the value \( N(\epsilon_{12} - gNT_1)/2gT_0 \), which approximates the value in (22) for \( N \gg 1 \). For typical double-well potentials, where \( N g |T_1| \ll |\epsilon_{12}| \), \( \gamma \) is well approximated by \( N(\epsilon_{12})/2gT_0 \) to leading order in \( 1/N \). In this case, the transition from a completely fragmented condensate to one that shows some coherence across the barrier occurs when the number of particles times the ratio of the inversion frequency to the self-interaction energy becomes non-negligible. Thus, for a given shape of the trap and a fixed barrier strength, the degree of fragmentation decreases as the number of particles is increased but increases as the strength of the interaction is increased.

**C. Numerical solutions**

The form of the double-well potential in the MIT condensate interference experiment [1] is well modelled by a term that is harmonic along all three Cartesian axes, with frequencies \( \omega_x, \omega_y \) and \( \omega_z \) respectively, to which is added a Gaussian barrier of width \( \delta \) and strength \( \alpha \) centered at \( x = 0 \),

\[ U(r) = m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) + \frac{\alpha}{\sqrt{2\pi}\delta} e^{-\frac{2}{\omega_x^2}}. \]

The parameter values appropriate for Ref. [1] are \( \omega_x = 2\pi \times 19 \text{ Hz}, \omega_y = \omega_z = 2\pi \times 250 \text{ Hz}, \) and \( \delta = 6 \text{ µm} \). Within such a trap, the criterion (8) for the applicability of our perturbative approach becomes \( N \ll 100 \), which is much smaller than the number of condensate atoms in their experiment. We consider instead a larger trap, specifically, one which is isotropic with the trapping frequency of the axis of weakest confinement in the MIT trap, \( \omega_x = \omega_y = \omega_z = 2\pi \times 19 \text{ Hz} \). In this case our perturbative approach is good for up to approximately \( N = 100 \) particles, and this is the example we consider. The scattering length of \( ^{23}\text{Na} \) is taken to be \( a_{sc} = 3 \text{ nm} \).

In Fig. 1 we plot the profile along the \( x \)-axis of the external potential \( U(r) \) and the wavefunctions \( \phi_1(r) \) and \( \phi_2(r) \), together with the coefficients \( C_i \) for several values of the barrier strength. Fig. 2 displays the degree of first-order spatial coherence, \( C^{(1)} \), and the variance, \( \Delta N_1 \), in the number of particles occupying the localized state \( \phi_1 \) as a function of the barrier strength. The generic features of these results persist for different choices of parameters in \( (28) \) as well as for different choices of the form of \( U(r) \).

Also displayed in Fig. 2 are the values for \( C^{(1)} \) and \( \Delta N_1 \) given by the continuum approximation, as specified by eqs. (14) and (23), and given by the two-coefficient approximation, as specified by eqs. (26) and (27), for the same choice of external potential. For their respective ranges of validity, the analytic approximations are found to fit the numerical results extremely well.

From these calculations arise the following picture of the transition between a single and a fragmented condensate. Moving up from zero barrier strength, there is a range of barrier strengths over which \( C^{(1)} \) is close to unity, while \( \Delta N_1 \) falls from its single condensate value of \( 1/2\sqrt{N} \) to a value of 1. Moving down from infinite barrier strength, there is a range of barrier strengths over which \( C^{(1)} \) and \( \Delta N_1 \) are both much less than 1. Between these two domains, there is a narrow range of barrier strengths wherein the greatest part of the transition in \( C^{(1)} \) is made. The barrier strengths delimiting these domains can be estimated analytically using the approximations presented in this section.

**IV. DISCUSSION**

**A. The experimental signature of fragmentation**

Herein we consider a measurement of the first-order degree of spatial coherence. This is accomplished by a type of interference experiment that has been widely discussed in the literature [1] [4] [6] [7] [13]. Essentially, it constitutes a double-slit experiment for Bose condensates. The thought experiment runs as follows. After preparation of the condensate, the trap potential is removed and the atoms fall under the force of gravity through a pair of slits, located symmetrically about \( x = 0 \). These slits can be formed by changing the shape of the trapping potential, as long as this change is not so rapid that excitations
are induced, and not so slow that the system has time to relax to a new many-body ground state. For simplicity of the analysis, we also assume that the particles on the left and right are each given momentum translations of magnitude $\hbar k$ towards one another \([3]\). In the absence of such translations, the interference pattern is simply more complicated, and has been studied by Röhrl et al. \([4]\). We make the approximation that the inter-particle interactions are insignificant during this expansion period. In this case, only the single-particle wavefunctions evolve, while the coefficients $C_{N_i}$ in the many-body state \([4]\) remain unchanged.

Suppose the slits are centered at points $r = (x, y, z)$ and $r' = (-x, y, z)$, where $x$ is positive and chosen so that the barrier acquire complex phase factors of $e^{ikx}$ and $e^{-ikx}$ and magnitudes we denote by $\phi_1(r)$ and $\phi_2(r)$ respectively. For many-body states that are symmetric under a reflection about $x = 0$, these magnitudes are roughly uniform and of equal magnitude in the far field, so that the many-body state in the far field can be approximated by the many-body state prior to removal of the trap, with $\phi_1(r)$ and $\phi_2(r)$ replaced by $e^{ikx}$ and $e^{-ikx}$ respectively.

We now imagine detectors in the far field that are assumed to remove atoms from the condensate \([16]\). The probability distribution over the position, $r_1$, of the first detection is given by the expectation value of normally ordered field operators $P^1(r_1) = \frac{1}{N} \langle \hat{\Psi}^\dagger(r_1) \hat{\Psi}(r_1) \rangle$. The probability distribution over the positions $r_1, r_2, ..., r_m$ of the first $m$ detections is given by $P^m(r_1, r_2, ..., r_m) = \frac{(N-m)!}{N!} \langle \hat{\Psi}^\dagger(r_1) \hat{\Psi}^\dagger(r_2) ... \hat{\Psi}^\dagger(r_m) \hat{\Psi}(r_m) ... \hat{\Psi}(r_2) \hat{\Psi}(r_1) \rangle$. The density of detection events that emerges in a single run of the double-slit experiment has the form $\bar{\rho}^m(r) = \frac{N}{m} \sum_{i=1}^{m} \delta(r - r_i)$ where the set of positions $\{r_i\}$ are obtained from the probability distribution $P^m(r_1, r_2, ..., r_m)$. Of course, the finite resolution of any realistic detector can be accounted for by replacing the delta function in this expression with a suitably broadened distribution; as long as the resolution is finer than the distance between the fringes of the interference pattern, the difference will not be significant.

In a single run of the double-slit experiment, both the single and dual condensates typically yield a distribution $\bar{\rho}^m(r)$ with essentially the maximum possible fringe visibility. This is obviously true for a single condensate, and has been shown to be true for a dual condensate in the seminal paper of Javanainen and Yoo \([14]\). Thus, the mere presence of such interference is not indicative of a non-zero degree of first-order coherence. However, suppose the experiment is repeated many times with the same initial many-body state. In this case, the spatial phase of the interference pattern will vary randomly from one run to the next if the initial state is a dual condensate, while it will remain fixed if the initial state is a single condensate \([14]\). We therefore expect the degree of first-order spatial coherence to be revealed by the variance in the spatial phase of the interference pattern over many runs, or equivalently, the fringe visibility of the average detection pattern over many runs. Indeed, if one averages the pattern of detections from an infinite number of runs of the double-slit experiment, all prepared initially in the same many-body state, and each involving $m$ detection events, one obtains:

$$
\bar{\rho}^m(r) = \int d^3r_1 ... d^3r_m \left( \frac{N}{m} \sum_{i=1}^{m} \delta(r - r_i) \right) P^m(r_1, r_2, ..., r_m)
$$

$$
= \frac{N}{m} \sum_{i=1}^{m} \int d^3r_1 ... d^3r_{i-1} d^3r_{i+1} ... d^3r_m 
\times P^m(r_1, ..., r_{i-1}, r, r_{i+1}, ..., r_m)
= \left\langle \hat{\Psi}^\dagger(r) \hat{\Psi}(r) \right\rangle.
$$

The final equality follows from the fact that each element of the sum is simply equal to $P^1(r)$. If the fringe visibility of the average detection pattern, $\bar{\rho}^m(r)$, is evaluated for the many-body state in the far field, it is found to be precisely equal to our definition of $C^{(1)}$, the degree of first-order spatial coherence across the barrier, and thus enables a measurement of the latter.

Another possibility for an experimental study of fragmentation is a measurement of the degree of second-order spatial coherence; this may be accessible through non-resonant imaging \([19]\).

B. Finite temperatures

We close this section with a few comments on the effect of finite temperatures on the coherence properties of the condensate. The excited states of the system are not in general well approximated by a state of the form of \([3]\). Nonetheless it can be shown that at infinite barrier strength the first-order degree of spatial coherence across the barrier is zero for thermal equilibrium at any finite temperature. The proof is as follows. For an infinitely strong barrier the Hamiltonian is separable into two terms each involving only operators pertaining to particles on one side of the barrier. Consequently, any non-degenerate energy eigenstates are tensor products of states describing particles on one side of the barrier only. For any set of energy eigenstates that are degenerate, the subspace of Hilbert space spanned by this set has a basis of such product states. Thus, one can always identify a basis of energy eigenstates that are product states of this sort. Since the density operator that represents thermal equilibrium, $\bar{\rho}$, is a mixture of these energy eigenstates,
we will necessarily have $Tr(\hat{\rho}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}')) = 0$ if $r$ and $r'$ are on opposite sides of the barrier, and consequently the degree of first-order spatial coherence across the barrier for such a mixed state is zero as well. In the absence of any barrier, as long as the temperature is small enough that most of the particles are in the lowest single-particle energy level, the first-order degree of spatial coherence for the thermal state should be close to unity. For such temperature, if the barrier strength is varied from zero to infinity, the first-order degree of spatial coherence of the thermal state will vary from nearly unity to zero. Thus, a significant transition must still occur at such temperatures.

**V. CONCLUSIONS**

A theoretical treatment of fragmentation in Bose condensates must go beyond a mean-field analysis. For the case of repulsive inter-particle interactions and a double-well trapping potential, we have proposed an approach wherein an approximation to the many-body ground state is obtained by a restricted variational principle. We have implemented this proposal for the case of nearly non-interacting particles.

The coherence properties that we have considered are the degrees of first-order and second-order coherence across the central barrier of the potential. The first of these quantifies the variance over many runs in the spatial phase of the fringe pattern arising from the interference of atoms on either side of the barrier. The second is essentially the density-density correlation across the barrier, and for the states we consider it is a simple function of the variance in the number of particles in one of the wells. We find that as the barrier strength is increased, this variance is continuously squeezed down from its value for a single condensate. The degree of first-order spatial coherence is close to unity when this variance is greater than one, but thereafter drops off rapidly. Above a certain critical barrier strength we find that both quantities become much less than one, indicating that the condensate is essentially completely fragmented.

We have discussed how the degree of first-order coherence might be measured through interference experiments, and argued that a significant effect should be present even at finite temperatures. A concern, however, is that the ground state might be difficult to prepare if the relaxation time of the system is long compared to the lifetime of the condensate. This could arise if the only way for the particles to be redistributed across the barrier is by tunneling through it. However for numbers of particles that are not too large, this tunneling time need not be restrictive. For instance, in the example presented in Section III.C, the single particle tunneling time at the barrier strength where $C^{(1)} = 0.88$ is approximately one minute, while at the barrier strength where $C^{(1)} = 0.1$ it is roughly one hour.

Our variational approach can be extended in a straightforward manner to the determination of the many-body ground state in systems where the external potential has an arbitrary number, $n$, of minima. In such cases, one would simply introduce states that are arbitrary superpositions of Fock states where up to $n$ single-particle wavefunctions are occupied. Such an analysis should be of relevance to the determination of the coherence properties of Bose condensates in optical lattices. Moreover, at extremely high densities, where the interaction energy is dominant, it may become energetically favorable for a condensate to begin to fragment even in the presence of a perfectly uniform potential. We hope to address these possibilities in future work.

**VI. ACKNOWLEDGMENTS**

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Fig. 1. Numerical solutions for the single-particle wavefunctions $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$ and the coefficients $C_{N_1}$ for $N = 100$ particles and double-well potentials with barrier strengths of $\alpha = 0, 15, 30, 45, \text{ and } 60$ in units of $\sqrt{\hbar \omega_x / m}$. The remaining parameter values are specified in the text. The dotted curve is the external potential along the $x$-axis, $U(x, y = 0, z = 0)$, in units of $\hbar \omega_x$. The solid and dashed curves are $\phi_1(x, y = 0, z = 0)$ and $\phi_2(x, y = 0, z = 0)$ respectively, in arbitrary units.

Fig. 2. (a) The degree of first-order spatial coherence across the barrier, $C^{(1)}$, and (b) the variance in the occupation number of one of the wells, $\Delta N_1$, as a function of the barrier strength, $\alpha$, in units of $\sqrt{\hbar \omega_x / m}$ for $N = 100$ particles and the parameter values specified in the text. The solid curve is the numerical solution, the dashed curve is the continuum approximation, and the dotted curve is the two-coefficient approximation.
