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 interparticle 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 an approximate analytic solution as well as a numerical solution of our model, in the regime where the interparticle interactions can be treated perturbatively. The degree of fragmentation of the condensate is characterized by the degrees of first- and second-order spatial coherence across the barrier. [S1050-2947(99)06605-6]

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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 wave functions. If the occupied single-particle wave functions 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 interparticle interactions it is the exchange energy that typically prevents fragmentation into a number of degenerate (or nearly degenerate) single-particle wave functions. However, this argument is inapplicable for bosons in an external potential with several local minima, since single-particle wave functions 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 of 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 wave functions, 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 interparticle 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 setup. 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. Röhrl *et al.* [4] 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 interparticle 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] considered the energy eigenstates of a Bose-Einstein condensate in a double-well potential, and predicted fragmentation when the interparticle interactions are sufficiently strong. However, these authors considered only traps with weakly coupled wells, and therefore could not 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 did 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.* [7] determined the probability distributions and lifetimes of two interacting condensates in different internal states confined to the same trap, while Cirac *et al.* [8] as well as Steel and Collett [9] considered 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 wave functions. 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 wave functions that determines the degree of fragmentation in the system.

The remainder of the paper is organized as follows. In Sec. II we present our model and define some useful measures of spatial coherence of the condensate. In Sec. III we present approximate analytic solutions of our model in the regime of nearly noninteracting 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 Sec. V, followed by our concluding remarks in Sec. VI.

II. MODEL

A. 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, $V(\mathbf{r},\mathbf{r}')=g\,\delta(\mathbf{r}-\mathbf{r}')$ with an interaction strength $g=4\pi a_{\rm sc}\hbar^2/m$, where $a_{\rm sc}$ is the s-wave scattering length, and m is the mass of the bosons. The Hamiltonian is given by [10]

$$\hat{H}=\int d^3r\left[-\frac{\hbar^2}{2m}\hat{\Psi}^\dagger(\mathbf{r})\boldsymbol{\nabla}^2\hat{\Psi}(\mathbf{r})+U(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})+\frac{g}{2}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r})\right], \tag{1}$$

where $\hat{\Psi}(\mathbf{r})$ is the quantum field operator, and $U(\mathbf{r})$ 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

$$|\psi\rangle=\sum_{N_1=0}^{N} C_{N_1}|N_1,N_2\rangle_{(\phi_1,\phi_2)}, \tag{2}$$

where

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

is the Fock state in which N_1 particles occupy the single-particle state $\phi_1(\mathbf{r})=\langle\mathbf{r}|a_1^\dagger|\mathrm{vac}\rangle$ and N_2 particles occupy $\phi_2(\mathbf{r})=\langle\mathbf{r}|a_2^\dagger|\mathrm{vac}\rangle$. 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 wave functions ϕ_1 and ϕ_2 are both normalized and orthogonal to one another.

State (2) is certainly not the most general state one can consider. Indeed, such a state 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 [3]. 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 Eq. (2), we consider only those which have the same symmetry as the Hamiltonian under reflections about $x=0$. This implies that the single-particle wave functions 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 ϕ_1 and ϕ_2 to be real, the Hamiltonian takes the form

$$\hat{H}_2=\epsilon_{11}\hat{N}+(\epsilon_{12}+gT_1(\hat{N}-1))(a_1^\dagger a_2+a_2^\dagger a_1)+\frac{gT_0}{2}(\hat{N}_1^2+\hat{N}_2^2-\hat{N})+\frac{gT_2}{2}(a_1^\dagger a_1^\dagger a_2 a_2+a_2^\dagger a_2^\dagger a_1 a_1+4\hat{N}_1\hat{N}_2), \tag{3}$$

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

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

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

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

$$T_1=\int d^3r\,\phi_1^3(\mathbf{r})\phi_2(\mathbf{r}),$$

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

These quantities have the following physical interpretation: ϵ_{11} is the single-particle energy for the state ϕ_1; ϵ_{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 [6,9], 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

$$\hat{J}_z=\frac{1}{2}(a_2^\dagger a_1+a_1^\dagger a_2),$$

$$\hat{J}_y=\frac{i}{2}(a_2^\dagger a_1-a_1^\dagger a_2),$$

$$\hat{J}_x=\frac{1}{2}(\hat{N}_2-\hat{N}_1),$$

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

$$\hat{H}_2=E_0+2(\epsilon_{12}+gT_1(N-1))\hat{J}_z+2gT_2\hat{J}_z^2+g(T_0-T_2)\hat{J}_x^2, \tag{4}$$

where

$$E_0\equiv\epsilon_{11}N+\tfrac{1}{4}N(N-2)(gT_0+gT_2),$$

and where we have used $\hat{J}_x^2+\hat{J}_y^2+\hat{J}_z^2=j(j+1)$ to eliminate $\hat{J}_y^2$ from the expression. The observable corresponding to $\hat{J}_x$ is the particle number difference between the localized states ϕ_1 and ϕ_2. Defining the wave functions $\phi_s=2^{-1/2}(\phi_1+\phi_2)$ and $\phi_a=2^{-1/2}(\phi_1-\phi_2)$, which are, respectively, symmetric and antisymmetric about $x=0$, one sees that $\hat{J}_z$ can be rewritten as $\frac{1}{2}(a_s^\dagger a_s-a_a^\dagger a_a)$, where $a_s^\dagger$ and $a_a^\dagger$ are the creation operators associated with ϕ_s and ϕ_a, respectively. Thus, $\hat{J}_z$ corresponds to the particle number difference between the symmetrized states ϕ_s and ϕ_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 wave function ϕ_1, subject to the constraints that the set of coefficients is normalized, and ϕ_1 is both normalized and orthogonal to ϕ_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 ϕ_s and ϕ_a rather than ϕ_1. The reason for this is that no constraint corresponding to orthogonality is required when working with ϕ_s and ϕ_a, since they are orthogonal by construction; as a result the analysis is simplified.

We begin with the variation of ϕ_s and ϕ_a, implementing the normalization constraints through Lagrange multipliers E_s and E_a, respectively. This results in two coupled nonlinear Schrödinger equations for ϕ_s and ϕ_a,

$$\left[-\frac{\hbar^2\nabla^2}{2m}+U(\mathbf{r})+g\Gamma^{\circ}_{\alpha}\phi_\alpha^2(\mathbf{r})+g\Gamma^{x}_{\alpha}\phi_\beta^2(\mathbf{r})\right]\phi_\alpha(\mathbf{r})=E_\alpha\phi_\alpha(\mathbf{r}), \tag{5}$$

where

$$\Gamma^{\circ}_{\alpha}=\langle(a_\alpha^\dagger a_\alpha)^2-a_\alpha^\dagger a_\alpha\rangle/\langle a_\alpha^\dagger a_\alpha\rangle,$$
$$\Gamma^{x}_{\alpha}=\langle a_\alpha^\dagger a_\alpha^\dagger a_\beta a_\beta+a_\beta^\dagger a_\beta^\dagger a_\alpha a_\alpha+4a_\alpha^\dagger a_\alpha a_\beta^\dagger a_\beta\rangle/\langle a_\alpha^\dagger a_\alpha\rangle, \tag{6}$$

and where the indices (α,β) take the values (s,a) and (a,s).

We now minimize the expectation value of $\hat{H}_2$ with respect to variations in the coefficients 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,

$$\left[N\epsilon_{11}+\frac{gT_0}{2}(N_1^2+N_2^2-N)+2gT_2N_1N_2-E\right]C_{N_1}+[\epsilon_{12}+gT_1(N-1)][\sqrt{N_1(N_2+1)}C_{N_1-1}+\sqrt{N_2(N_1+1)}C_{N_1+1}]$$
$$+\frac{gT_2}{2}[\sqrt{(N_1-1)N_1(N_2+1)(N_2+2)}C_{N_1-2}+\sqrt{(N_2-1)N_2(N_1+1)(N_1+2)}C_{N_1+2}]=0, \tag{7}$$

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 ϵ_{11}, ϵ_{12}, T_0, T_1, and T_2, we can solve this equation by diagonalizing an $N\times N$ matrix with nonzero entries along five diagonals, a problem which is numerically tractable if the number of nonzero coefficients is not too large.

Since Eqs. (5) and (7) form a coupled set of equations for ϕ_s, ϕ_a, and 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. Regime of nearly noninteracting particles

The full problem outlined above is rather complex. In this paper, we consider only perturbative solutions of Eq. (5) in the nearly noninteracting 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 single-particle excited state of the external potential, and ϵ_s, the energy of the ground state. This is ensured by the criterion

$$gNT_0\ll\epsilon_s^{(1)}-\epsilon_s. \tag{8}$$

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 nonlinear terms in Eq. (5) 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

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

for $\alpha=s$, a. In this case, the wave functions ϕ_s and ϕ_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 ϵ_{11}, ϵ_{12}, T_0, T_1, and T_2, and these subsequently define the form of the recurrence relation (7) that must be solved to obtain the coefficients C_{N_1}. Although the full results are presented in Sec. 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, $|\epsilon_{12}|\simeq\epsilon_s^{(1)}-\epsilon_s$, and since $|T_1|$ and T_2 are on the order of T_0 or less, it follows from criterion (8) that $|\epsilon_{12}|\gg NgT_0, Ng|T_1|, NgT_2$. If we provisionally assume that the ground state fulfills the conditions that $N|\langle\hat{J}_z\rangle|\gtrsim\langle\hat{J}_z^2\rangle,\langle\hat{J}_x^2\rangle$, then we are led to approximate the Hamiltonian by

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

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 ϕ_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 noninteracting 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 ϕ_0, as a ''single condensate.'' In this paper, we are concerned only with single condensates wherein the single-particle wave function ϕ_0 is symmetric about $x=0$. We do not introduce any additional terminology to distinguish such a state from one with arbitrary ϕ_0, since no confusion is likely to arise.

In the limit of infinite barrier strength, the amplitudes of ϕ_s and ϕ_a at $x=0$ are necessarily zero, while ϕ_s and ϕ_a at $x\neq0$ satisfy the same equation. Consequently, ϕ_s and ϕ_a differ only in their symmetry under reflection about $x=0$ and thus $\epsilon_{12}=T_1=T_2=0$. The Hamiltonian of Eq. (4) then reduces to

$$\hat{H}_2=E_0+gT_0\hat{J}_x^2. \tag{11}$$

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 ϕ_1 and ϕ_2 are orthogonal, as a ''dual condensate'' [11]. In this paper we will be concerned only with dual condensates wherein $N_1=N_2=N/2$, and ϕ_1 and ϕ_2 are mirror images of one another across $x=0$.

The analysis above confirms, for the limit of nearly noninteracting particles, the results of an earlier study [3]: 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 [12], 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 $\mathbf{r}'$,

$$g^{(1)}(\mathbf{r},\mathbf{r}')=\frac{\rho_1(\mathbf{r},\mathbf{r}')}{[\rho_1(\mathbf{r},\mathbf{r})\rho_1(\mathbf{r}',\mathbf{r}')]^{1/2}}. \tag{12}$$

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 $|\phi_1(\mathbf{r})|\ll|\phi_2(\mathbf{r})|$ and $|\phi_1(\mathbf{r}')|\gg|\phi_2(\mathbf{r}')|$, for any state of the form of Eq. (2) that is symmetric under reflection about $x=0$, the quantity $g^{(1)}(\mathbf{r},\mathbf{r}')$ is in fact independent of $\mathbf{r}$ and $\mathbf{r}'$, and has the value

$$\mathcal{C}^{(1)}=\frac{\langle a_1^\dagger a_2+a_2^\dagger a_1\rangle}{N}. \tag{13}$$

We refer to $\mathcal{C}^{(1)}$ 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 $\rho_2(\mathbf{r},\mathbf{r}')=\langle\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r})\rangle$, which is simply the normally ordered density-density correlation, can be normalized to obtain the degree of second-order spatial coherence between points $\mathbf{r}$ and $\mathbf{r}'$,

$$g^{(2)}(\mathbf{r},\mathbf{r}')=\frac{\rho_2(\mathbf{r},\mathbf{r}')}{[\rho_2(\mathbf{r},\mathbf{r})\rho_2(\mathbf{r}',\mathbf{r}')]^{1/2}}. \tag{14}$$

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

$$\mathcal{C}^{(2)}=\frac{1-4\left(\frac{\Delta N_1}{N}\right)^2}{\frac{N-2}{N}+4\left(\frac{\Delta N_1}{N}\right)^2}, \tag{15}$$

where $\Delta N_1 \equiv (\langle \hat{N}_1^2\rangle - \langle \hat{N}_1\rangle^2)^{1/2}$ is the variance in the number of particles occupying the localized state ϕ_1. We refer to $\mathcal{C}^{(2)}$ as the degree of second-order spatial coherence across the barrier. The variance in N_1 for a single condensate $|N\rangle_{\phi_s}$ 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, $\mathcal{C}^{(2)}-1=0$ for a single condensate $|N\rangle_{\phi_s}$, and $\mathcal{C}^{(2)}-1=2/(N-2)$ for a dual condensate. Since ΔN_1 is sufficient to specify $\mathcal{C}^{(2)}$, while being simpler to interpret, we use ΔN_1 together with $\mathcal{C}^{(1)}$ 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 (9). The localized single-particle states ϕ_1 and ϕ_2 are simply the sum and difference of the single-particle ground and first excited states. Using these wave functions, the coefficients C_{N_1} can be obtained by solving the recurrence relation (7).

Here we 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 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 (7) 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 where $u \lesssim \sqrt{1/N}$. 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 ΔN_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 $\overline{C}(u)=C(u)\exp(-\Sigma_n a_{2n}u^{2n})$ with an appropriate choice of the constants a_{2n}. It then follows that $\overline{C}(u)$ 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 $\overline{C}(u)=C(u)\exp(-\pi u^2/2)$ satisfies the equation for the modes of a simple harmonic oscillator:

$$-\overline{C}''(u)+(\nu^2+\tau^2)u^2\overline{C}(u)=(\eta+\tau)\overline{C}(u), \tag{16}$$

where, after expanding the I_n and J_n to leading order in $1/N$,

$$\eta = 2N^2\frac{E/N-\left[\epsilon_{11}+\epsilon_{12}+Ng\left(\frac{1}{4}T_0+T_1+\frac{3}{4}T_2\right)\right]}{-\epsilon_{12}-Ng(T_1+T_2)},$$

$$\nu^2=\frac{2N^2}{-\epsilon_{12}-Ng(T_1+T_2)}\left[\left(2-\frac{\eta}{N^2}\right)(-\epsilon_{12}-NgT_1)+Ng\left(T_0+\left(2\frac{\eta}{N^2}-3\right)T_2\right)\right], \tag{17}$$

$$\tau=2.$$

Thus the solution for $C(u)$ that minimizes η, thereby minimizing the energy E, is a Gaussian,

$$C(u)=\frac{1}{\sqrt{N}}\frac{1}{(2\pi)^{1/4}\sqrt{\sigma}}e^{-u^2/4\sigma^2}, \tag{18}$$

with width

$$\sigma=\frac{1}{2\sqrt{N}}\frac{1}{\sqrt{-A+\sqrt{A^2+B}}}, \tag{19}$$

where

$$A=\frac{3}{2N}\frac{-\epsilon_{12}-Ng\left(T_1+\frac{4}{3}T_2\right)}{-\epsilon_{12}-Ng(T_1+T_2)},$$

$$B=\frac{-\epsilon_{12}-Ng\left(T_1+\frac{3}{2}T_2-\frac{1}{2}T_0\right)}{-\epsilon_{12}-Ng(T_1+T_2)},$$

and with energy

$$E=N\left[\frac{-\epsilon_{12}-Ng(T_1+T_2)}{4N^2\sigma^2}+(\epsilon_{11}+\epsilon_{12})+Ng\left(\frac{1}{4}T_0+T_1+\frac{3}{4}T_2\right)\right]. \tag{20}$$

The variance in N_1 for this solution is simply $N\sigma$, while the degree of first-order spatial coherence is given by

$$\mathcal{C}^{(1)}=e^{-1/8\sigma^2N^2}\left(1+\frac{1}{N}-2\sigma^2\right). \tag{21}$$

In the absence of any barrier, $|\epsilon_{12}| \gg NgT_0, Ng|T_1|, NgT_2$, and it can be verified that Eq. (19) predicts the appropriate value for this limit, namely, $\Delta N_1 \simeq \sqrt{N}/2$, the value for a single condensate. As the barrier strength is increased, the magnitudes of ϵ_{12}, T_1, and T_2 decrease, while the magnitude of T_0 does not vary significantly; it therefore follows from Eq. (19) that ΔN_1 will decrease with barrier strength. When ΔN_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, $\mathcal{C}^{(1)} \gtrsim 0.88$.

If the potential is such that $Ng|T_1|, NgT_2 \ll |\epsilon_{12}|$ continues to hold as the barrier strength is raised from zero, then to leading order in $1/N$ the expression for σ simplifies to

$$\sigma=\frac{1}{2\sqrt{N}}\frac{1}{\sqrt{1+\frac{N}{2}\frac{gT_0}{(-\epsilon_{12})}}},$$

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:

$$|\gamma| \ll 1, \tag{22}$$

where

$$\gamma \equiv \frac{\sqrt{\frac{N}{2}\left(\frac{N}{2}+1\right)}(-\epsilon_{12}-g(N-1)T_1)}{gT_0}$$

and

$$|\zeta| \ll 1, \tag{23}$$

where

$$\zeta \equiv \frac{N^2 gT_2}{\sqrt{\frac{N}{2}\left(\frac{N}{2}+1\right)}(-\epsilon_{12}-g(N-1)T_1)}.$$

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_1} that satisfy the recurrence relation (7) to first order in γ and ζ. Dividing the recurrence relation by gT_0, one finds that all terms involving N^2gT_2 have a magnitude on the order of $\gamma\zeta$ and can therefore be neglected. In this limit, the following set of coefficients are a solution:

$$\begin{aligned} C_{N_1} &= \sqrt{1-2\gamma^2} \quad \text{for } N_1=\frac{N}{2} \\ &= \gamma \quad \text{for} \quad N_1=\frac{N}{2}+1,\ \frac{N}{2}-1 \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{24}$$

The energy in this case is

$$E=N\epsilon_{11}+\left(\frac{N(N-2)}{4}-2\gamma^2\right)gT_0. \tag{25}$$

We refer to this approximation as the *two-coefficient approximation*, and we dub any state of the form of Eq. (24) a *perturbed dual condensate*. For such a state, $\mathcal{C}^{(1)}$ and ΔN_1 are given by

$$\mathcal{C}^{(1)}=2\gamma\sqrt{1-2\gamma^2}\sqrt{1+\frac{2}{N}}, \tag{26}$$

$$\Delta N_1=\sqrt{2}\gamma. \tag{27}$$

Keeping terms to first order in γ, and to leading order in powers of $1/N$, we have $\mathcal{C}^{(1)}=2\gamma$. The range of validity of

the two-coefficient approximation is the range of barrier strengths for which $\mathcal{C}^{(1)} \ll 1$ 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 Eq. (24) and showing that the value of γ that minimizes the energy is indeed the value given in Eq. (22). We begin by recalling the form of $\hat{H}_2$, exhibited in Eq. (3). Assuming that $|\zeta| \ll 1$, the T_2 term in $(\hat{H}_2)$ can safely be neglected. If we introduce the operators

$$\hat{n}_1 = \hat{N}_1 - \frac{N}{2},$$

$$\hat{n}_2 = \hat{N}_2 - \frac{N}{2},$$

then we find that

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

where E_{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 ϵ_{12} term, can be considered as an effective single-particle energy. To first order in γ 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 γ, while the self-interaction energy increases quadratically with this parameter. The minimum occurs precisely when γ has the value $N(-\epsilon_{12} - gNT_1)/2gT_0$, which approximates the value in Eq. (22) for $N \gg 1$.

For typical double-well potentials, where $Ng|T_1| \ll |\epsilon_{12}|$, γ 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 modeled by a term that is harmonic along all three Cartesian axes, with frequencies ω_x, ω_y, and ω_z, respectively, to which is added a Gaussian barrier of width δ and strength α centered at $x = 0$:

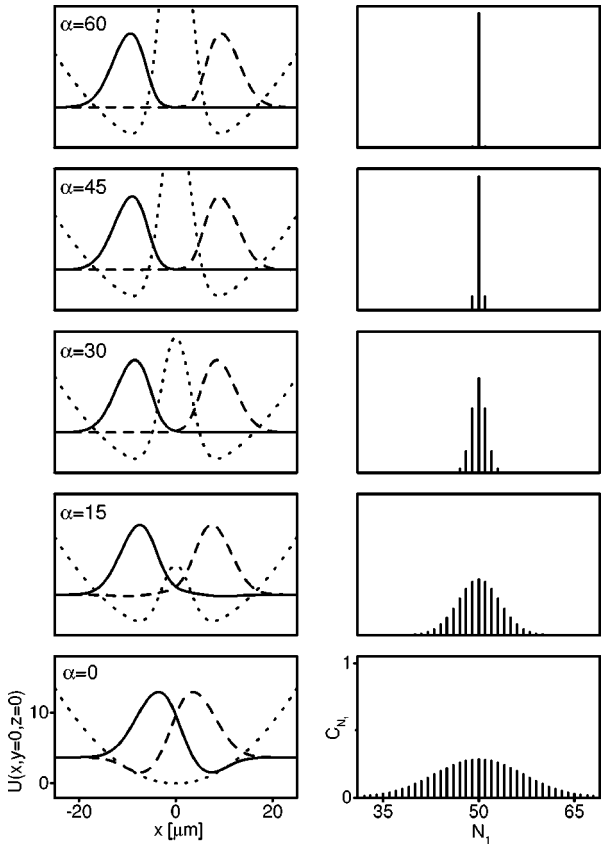

FIG. 1. Numerical solutions for the single-particle wave functions $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$ and the coefficients C_{N_1} for $N = 100$ particles and double-well potentials with barrier strengths of $\alpha = 0$, 15, 30, 45, and 60 in units of $\sqrt{\hbar^3 \omega_x / m}$. The remaining 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.

$$U(\mathbf{r}) = m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) + \frac{\alpha}{\sqrt{2\pi}\delta} e^{-x^2/2\delta^2}. \quad (28)$$

The parameter values appropriate for Ref. [1] are $\omega_x = 2\pi \times 19$ Hz, $\omega_y = \omega_z = 2\pi \times 250$ Hz, and $\delta = 6$ μm. Within such a trap, 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, $\omega_x = \omega_y = \omega_z = 2\pi \times 19$ 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}Na is taken to be $a_{\text{sc}} = 3$ nm [13].

In Fig. 1 we plot the profile along the x axis of the external potential $U(\mathbf{r})$ and the wave functions $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$, together with the coefficients C_{N_1} for several values of the barrier strength. Figure 2 displays the degree of first-order spatial coherence, $\mathcal{C}^{(1)}$, and the variance, ΔN_1, in the number of particles occupying the localized state ϕ_1 as a function of the barrier strength. The generic features of these results per-

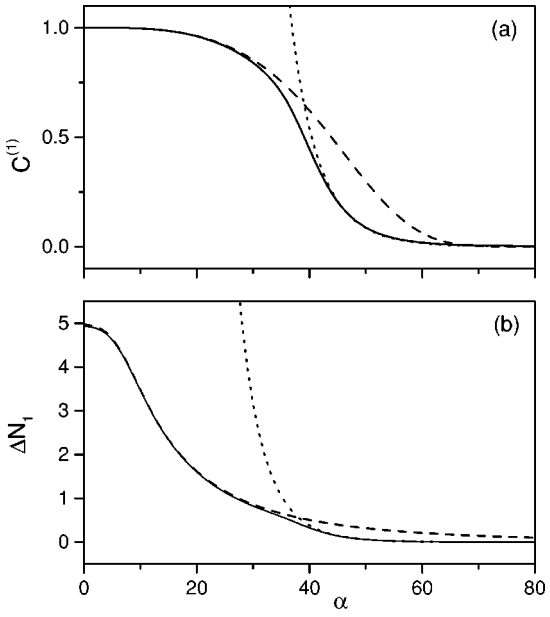

FIG. 2. (a) The degree of first-order spatial coherence across the barrier, $\mathcal{C}^{(1)}$, and (b) the variance in the occupation number of one of the wells, ΔN_1, as a function of the barrier strength, α, in units of $\sqrt{\hbar^3\omega_x/m}$ for $N=100$ particles and the parameter values specified 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.

sist for different choices of parameters in Eq. (28) as well as for different choices of the form of $U(\mathbf{r})$.

Also displayed in Fig. 2 are the values for $\mathcal{C}^{(1)}$ and ΔN_1 given by the continuum approximation, as specified by Eqs. (19) and (21), 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 condensate and a fragmented condensate. Moving up from zero barrier strength, there is a range of barrier strengths over which $\mathcal{C}^{(1)}$ is close to unity, while ΔN_1 falls from its single condensate value of $\sqrt{N}/2$ to a value of 1. Moving down from infinite barrier strength, there is a range of barrier strengths over which $\mathcal{C}^{(1)}$ and ΔN_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 $\mathcal{C}^{(1)}$ is made. The barrier strengths delimiting these domains can be estimated analytically using the approximations presented in this section.

IV. DISCUSSION

A. 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 [1,14–17]. 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 $\hbar k$ toward one another [14]. In the absence of such translations, the interference pattern is simply more complicated, and has been studied by Rörhl *et al.* [4]. We make the approximation that the interparticle interactions are insignificant during this expansion period. In this case, only the single-particle wave functions evolve, while the coefficients C_{N_1} in the many-body state (2) remain unchanged.

Suppose the slits are centered at points $\mathbf{r}=(x,y,z)$ and $\mathbf{r}'=(-x,y,z)$, where x is positive and chosen to be sufficiently large so that $|\phi_1(\mathbf{r})| \ll |\phi_2(\mathbf{r})|$ and $|\phi_1(\mathbf{r}')| \gg |\phi_2(\mathbf{r}')|$. In this case, the single-particle wave functions $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$ evolve to wave functions localized entirely at just one of the slits. After the momentum translation and a period of free expansion the single-particle wave functions originating from the left and right of the barrier acquire complex phase factors of e^{ikx} and e^{-ikx} and magnitudes we denote by $\tilde{\phi}_1(\mathbf{r})$ and $\tilde{\phi}_2(\mathbf{r})$, respectively. For many-body states that are symmetric under a reflection about $x=0$, these magnitudes are roughly uniform and equal in the far field of the double slit, 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 $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$ 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 [15]. The probability distribution over the position $\mathbf{r}_1$ of the first detection is given by the expectation value of normally ordered field operators $P^1(\mathbf{r}_1)=(1/N)\langle\hat{\Psi}^\dagger(\mathbf{r}_1)\hat{\Psi}(\mathbf{r}_1)\rangle$. The probability distribution over the positions $\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m$ of the first m detections is given by $P^m(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m)=[(N-m)!/N!]\langle\hat{\Psi}^\dagger(\mathbf{r}_1)\hat{\Psi}^\dagger(\mathbf{r}_2)\cdots\hat{\Psi}^\dagger(\mathbf{r}_m)\hat{\Psi}(\mathbf{r}_m)\cdots\hat{\Psi}(\mathbf{r}_2)\hat{\Psi}(\mathbf{r}_1)\rangle$. The density of detection events that emerges in a single run of the double-slit experiment has the form $\rho^m(\mathbf{r})=(N/m)\Sigma_{i=1}^m\delta(\mathbf{r}-\mathbf{r}_i)$ where the set of positions $\{\mathbf{r}_i\}$ is obtained from the probability distribution $P^m(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m)$. Of course, the finite resolution of any realistic detector can be accounted for by replacing the δ 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 $\rho^m(\mathbf{r})$ 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 [15]. Thus the mere presence of such interference is not indicative of a nonzero 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 [15]. 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

$$\overline{\rho}^m(\mathbf{r}) = \int d^3r_1 \cdots d^3r_m \left(\frac{N}{m} \sum_{i=1}^{m} \delta(\mathbf{r}-\mathbf{r}_i) \right) P^m(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_m)$$

$$= \frac{N}{m} \sum_{i=1}^{m} \int d^3r_1 \cdots d^3r_{i-1} d^3r_{i+1} \cdots d^3r_m P^m(\mathbf{r}_1, \ldots, \mathbf{r}_{i-1}, \mathbf{r}, \mathbf{r}_{i+1}, \ldots, \mathbf{r}_m) = \langle \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \rangle. \tag{29}$$

The final equality follows from the fact that each element of the sum is simply equal to $P^1(\mathbf{r}_i)$. If the fringe visibility of the average detection pattern, $\overline{\rho}^m(\mathbf{r})$, is evaluated for the many-body state in the far field, it is found to be precisely equal to our definition of $\mathcal{C}^{(1)}$, 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 nonresonant imaging [18].

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 Eq. (2). 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 nondegenerate 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, $\hat{\rho}$, is a mixture of these energy eigenstates, we will necessarily have $\mathrm{Tr}(\hat{\rho}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}'))=0$ if $\mathbf{r}$ and $\mathbf{r}'$ 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 temperatures, 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 interparticle 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 noninteracting particles.

The coherence properties that we have considered are the degrees of first- 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 1, but thereafter drops off rapidly. Above a certain critical barrier strength we find that both quantities become much less than 1, 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 Sec. III C, the single-particle tunneling time at the barrier strength where $\mathcal{C}^{(1)}=0.88$ is approximately 1 min, while at the barrier strength where $\mathcal{C}^{(1)}=0.1$ it is roughly 1 h.

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 wave functions are occupied.

Such an analysis is of relevance to the determination of the coherence properties of Bose condensates in optical lattices [19]. 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 this possibility in future work.

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