

Ground-state fragmentation of repulsive Bose-Einstein condensates in double-trap potentials

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The fragmentation of the ground state of a repulsive condensate immersed into a double-trap potential is found to be a general and critical phenomenon. It takes place for a given number of bosons if their scattering length is larger than some critical value or for a given value of the scattering length if the number of bosons is above some critical number. We demonstrate that the geometry of the inner trap determines these critical parameters while the number of the fragments and the fraction of bosons in the various fragments can be manipulated by the outer trap. There is also a maximal number of bosons for which the ground state is fragmented. If this number is exceeded, the fragmented state becomes a very low-lying excited state of the condensate. This maximal number of bosons can be substantially manipulated by varying the inner and outer traps. To study threefold fragmentation we have chosen a potential well with two barriers as the inner trap and embedded in two types of outer ones. A manifold fragmentation is also addressed.

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I. INTRODUCTION

The general mathematical formulation of the condensation phenomenon for an ideal gas in equilibrium was given by Penrose and Onsager [1] in 1956. They considered a system of N interacting bosons and its reduced one-particle density matrix. The eigenvalues of this matrix are called *occupation numbers* and the eigenvectors are referred to as *natural orbitals*. If an ideal gas of free bosons forms a Bose-Einstein condensate (BEC), then only a single natural orbital is macroscopically occupied. The extension of this concept to several macroscopically occupied orbitals is the basis of the fragmentation phenomenon. The BEC is called *fragmented* if several natural orbitals have macroscopic occupation numbers [2]. Although these original definitions have been formulated in the thermodynamic limit $N \rightarrow \infty$, the reduced one-particle density matrix can also be applied to study condensation [3] and fragmentation [4] in finite- N bosonic systems.

The first measurements of an interference between two expanding and overlapping condensates [5] have stimulated a great interest in theoretical studies of fragmentation. An initial quantum state of such a system is supposed to be twofold fragmented, i.e., two spatially separated orbitals are macroscopically occupied. Theoretical studies on the relative phase [6–8] between the fragments, its dynamical stability [9,10], and related questions on the evolution of this state [11,12] have been a subject of numerous discussions. A natural extension of these effects to an array of multiple wells with a manifold fragmented initial state [13] has been initiated by the recent experiments in optical [14] and hybrid traps [15].

In contrast, the fragmentation of the ground state of a BEC has been predicted only for a few systems where it is enforced by the spatial or spin symmetry of the system. In particular, the ground state of an attractive condensate in a

perfect ring is found to be fragmented [16]. The rotational symmetry of the corresponding Hamiltonian permits as natural orbitals only plane waves [17]. The many-body wave function of this system starts to differ from a function composed by plane waves for any nonzero attractive interaction and the respective one-particle density matrix having plane waves as natural orbitals must exhibit several nonzero eigenvalues. This eventually leads to fragmentation and its origin is spatial (rotational) symmetry. Another example is an attractive BEC in a symmetric double-well potential where the ideal symmetry of the potential [18] causes the fragmentation of the ground state. The stability of all these fragmented states with respect to a small asymmetric perturbation is still an open question. There are indications that these symmetry related fragmentations disappear upon symmetry breaking. Fragmentation can also take place if bosons have additional internal degrees of freedom. An example of such a system is a system made of Bose particles with nonzero spin, a so-called spinor condensate. In spinor condensates different spin components may have different spatial extensions in the presence of an external magnetic field. Indeed, the ground state of a spin-1 Bose gas in a uniform magnetic field was proved to be fragmented [19].

The single-condensate picture and its mean-field description via the Gross-Pitaevskii (GP) equation has been a very successful approximation and can explain many experiments; see, e.g., Refs. [20,21] and references therein. However, this mean field is incapable by definition of describing fragmentation, since only one orbital is involved. Recently, a more flexible mean-field approach allowing for bosons to reside in different orthonormal one-particle functions has been formulated [18]. This intrinsic ability to describe fragmentation makes it very attractive for theoretical investigations and predictions. In the framework of this best mean field (BMF) it is possible to answer the question whether fragmentation is energetically favorable or not. In particular,

a repulsive BEC in an asymmetric double-well potential can be in a stable twofold fragmented state [22], but the energy of this state is higher than the energy of the corresponding nonfragmented ground state of the condensate, i.e., it is an excited state of the BEC. This result is in agreement with general predictions derived by Nozieres [2] that interaction prevents fragmentation in repulsive condensates. We shall demonstrate below, however, that in appropriate traps, repulsive BECs can exhibit fragmentation in the ground state.

In the present paper we use the best mean-field approach to study the ground state of a system of N identical bosons with positive scattering length immersed into a double-trap external potential. A double-trap potential consists of an inner trap embedded in a wider outer trap. The paper is organized as follows. In Sec. II we briefly discuss the three-orbital best mean-field formalism. We also provide a very transparent example which illustrates that a finite number of particles and well-separated multiple potential wells are favorable conditions for fragmentation. In Sec. III, we propose specific shapes of trap potentials and discuss why fragmentation is expected. We demonstrate in Sec. IV that indeed in the ground state macroscopic occupation of three single-particle functions is energetically more favorable than accumulation of all particles in a single orbital. We also show that fragmentation is a general phenomenon which, depending on the trap potentials, may take place for any number of particles. In Sec. V we demonstrate that the number of fragments, the shapes of the corresponding one-particle orbitals, and their occupation numbers can be manipulated by the proper choice of the outer trap. Here, we also verify that fragmentation of the ground state is a critical phenomenon, because it occurs when the number of bosons exceeds some critical number at a fixed scattering length, or at some critical scattering length if the number of bosons is fixed. The interplay between critical parameters of the fragmentation and the geometry of the inner trap forms the content of Sec. VI. A discussion of the factors suppressing fragmentation in the ground state is given in Sec. VII. Next, we briefly address manifold fragmentation in multiple wells in Sec. VIII. Finally, Sec. IX summarizes our results and conclusions.

II. MEAN-FIELD THEORIES

We consider a system of N identical bosons interacting via a δ -function contact potential $W(\vec{r}_i - \vec{r}_j) = \lambda_0 \delta(\vec{r}_i - \vec{r}_j)$, where \vec{r}_i is the position of the i th boson and the nonlinear parameter λ_0 is related to the s -wave scattering length of the bosons [21].

The standard mean-field description of the interacting system is obtained by assuming the ground state wave function Ψ to be a product of identical spatial orbitals φ : $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \varphi(\vec{r}_1)\varphi(\vec{r}_2)\cdots\varphi(\vec{r}_N)$. The energy $E \equiv \langle \Psi | \hat{H} | \Psi \rangle$, defined as the expectation value of the \hat{H} , reads

$$E_{GP} = N \left\{ \int \varphi^* h \varphi d\vec{r} + \frac{\lambda}{2} \int |\varphi|^4 d\vec{r} \right\}, \quad (1)$$

where $\lambda = \lambda_0(N-1)$ is the interaction parameter and $h(\vec{r}) = \hat{T} + \hat{V}(\vec{r})$ is the one-particle Hamiltonian consisting of the ki-

netic operator \hat{T} and the external potential $\hat{V}(\vec{r})$. The mean-field equation for bosons residing in a single orbital obtained by minimizing this energy is the well-known Gross-Pitaevskii equation [23,24]

$$\{h(\vec{r}) + \lambda_0(N-1)|\varphi(\vec{r})|^2\}\varphi(\vec{r}) = \mu_{GP}\varphi(\vec{r}). \quad (2)$$

By definition, this equation cannot describe fragmentation because all bosons reside in a single orbital. The reduced one-particle density operator and the corresponding spatial density are given by $\rho_{GP}(\vec{r}, \vec{r}') = \varphi^*(\vec{r}')\varphi(\vec{r})$ and $\rho_{GP}(\vec{r}) = |\varphi(\vec{r})|^2$, respectively.

In order to describe the fragmentation on a mean-field level, a more general ansatz for the wave function must be used. In the present study three orbitals ϕ_1 , ϕ_2 , and ϕ_3 with particle occupations n_1 , n_2 , and n_3 and $n_1 + n_2 + n_3 = N$ are utilized. It will become evident below why three orbitals have to be used in the present investigation. Since the details of the general derivation have already been published elsewhere [18,22], we outline here only the main steps. With this ansatz the wave function now reads

$$\Psi(\vec{r}_1, \dots, \vec{r}_N) = \hat{S} \phi_1(\vec{r}_1) \cdots \phi_1(\vec{r}_{n_1}) \phi_2(\vec{r}_{n_1+1}) \cdots \phi_2(\vec{r}_{n_1+n_2}) \times \phi_3(\vec{r}_{n_1+n_2+1}) \cdots \phi_3(\vec{r}_{n_1+n_2+n_3}), \quad (3)$$

where \hat{S} is the symmetrizing operator. The energy expression takes the form

$$\begin{aligned} E = & n_1 h_{11} + n_2 h_{22} + n_3 h_{33} + \lambda_0 \frac{n_1(n_1-1)}{2} \int |\phi_1|^4 d\vec{r} \\ & + \lambda_0 \frac{n_2(n_2-1)}{2} \int |\phi_2|^4 d\vec{r} + \lambda_0 \frac{n_3(n_3-1)}{2} \int |\phi_3|^4 d\vec{r} \\ & + 2\lambda_0 n_1 n_2 \int |\phi_1|^2 |\phi_2|^2 d\vec{r} + 2\lambda_0 n_1 n_3 \int |\phi_1|^2 |\phi_3|^2 d\vec{r} \\ & + 2\lambda_0 n_2 n_3 \int |\phi_2|^2 |\phi_3|^2 d\vec{r}. \end{aligned} \quad (4)$$

By minimizing this energy with respect to the orbitals under the constraints that they are orthogonal and normalized, i.e., $\langle \phi_i | \phi_j \rangle = \delta_{ij}$, we get the following three coupled equations for the optimal orbitals:

$$\begin{aligned} \{h(\vec{r}) + \lambda_0(n_1-1)|\phi_1(\vec{r})|^2 + 2\lambda_0 n_2 |\phi_2(\vec{r})|^2 \\ + 2\lambda_0 n_3 |\phi_3(\vec{r})|^2\} \phi_1(\vec{r}) &= \mu_{11} \phi_1(\vec{r}) + \mu_{12} \phi_2(\vec{r}) + \mu_{13} \phi_3(\vec{r}), \\ \{h(\vec{r}) + \lambda_0(n_2-1)|\phi_2(\vec{r})|^2 + 2\lambda_0 n_1 |\phi_1(\vec{r})|^2 \\ + 2\lambda_0 n_3 |\phi_3(\vec{r})|^2\} \phi_2(\vec{r}) &= \mu_{21} \phi_1(\vec{r}) + \mu_{22} \phi_2(\vec{r}) + \mu_{23} \phi_3(\vec{r}), \\ \{h(\vec{r}) + \lambda_0(n_3-1)|\phi_3(\vec{r})|^2 + 2\lambda_0 n_1 |\phi_1(\vec{r})|^2 \\ + 2\lambda_0 n_2 |\phi_2(\vec{r})|^2\} \phi_3(\vec{r}) &= \mu_{31} \phi_1(\vec{r}) + \mu_{32} \phi_2(\vec{r}) + \mu_{33} \phi_3(\vec{r}). \end{aligned} \quad (5)$$

Several key features of this approach should be mentioned. First, this mean-field includes the GP equation as a special case: when the occupation of two of the three orbitals vanishes, i.e., $n_2 = n_3 = 0$, the system of equations (5) is re-

duced to the single equation (2) and the corresponding energy in Eq. (4) coincides with the GP one [compare Eq. (4) and Eq. (1)]. Second, by construction, this method can describe fragmentation for a finite number of fragments. Indeed, in this three-orbital case the reduced one-particle density operator can be written as $\rho_{BMF}(\vec{r}, \vec{r}') = \sum_i^3 \phi_i^*(\vec{r}') \phi_i(\vec{r}) n_i$ and the corresponding spatial density becomes $\rho_{BMF}(\vec{r}) = n_1 |\phi_1(\vec{r})|^2 + n_2 |\phi_2(\vec{r})|^2 + n_3 |\phi_3(\vec{r})|^2$. Third, the occupation numbers n_i of all fragments are variational parameters, minimizing the full energy. In order to find this optimal value of the energy, Eqs. (5) are solved for all possible occupation numbers, and the corresponding energies Eq. (4), are evaluated and compared. As we discussed before, the results obtained for the specific occupation numbers $n_2 = n_3 = 0$ are identical to the standard GP ones. Therefore, within this computational scheme we automatically clarify the question on the favorability of fragmentation. Fourth, $\lambda = \lambda_0(N-1)$ is the only parameter involved in the GP energy per particle expression [see Eq. (1)]. Therefore, the one-orbital mean field cannot distinguish energetically between two systems made of different numbers of bosons if they are characterized by the same λ . In contrast to that, the BMF treats these systems differently. For example, at the GP mean-field level two systems made of 11 bosons with $\lambda_0 = 0.1$ and of 1 000 001 bosons with $\lambda_0 = 0.000\,001$ are characterized by the same energy per particle. At the BMF level of description, if one of the systems is fragmented, the respective energies are different due to different relative occupation numbers. This observation defines λ , N as a very natural choice of the parameters to study fragmentation at the general mean-field level. If fragmentation takes place, then the number of particles becomes a relevant parameter. In the following, to compare systems made of different numbers of bosons we adjust their λ_0 's in such a way that λ is the same for each system. Then, for a given trap potential the GP ansatz gives the same energy per particle for all these systems.

Large numbers of bosons and well-separated quantum levels of the single-well trap potential provided [21] a justification for the single-orbital mean-field description of BEC. However, recent experiments on optical trapping of BECs have initiated interest in studies of multiwell systems and questioned the validity of the one-orbital mean field description. The ground and lowest excited states of a multiwell trap potential can be almost degenerate and this opens a competition among the involved single-particle levels and the degree of their occupations. Therefore, the one-orbital mean field description may be insufficient. Another difficulty for the one-orbital mean field arises when the number of wells is comparable to the number of particles. In this case the average occupation number of each well (so-called filling factor per lattice site) can be of the order of several atoms. It is worthwhile to demonstrate that for such a situation a many-orbital mean field is the best mean field, since it is energetically and physically more favorable than the one-orbital ansatz.

Let us consider a system of three repulsive bosons trapped in three equivalent, infinitely separated wells which we denote left (*l*), central (*c*) and right (*r*). Without loss of gener-

ality, we can assume that the lowest total energy is obtained if each well contains only one particle, i.e., $n_l = n_c = n_r = 1$. Since the wells are equivalent and infinitely separated, the wave functions (orbitals) of each boson ψ_l , ψ_c , ψ_r are the same but localized at the different wells. This implies also zero overlap between each pair of orbitals. In other words, we have a system of three noninteracting bosons. The GP orbital now reads $\varphi = (\psi_l + \psi_c + \psi_r) / \sqrt{3}$ while the BMF orbitals are the three orbitals $\phi_1 = \psi_l$, $\phi_2 = \psi_c$, and $\phi_3 = \psi_r$. Substitution of these functions into Eq. (1) and Eq. (4) gives

$$E_{1 \text{ orb}} = h_{ll} + h_{cc} + h_{rr} + \frac{3(3-1)\lambda_0}{2} \\ \times \int \left(\frac{1}{9} |\psi_l|^4 + \frac{1}{9} |\psi_c|^4 + \frac{1}{9} |\psi_r|^4 \right) d\vec{r}, \\ E_{3 \text{ orb}} = h_{ll} + h_{cc} + h_{rr}.$$

Inspection of these energies clearly shows that for repulsive interaction $\lambda_0 > 0$ the three-orbital description is energetically more favorable than the one-orbital (GP) approach. The total energy of three equivalent noninteracting bosons is expected to be a sum of the energies of each particle. Therefore, only the BMF describes the physics correctly, while the GP energy contains an artificial term which can be considered as an interaction between the actually noninteracting subsystems. For this example of three infinitely separated wells, the energy provided by the many-orbital mean field (BMF) is lower than the GP one for any finite number of particles. At the limit of very large N the energy difference between the GP and BMF approaches vanishes while the physics in the GP case still remains wrong. For this trivial case the three-orbital ansatz is evident. However, the question whether the number of the fragments is always equal to the number of wells deserves a more detailed investigation and will be reported elsewhere [25].

We close this section with a general remark concerning the BMF. For a given number of orbitals m_0 , three in the present case, the BMF approach determines their optimal occupation numbers by minimizing the energy functional in Eq. (4). We call the result BMF(m_0). As mentioned above, the calculation may provide the result that some of these orbitals are not occupied, i.e., their occupation number is equal to zero. This, of course, implies that the overall best mean field is achieved with fewer than m_0 orbitals. Generally, we arrive at the overall best mean field if inclusion of more orbitals does not improve the description. In the present study $m_0 = 3$ and we have arguments that this choice leads to the overall best mean field.

III. PROPOSED DOUBLE-TRAP POTENTIAL

Our proposed one-dimensional double-trap potential is shown in Fig. 1. Effectively such a trap may be obtained as a superposition of two potentials (inner and outer). We model the inner potential as

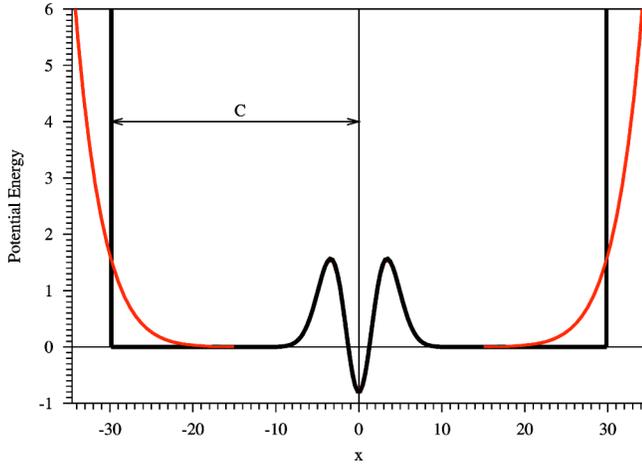


FIG. 1. (Color online) Proposed double-trap potential made of an inner trap of the form given in Eq. (6) and an outer trap. As outer traps we use either infinite walls at $\pm C$ (black) or a smooth power potential (red). Potential energy is given in units of ω ; x is a dimensionless coordinate.

$$V_{inner}(x) = \omega \left(\frac{x^2}{2} - A \right) e^{-Bx^2} \quad (6)$$

where A and B are parameters of the inner trap. As an outer trap embedding the inner one we used either an infinitely deep square potential well (infinite square well) with half-width equal to C or a smooth power potential $V_{outer}(x) = (0.035x)^{10}$. The infinite square well is obtained by placing the infinite walls at $[-(C+\delta); +(C-\delta)]$. We introduced a small asymmetry parameter $\delta=0.01\pi$ to destroy the exact symmetry of the trap potential in order to get rid of the effects of symmetry. In the following, as a default outer trap we use a square well with walls at $C_0=9.5\pi$ and $A_0=0.8$, $B_0=0.1$ as reference parameters of the inner trap. The corresponding kinetic energy reads $\hat{T} = -(\omega/2)(\partial^2/\partial x^2)$ implying that coordinate x and all the parameters A , B , C of the double-trap potential are dimensionless while all energies and λ_0 are now in units of the frequency ω .

An inner trap potential of the form given in Eq. (6) was originally proposed to study BEC tunneling [26,27]. For the above reference parameters and one particle this potential has only a single bound state and a set of metastable states at positive energies (so-called resonances). In the limit of non-interacting particles, all bosons will occupy this bound orbital, while for a nonzero repulsive interaction the bosons trapped inside the well may “flow out.” In this case, a competition between the bound state localized inside the well and the continuum states outside the barriers has been predicted [27]. The experimental observation of the continuum outgoing waves is a delicate problem. By placing a secondary trap potential beyond the barriers the continuum outgoing wave functions are discretized and “transformed” to real functions which can be occupied by bosons and observed experimentally. We shall demonstrate later that the specific shape of the secondary trap potential is of rather minor importance, while its width is a major factor. The secondary trap potential

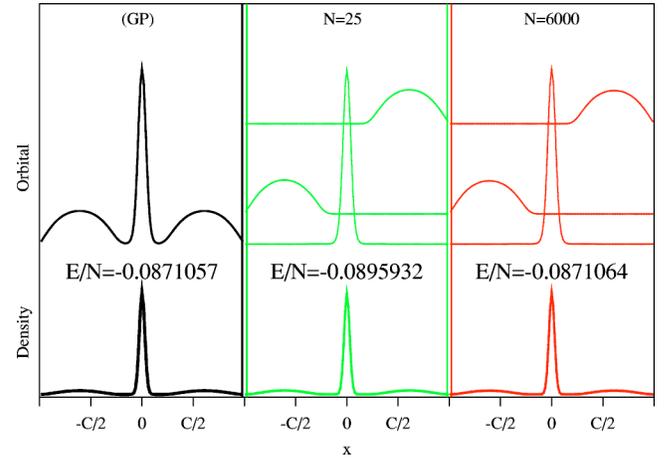


FIG. 2. (Color online) The orbitals and densities for the double-trap potential with infinite walls (see Fig. 1). The orbitals $\phi_1(x)$, $\phi_2(x)$, and $\phi_3(x)$ and the corresponding density per particle $\rho_{BMF} = (n_1|\phi_1|^2 + n_2|\phi_2|^2 + n_3|\phi_3|^2)/N$ of the threefold fragmented ground state [for convenience the $(n_i/N)^{1/2}\phi_i(x)$ are depicted in comparison with the GP orbital φ and its density $\rho_{GP} = |\varphi|^2$ for $N=25$ and $N=6000$ and $\lambda=1.3$. The energy per particle is indicated. For convenience, the baseline of the orbitals $\phi_2(x)$ and $\phi_3(x)$ has been moved upward artificially from zero. All orbitals and densities are dimensionless and plotted as functions of the dimensionless coordinate x ; $C=C_0=9.5\pi$.

should have a width capable of accumulating particles. The simplest choice is to place two infinite walls at some distance from the origin. The fixed infinite walls can be replaced by some external embedding potentials with a smooth profile. From an experimental point of view this means that the fragmentation phenomenon may be observed in outer ordinary traps.

IV. FRAGMENTATION

The combined potential ($V_{inner} + V_{outer}$) has three well-separated wells (see Fig. 1). Therefore, if fragmentation takes place, bosons will be accumulated in each of these three wells. More precisely, the reduced one-particle density of the system of N identical bosons in this double-trap potential will have three *macroscopic* (with respect to N) eigenvalues. The condition that all three wells are well separated from each other implies that the respective eigenvectors (natural orbital) will be predominantly localized in each of these wells.

Indeed, within the framework of BMF(3) the ground state of the system of N bosons becomes threefold fragmented. In Fig. 2 we present two sets of the orthonormal BMF orbitals and the respective densities corresponding to the system of $N=25$ and $N=6000$ bosons and compare them with the GP results. The interaction strengths of these systems have been chosen to keep the quantity $\lambda = \lambda_0(N-1) = 1.3$ fixed for both systems as explained above. BMF(3) predicts fragmentation of the ground state as it provides a lower energy than the GP equation does.

From Fig. 2 one can see that the spatial densities (not to be confused with the reduced one-particle density) of the GP

method, $\rho_{GP}=|\varphi|^2$, and of the three-orbital BMF approach, $\rho_{BMF}=n_1|\phi_1|^2+n_2|\phi_2|^2+n_3|\phi_3|^2$, are rather similar. At the same time the energy per particle provided by the BMF method is lower than the corresponding GP one. Despite the fact that the spatial densities provided by the GP and BMF approaches are similar, there is a substantial physical difference between the methods. At the one-orbital level of description the systems are unfragmented, while at the three-orbital one they are threefold fragmented.

By solving Eqs. (5) for different occupation patterns we obtained the optimal relative occupation numbers for the systems of $N=6000$ and $N=25$ bosons. For the sake of convenience we will from now on also use the term relative occupation number for n_i/N and express this quantity in % $[(n_i/N) \times 100\%]$. These are found to be similar for both systems: $n_1/N \approx 68.58\%$ for the orbital localized in the central well and $n_2/N \approx n_3/N = 17.71\%$ for the orbitals localized in the outer wells for $N=6000$ and $n_1/N \approx 67.5\%$ and $n_2/N \approx n_3/N = 16.25\%$ for $N=25$. The fact that the occupation numbers of the orbitals localized in the left and right wells are approximately the same is explained by the slight asymmetry of the double-trap potential. This observation allowed us to simplify the numerical search for the optimal values of the occupation numbers. Instead of searching for the minimum of a functional $E(n_1, n_2, n_3)$ of two independent variables ($n_3 \equiv N - n_1 - n_2$), we can start the search using $n_2 = n_3$ and then relax this condition.

It is convenient to use the relative occupation n_1/N of the orbital localized in the central well as a characteristic parameter of fragmentation. If the relative occupation $n_1/N = 100\%$ then there is no fragmentation at all, while for any other values of n_1/N the fraction of bosons accumulating in the outer wells is defined as $100\% - n_1/N$. In the following we call the latter quantity the *fragmented* fraction in the outer wells or briefly the fragmented fraction. For the specific examples depicted in Fig. 2 ($\lambda=1.3$), the fragmented fractions of the systems with $N=25$ and $N=6000$ bosons are 32.5% and 31.42%, respectively.

This observation allows us to conclude that if the ground state of a system made of a large number of bosons is fragmented, then any other system of bosons characterized by the same λ and made of a smaller number of particles (of course, $N > 1$) is also fragmented. The opposite does not apply, however. For a given value of λ there is a maximal number of bosons for which the ground state is fragmented. This number depends on the trap potentials used and can be manipulated by changing these potentials. For a discussion of this issue, see Sec. VII.

In the following study we confine ourselves to the system of $N=25$ particles, keeping in mind that for a larger number of particles the occupation numbers may differ within less than 5% as long as the condensate is fragmented (this has been verified numerically).

V. MANIPULATING FRAGMENTATION BY VARYING THE OUTER TRAP

By “manipulation of the fragmentation” we mean the possibility to choose the shape of the trap potential as well as the

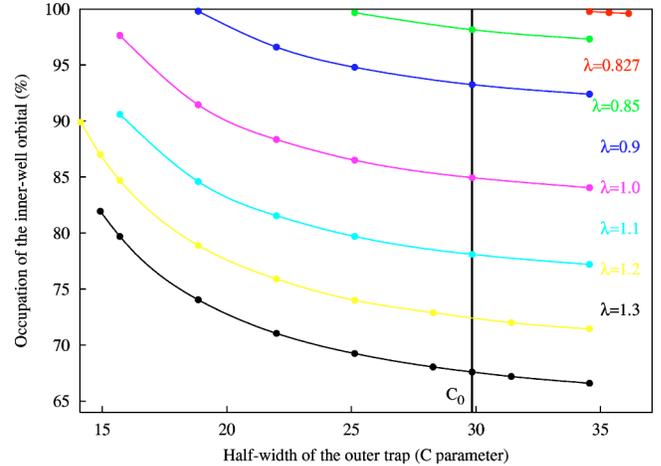


FIG. 3. (Color online) Manipulating the fragmentation by varying the outer trap. Shown is the relative occupation of the orbital localized in the inner well as a function of C (half-width of the outer trap). All other parameters are kept at their reference values A_0 and B_0 . All parameters of the double-trap potential are dimensionless.

number of bosons (and possibly also their scattering length) in such a way that all fragments acquire the desired occupation numbers.

As we briefly mentioned above, the bosons trapped by the inner potential alone in the absence of the outer trap occupy the bound state (localized in the central well) as long as $\lambda < \lambda_{cr}$. Any change in the number of particles or in the scattering length such that $\lambda = \lambda_0(N-1)$ becomes larger than λ_{cr} immediately initiates tunneling—the flow of bosons out of the central well [27]. If infinite walls are placed beyond the barriers, the system becomes closed and bosons are collected in the outer wells. If all three wells are macroscopically occupied the system is fragmented.

Several questions arise in the presence of the outer trap. Does the fragmentation phenomenon exist for any λ or is it characterized by some critical parameters, similarly to tunneling in the open system? The second question may be formulated as follows: Do the relative occupation numbers depend upon the positions $\pm C$ of the walls of the outer trap and on the particular shape of this trap?

Figure 3 shows the relative occupation of the orbital localized in the central well as a function of the positions $\pm C$ of the outer walls (see Fig. 1) for several values of λ . From this figure it is clear that the fragmentation starts to take place when λ exceeds some threshold (for the example of 25 bosons and $C = 11\pi$ $\lambda_{cr} = 0.8249$). It is interesting to notice that the exact value of this threshold for a system with a finite number of bosons is slightly smaller than that for the open system, i.e., $C \rightarrow \infty$. As N grows, the critical value of λ obtained for the closed system approaches the numerical result $\lambda_{cr} = 0.8279$ for the open one where tunneling through the barriers begins [27].

Further increasing the boson interaction strength λ beyond λ_{cr} (at least up to $\lambda = 3.0$) leads to a more pronounced fragmentation of the ground state. Here, we have to mention that there is another limit where fragmentation must disappear, namely, when λ becomes so large that the chemical

potential is larger than the barrier heights of the inner trap and particles can flow freely into the outer trap.

These observations reveal that fragmentation of the ground state is a critical phenomenon initiated when the number of bosons exceeds some critical number, for a fixed scattering length, or at some critical scattering length if the number of bosons is fixed.

Figure 3 also illustrates that fragmentation can be observed if the width of the outer trap is quite large or more specifically, if the infinite walls are placed at comparatively large distances from the barriers. For example, for the chosen shape of the inner trap (A_0, B_0) with the barriers at $x_b \approx \pm 3.4$, and $\lambda = 1.3$, about 30% of bosons are shared by the outer wells if the walls are at $C \approx 25$. By pushing the walls toward the barriers, the fragmentation gradually decreases: for $C \approx 16$ the fragmentation is 20%, and for walls at $C < 10$ the fragmentation totally disappears—all bosons are accumulated in the inner trap. Therefore, by pushing the walls toward the barriers the fragmentation can be reduced or even totally suppressed. These results show that fragmentation in the double-trap potential may be manipulated by the outer trap: *fragmentation can be suppressed by squeezing the outer trap and enhanced by its expansion.*

On the other hand, when the walls are moving outward from the barriers, the fragmented fraction in the outer wells becomes larger and converges to some constant value which depends on λ , of course. This value can be extracted from the results of Fig. 3 and also from the results obtained for the open system; an open system may be thought of as a closed one with walls placed at infinity. From this we conclude that for a given value of λ , the maximal fraction of the bosons in the outer wells is defined by the inner-trap potential only.

The relevant factor for the fragmentation is the width of the outer trap and we may suppose that the specific shape of the outer trap is of lesser importance. To support this expectation, we study the fragmentation for $\lambda = 1.3$ in the systems of $N = 3000$ and $N = 25$ bosons trapped in the double trap, with the same inner potential as before and the smooth power $(0.035x)^{10}$ outer potential [solid (red) line in Fig. 1]. As seen in Fig. 4, the threefold fragmentation of the ground state is again favorable energetically for these systems. Moreover, the optimal occupations of the inner orbital for $N = 3000$ and $N = 25$ are $n_1/N \approx 72.2\%$ and $n_1/N \approx 71\%$, respectively, and hence similar to those discussed above for the infinite walls case. In Fig. 4 we plotted the orbitals and the spatial densities determined for the smooth power outer trap. By comparing these orbitals with those shown in Fig. 2 for the infinite square outer trap, we conclude that the shape of the orbital localized in the inner trap does not depend upon the specific shape of the outer potential. The profiles of the orbitals localized in the outer wells exhibit differences which may be experimentally observed. In the case of the smooth power outer trap the density profiles of the outer orbitals are Gaussian-like, whereas those for the infinite square outer trap are of a sinusoidal type.

VI. MANIPULATING FRAGMENTATION BY VARYING THE INNER TRAP

Here, we investigate how fragmentation of BEC depends upon the shape of the inner potential. This potential permits

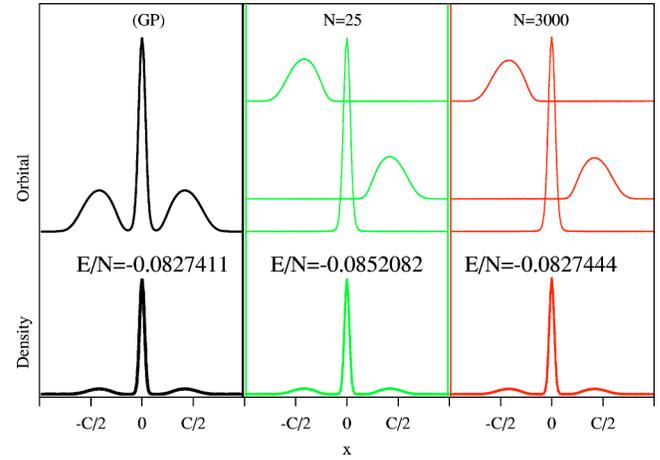


FIG. 4. (Color online) The orbitals and densities for the double-trap potential with a smooth power outer trap (see Fig. 1). The orbitals $\phi_1(x)$, $\phi_2(x)$, and $\phi_3(x)$ and the corresponding density per particle $\rho_{BMF} = (n_1|\phi_1|^2 + n_2|\phi_2|^2 + n_3|\phi_3|^2)/N$ of the threefold fragmented ground state [for convenience the $(n_i/N)^{1/2}\phi_i(x)$ are shown] are depicted in comparison with the GP orbital φ and its density $\rho_{GP} = |\varphi|^2$ for $N = 25$ and $N = 3000$ and $\lambda = 1.3$. The energy per particle is indicated. For convenience, the baseline of the orbitals $\phi_2(x)$ and $\phi_3(x)$ has been moved upward artificially from zero. All orbitals and densities are dimensionless and plotted as functions of the dimensionless coordinate x ; $C = C_0 = 9.5\pi$.

two degrees of manipulation by varying the depth of the inner well and by varying the height of the barriers. The parameter A of the inner potential [see Eq. (6) and Fig. 5(a)] is directly related to the depth of the inner well. This depth grows as A is increased. In Fig. 5(b) we illustrate the potential dependence upon B , a parameter which defines the height of the barriers, their widths, and the positions of their maxima. By decreasing the value of B , the height of the barriers and their widths grow while the positions of their maxima are shifted outward.

In Fig. 6 we plot the relative occupation in the inner trap as a function of A for several values of λ . It is seen that

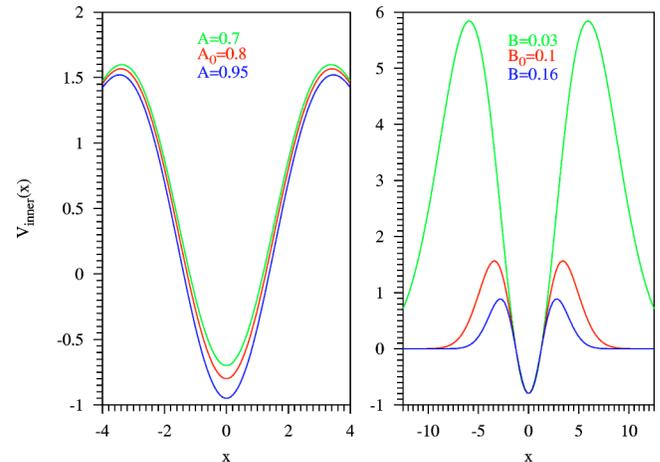


FIG. 5. (Color online) Parametrization of the inner trap. Left figure: Dependence on the parameter A . Right figure: Dependence on the parameter B . Potential energy is given in units of ω ; x is a dimensionless coordinate.

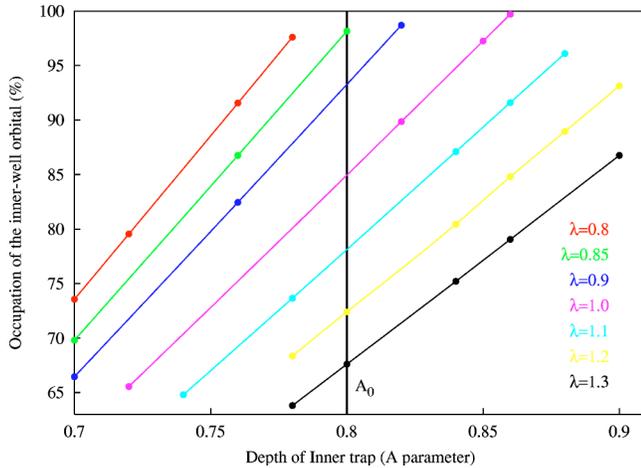


FIG. 6. (Color online) Manipulating the fragmentation by varying the inner trap. Shown is the relative occupation of the orbital localized in the inner well as a function of A . All other parameters are kept at their reference values B_0 and C_0 . All parameters of the double-trap potential are dimensionless.

fragmentation decreases monotonically with A . Qualitatively speaking, this finding implies that by increasing the depth of the inner potential more “room” becomes available for bosons in the inner well. Conversely, by decreasing A the capacity of the inner well becomes smaller and more particles “flow” out into the outer wells. This picture serves also as a verification and extension of the conclusions drawn above. We have established that at fixed trap geometries fragmentation takes place at $\lambda \approx \lambda_{cr}$ and becomes more pronounced as λ is increased. We may now add that there is a critical depth of the inner potential initiating fragmentation. For example, for $\lambda=0.8$ and $A=0.8$ ($B_0=0.1$, $C_0=9.5\pi$) fragmentation does not exist, while for $A=0.72$ the system becomes 20% fragmented.

Finally, we investigated the dependence of the fragmentation on the height of the barriers (B parameter). In Fig. 7, we plot the relative occupation of the inner well as a function of B ($A_0=0.8$, $C_0=9.5\pi$) for several $\lambda > \lambda_{cr}$. From this figure it is clear that as long as B is not too small or too large the fragmentation is not particularly sensitive to variations of B . Decreasing B from 0.16 to 0.02 corresponds to a substantial change of the barriers heights from 0.8 to 5.8 units. At the same time the respective relative occupation of the bosons in the central well varies by several percents only for any fixed value of λ . A further decrease of B causes, however, the disappearance of the fragmentation. Such a behavior is to be expected in this case, since a very small value of B corresponds to very broad barriers (see Fig. 5) diminishing thereby the size of the outer wells and hence their capacity to hold bosons at favorable energy cost (see Sec. V).

On the other hand, at large values of B the height of the barriers becomes very small and the fragmentation of the ground state is expected to be unfavorable energetically. This issue is further discussed in the subsequent section.

It is very important to note that the presence of barriers is an essential factor for the ground state fragmentation of the repulsive BEC. The specific shape of the barriers is of lesser relevance and its impact on fragmentation can be largely

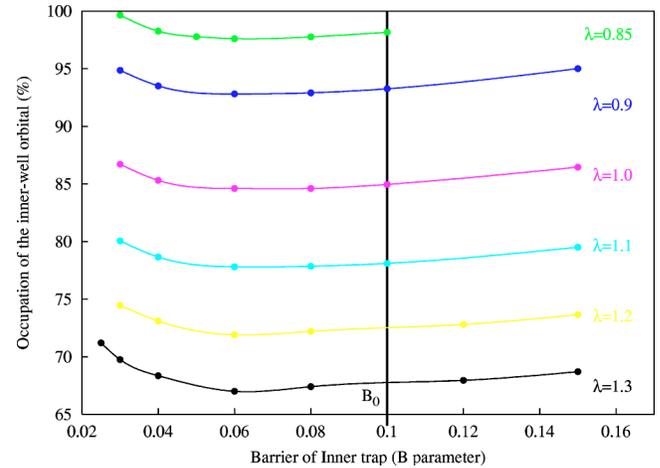


FIG. 7. (Color online) Manipulating the fragmentation by varying the inner trap. Shown is the relative occupation of the orbital localized in the inner well as a function of B . All other parameters are kept at their reference values A_0 and C_0 . All parameters of the double-trap potential are dimensionless.

compensated by moving the position of the walls of the outer trap. We expect, however, that for time-dependent studies this situation will be changed drastically, because the tunneling time (i.e., the time which is needed to tunnel through the barriers) is determined by the height and width of the barriers.

VII. MANIPULATING THE MAXIMAL NUMBER OF BOSONS IN THE FRAGMENTED GROUND STATE

There are several factors limiting the number of bosons in a fragmented ground state. The most transparent factor is the height of the barriers of the inner trap. Increasing the particle number N obviously enlarges $\lambda = \lambda_0(N-1)$ for a given scattering length. We have already pointed out that when λ becomes so large that the chemical potential is larger than the barrier heights, particles can flow freely out of the inner trap and the fragmentation disappears. Consequently, there is a maximal number N_{max} of bosons in a fragmented ground state and this number depends on the double-trap potential and on the scattering length.

For the open system we have seen that—at a fixed value of λ —once fragmentation in the ground state takes place, i.e., $\lambda > \lambda_{cr}$, this fragmentation persists for any number of bosons (N larger than 1, of course). This finding does not hold for closed systems. For these systems there is again an N_{max} even if λ is kept fixed at a value where the chemical potential is smaller than the barriers heights. As seen in the preceding sections, there is an enormous range of double-trap potentials giving rise to fragmented ground states as long as $\lambda > \lambda_{cr}$. The degree of fragmentation can be widely manipulated by varying the parameters of the trap potentials. Two major questions arise now: what is the origin of N_{max} and can this value be manipulated by varying the parameters of the trap potentials? The answer to the latter question is positive and we shall present numerical calculations below.

To facilitate the origin of the existence of N_{max} we recall that $\lambda = \lambda_0(N-1)$ where λ_0 is the interaction strength of two

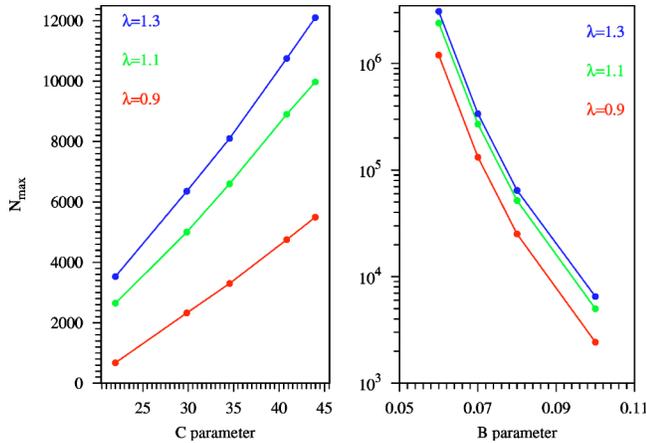


FIG. 8. (Color online) Manipulating the maximal number of bosons N_{max} in the fragmented ground state by varying the double-trap potential. Left figure: Dependence on the parameter C . All other parameters are kept at their reference values A_0 and B_0 . Right figure: Dependence on the parameter B (note the logarithmic scale). All other parameters are kept at their reference values A_0 and C_0 . All parameters of the double-trap potential are dimensionless.

interacting bosons. Increasing the number N of bosons while keeping the value of λ fixed obviously implies a weakening of the interaction strength. As N approaches infinity, the interaction strength λ_0 approaches zero and we may expect that the ground state takes on the appearance of a noninteracting system, i.e., that of the GP ansatz. Indeed, our numerical calculations show that while for $N \leq N_{max}$ the ground state is fragmented, fragmentation still persists even for $N > N_{max}$, but the state in question is an excited state of the condensate. This excited state is very low lying for *all* $N > N_{max}$; its energy is extremely close to that of the now unfragmented ground state (in the present examples the two energies per particle differ just at the seventh digit). The existence of a very low-lying fragmented excited state is of great interest by itself and should play a role in particular in time-dependent experiments.

In Fig. 8 we show N_{max} as a function of the outer trap parameter C for several values of λ keeping the parameters of the inner trap at their reference values. Also shown are the variations of N_{max} with the inner trap parameter B . In the range of parameters studied, the maximal number of bosons N_{max} grows linearly with the size of the outer trap and exponentially with the height and width of the barriers.

For a better understanding of the above findings we draw attention to Fig. 2. To maintain orthogonality, the three orbitals of the BMF exist in different regions of space. As long as the size of the outer traps is large enough, this is favored by the presence of broad and high barriers between the inner and outer wells. Since the condensate is repulsive, a large outer trap enables the wave function in this region of space to delocalize without the necessity to penetrate the inner well.

VIII. MANIPULATION OF FRAGMENTATION BY SEVERAL INNER TRAPS

Threefold fragmentation of the ground state is found to take place in suitable three-well potentials. The results ob-

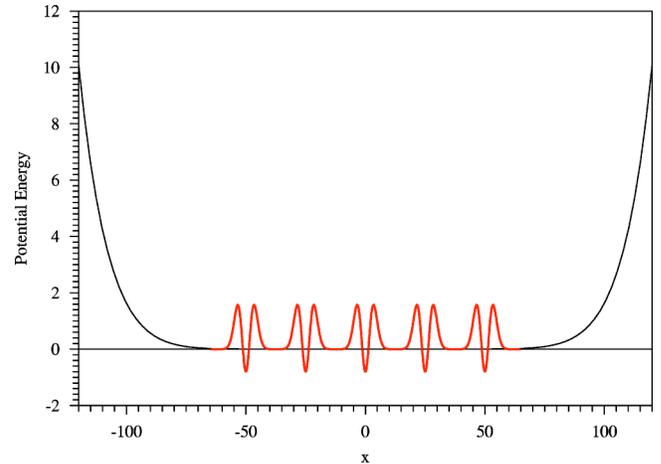


FIG. 9. (Color online) Proposed multiwell double-trap potential. Potential energy is given in units of ω ; x is a dimensionless coordinate.

tained for these potentials can naturally be extended to an array of multiple wells. This extension is particularly relevant due to the recent experimental efforts to investigate one-dimensional optical lattices [14]. For example, a multiwell potential may be formed if the inner-well trap given by Eq. (6) is translated several times and then embraced by an outer smooth power or infinite square trap. In these cases we expect manifold fragmentation and if the inner traps are well separated from each other and from the outer walls, then the critical value of λ scales according to the number of inner potentials. In Fig. 9 we plotted an example of such a trap. The critical value of λ for this system is approximately five times larger than the corresponding value obtained above for the single inner potential. This value as well as the extent of the fragmentation can be sensitively manipulated by varying the trap parameters. Of course, a many-orbital BMF must be used in order to correctly describe the situation. For the multiwell trap shown in Fig. 9 we expect that 11 orbitals should be used and that should be possible to do in the future.

IX. CONCLUSIONS

In this article we have investigated the fragmentation phenomenon in the ground state of a repulsive condensate immersed in a double-trap potential. We demonstrate that fragmentation can be successfully characterized by the best mean-field approach. To be able to correctly describe m -fold fragmentation, m orbitals are needed and are available in the m -orbital mean-field BMF (m) method. In this method the occupation number of each fragment as well as the optimal shape of the respective orbitals are determined variationally by minimizing the total energy functional. If more orbitals are included than needed, the occupation of the superfluous orbitals becomes zero by minimizing the total energy.

The double-trap potential studied here has three wells, obtained as the superposition of an inner trap exhibiting one well and two barriers and an outer trap embedding the inner one. For many choices of the potentials, the macroscopic occupation of the three orbitals may become energetically

more favorable than accumulating all the particles in a single orbital. The fragmentation of the ground state is found to occur when the number of bosons exceeds some critical value which depends on the scattering length and on the shape of the inner trap potential. For the example studied we found that if fragmentation is observed for a large number of bosons, then it exists also for any smaller number of bosons (of course $N > 1$) when λ is kept fixed. When λ is kept fixed, there exists, however, a maximal number of bosons for which the ground state is fragmented. This number can be strongly manipulated by varying the double-trap potential.

We have demonstrated that the geometry of the inner potential determines the values of the critical parameters. Moreover, for any given number of bosons this potential also determines the maximally possible fragmented fraction of bosons which is localized in the outer wells. The actual fragmented fraction of bosons may be effectively manipulated by the proper choice of the outer trap. The interplay between the

inner and outer trap potentials provides a sensitive tool to manipulate fragmentation of repulsive condensates. Varying the number of bosons in the condensate and the scattering length are also instrumental in this respect.

The results obtained for three-well potentials can naturally be extended to an array of multiple wells.

Finally, we would like to mention that in all our previous work we did not find fragmentation in the ground state of repulsive condensates. These previous studies have been performed in the large N limit. The present paper demonstrates that a finite particle number is needed to observe fragmentation of the ground state.

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