Bose-Einstein condensates on slightly asymmetric double-well potentials

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An analytical insight into the symmetry breaking mechanisms underlying the transition from Josephson to self-trapping regimes in Bose-Einstein condensates is presented. We obtain expressions for the ground state properties of the system of a gas of attractive bosons modeled by a two site Bose-Hubbard hamiltonian with an external bias. Simple formulas are found relating the appearance of fragmentation in the condensate with the large quantum fluctuations of the population imbalance occurring in the transition from the Josephson to the self-trapped regime.

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I. INTRODUCTION

The dynamics of cold bosonic atoms in double-well potentials has deserved a great deal of attention in the last decade. See [1, 2] for a careful review of the early findings, and [3] for a more recent update. Of particular interest here are the seminal works of Smerzi et al. [4] and Milburn et al. [5]. The latter managed to derive a simplified many-body hamiltonian with semiclassical predictions similar to those of [4] but with the important advantage of allowing the study of the quantum fluctuations on top of the semiclassical quantum averages. In both cases, the most remarkable feature reported was the existence of a new phenomenon, macroscopic self-trapping, directly linked to the atom-atom interaction. Most of the studies focused on the case of repulsive atom-atom interactions. However, more recently interest has grown on the properties of these systems when this interaction is made attractive and in particular on the appearance of cat like ground states whose description goes beyond the usual semiclassical approximations [6–8]. The structure of these ground states is determined by the ratio between interaction and tunneling strengths.

For repulsive interactions, the Bose-Hubbard model has been widely used to study the transition between the Josephson and the self-trapped regimes [6–8, 11]. It is also the natural choice for attractive interactions. Varying the parameters of the model allows to easily scan the properties of the system. The transition from the Josephson to the self-trapped regime is directly related to the properties of the spectrum of the system as we increase the atom-atom interactions. In a recent manuscript the strongly correlated nature of the ground state of the system (for attractive interactions) in the transition region has been described [12]. This state is similar to the cat-like states described in Ref. [13, 14] for the case of internal Josephson-like behavior. Both studies find a deep relation between the appearance of a bifurcation in the semi-classical description and the existence of strongly correlated, cat-like, ground states in the systems. Similar states also appear in the nucleation of vortices in BECs [12]. The presence of the bifurcation points to the

need of a fully quantum description that goes beyond the usual semiclassical approach. However the exact solution of the Bose-Hubbard model involves numerical calculations that complicate the interpretation of the results. It is thus highly desirable to develop also simplified models that give analytical insights into the relevant physics.

In this article we extend the previous work of Janvainen et al. [6], Jaaskelainen and Meystre [7], and the more recent one of Shchesnovich and Trippenbach [8, 16]. Starting from Bose-Hubbard Hamiltonians, these authors obtain approximate, Schrödinger-like, equations for the dynamics of the Fock space amplitudes of a system of N atoms on a double-well potential. We will first rederive these equations and, afterwards, will go one step further and obtain simple analytical solutions under certain premises. These are found to be in good agreement with the exact results and help to explain the delicate balances involved in the transition between the two regimes.

II. QUANTUM MODELS FOR THE GROUND STATE

The time dependent Schrödinger equation governing the evolution of the system of N atoms reads,

$$iN\partial_t |\Phi> = \hat{H} |\Phi> ,$$

(1)

with the (Bose-Hubbard) Hamiltonian written in reduced units as $^1$,

$$\hat{H} \equiv -\frac{1}{N}(a_1^+ a_2 + a_2^+ a_1) + \frac{\epsilon}{N} \tilde{n}_1 + \frac{\gamma}{N^2}(\tilde{n}_1^2 + \tilde{n}_2^2).$$

(2)

Where $\tilde{n}_i = a_i^+ a_i$, N is the total number of atoms in the system and $a_i$ ($a_i^+$) is the annihilation (creation) operator for well $i$. The Fock state basis is written as $|n_1, n_2>$ and

$^1$ To ease the comparison with the work in [8] we will make use of their notation.
has $N + 1$ vectors, $\{0, N, \ldots, |N, 0\}$. The two parameters governing the dynamics are $\gamma$, which measures the ratio between the contact atom-atom interactions and the hopping strength, and $\varepsilon$ which is a symmetry breaking bias, also divided by the hopping strength $k$. For this study we take $\varepsilon < 0$ which promotes $|1\rangle$.

With this sign convention, $\gamma > 0$ and $\gamma < 0$ correspond to repulsive and attractive atom-atom contact interactions.

The solution to (2) can be expanded in the Fock basis as, $\Phi(t) := \sum_{k=0}^{N} c_k(t) \ket{k, N - k}$, leading to an equation for the time evolution of the coefficients $c_k$ of the form $[\mathbf{S}]:$

$$i \frac{d}{dt} c_k = -(b_{k-1}c_{k-1} + b_kc_{k+1}) + a_k c_k,$$

with $b_k = \frac{1}{\sqrt{N}} \sqrt{(k+1)(N-k)}$, and $a_k = \frac{\gamma}{\sqrt{N}} [k^2 + (N-k)^2] + \frac{\varepsilon}{2} k$. Now, it is useful to introduce a new variable, $x = k/N$, and, assuming that $\hbar \equiv 1/N$ is small, we define $\Psi(x) = c_k/\sqrt{N}$ and $b(x) = b_k$. The next step is to make $x$ a continuous variable $\gamma$. This leads to Eq. (5) of $[\mathbf{S}]$,

$$i \hbar \partial_x \Psi(x) = -\left[ e^{i\varepsilon b(x)} + b(x)e^{-i\varepsilon} \right] \Psi(x) + a(x) \Psi(x),$$

(4)

where $\hat{p} \equiv -i \hbar \partial_x$, and

$$b(x) = [(x+h)(1-x)]^{1/2},$$

$$a(x) = \gamma [x^2 + (1-x)^2] + \varepsilon x.$$  

(5)

Eq. 4 describes the time evolution of $\Psi(x)$, which is a continuous interpolation of the $c_k/\sqrt{N}$. This interpolation assumes a certain degree of smoothness for the $c_k$, so that for most $k$: $\text{sign}(c_{k+1}) = \text{sign}(c_k)$. This is the case for the ground state with either repulsive or attractive interactions, provided the symmetric state is lower in energy than the antisymmetric one (our case) $\gamma$.

From the formally exact Eq. 4, we first retain up to terms of order $\hbar^2$,

$$e^{i\varepsilon \hat{p}} \simeq 1 \pm \hbar \partial_x - \frac{1}{2} \hbar^2 \partial_x^2$$

(6)

and

$$b_0(x) \simeq b_0(x) + \hbar \partial_x b_0(x)|_{h=0} + (1/2)\hbar^2 \partial_x^2 b_0(x)|_{h=0},$$

(7)

$$\hbar \partial_x \psi(x) = -\hbar^2 b_0(x)\psi''(x) - \hbar^2 b'_0(x)\psi'(x) + [a(x) + V_2(x)]\psi(x)$$

(8)

where

$$V_2(x) = -2\hbar_0(x) + \hbar(b_0(x) - 2\hbar b_0(x)|_{h=0}) - \hbar^2(\partial_x^2 b_0(x)|_{h=0} - \partial_x b_0(x)|_{h=0} + \frac{1}{2} b''_0(x)).$$

(9)

This equation is similar to Eq. (13) of $[\mathbf{S}]$ if we retain only the $h^0$ term in $V_2(x)$. This approximation respects the symmetry and behaves well at the edges of the Fock space. Besides, taking into account that

$$\hat{p}\sqrt{(1-x)\hat{p}}\psi = -\hbar^2 \partial_x (b_0\partial_x \psi) = -\hbar^2 (b_0\psi'' + b_0\psi''),$$

(10)

we arrive to

$$i \hbar \partial_x \psi = +\sqrt{(1-x)\hat{p}} \hat{p} + a(x) + V_0(x)\psi(x),$$

(11)

with $V_0(x) = -2\sqrt{(1-x)}$.

The range of $x$ is the interval $[0, 1]$. It will be convenient to introduce the variable $z \equiv 1 - 2x, x \in [-1, 1]$. In terms of the new variable, Eq. (11) becomes

$$i \hbar \partial_z \psi(z) = -2\hbar^2 \partial_z \sqrt{1 - z^2} \partial_z + V(z)\psi(z).$$

(12)

with $V(z) = (1/2)(\gamma z^2 - \varepsilon z) - \sqrt{1 - z^2}$. This equation is a Schrödinger-like equation with an effective $z$ dependent mass: $-\hbar^2/(2m) \equiv -\hbar^2 \sqrt{1 - z^2}$. For convenience, we normalize $\psi(z)$ as $\int_{-1}^{1} dz \psi(z)^2$.

As discussed in Refs. $[\mathbf{S}]$ and $[12]$, the population imbalance is an appropriate order parameter. It is defined as,

$$I = (\langle \Phi | \hat{n}_2 - \hat{n}_1 | \Phi \rangle) / N = \sum_{k=0}^{N} c_k^2 (1 - 2k/N),$$

(13)

FIG. 1: (color online) (a) The potential $V$ for several values of $\gamma$ and zero bias ($\varepsilon = 0$), (b) Separation between the two minima (solid-black) and height of the barrier as function of $\gamma$, (dashed-red), also in the case of zero bias.
which in the continuous variable reads, \( I = \int_{-\gamma}^{\gamma} dz |\psi(z)|^2 z \), where we have used \( \sum_{k=0}^{N} c_k^2 = 1 \) and the normalization of the \( \psi(z) \).

### A. Effective two mode model

We first study the solutions of Eq. (12) for the stationary case with zero bias, and concentrate on the region where the classical bifurcation appears, \( \gamma < -1 \). For \( \gamma < 1 \), \( V(z) \) has two symmetric minima, which get deeper as \( \gamma \) decreases, see panel (a) of Fig. 5. The separation between the two minima, \( 2\sqrt{1-1/\gamma^2} \) and the barrier height \( (\Delta = (1+\gamma)^2/(2\gamma)) \) are depicted in panel (b).

Since \( V(z) \) has pronounced minima and maximum we first determine the g.s. energy of the system by approximating these minima by parabolas, see Fig. 2.

\[
V(z) \simeq V(z_m) + \frac{1}{2} V''(z_m)(z \pm z_m)^2
\]

with \( z_m = \sqrt{1-1/\gamma^2} \), \( V(z_m) = \gamma/2 + 1/(2\gamma) \), and \( V''(z_m) = \gamma - \gamma^3 \). As an additional approximation, in the first term in the r.h.s. of Eq. (12) we replace \( z \) by \( z_m \), since the wavefunction, \( \psi(z) \), is sharply peaked around the minima at \( \pm z_m \). The stationary pseudo-Schrödinger equation can then be written as,

\[
\left[ -2h^2 \partial_z^2 + \frac{1}{2}(\gamma^4 - \gamma^2)(z - z_m)^2 \right] \psi = \left[ -\gamma E + (1 + 1/\gamma^2)/2 \right] \psi
\]

and its spectrum can be readily obtained by comparing to the harmonic oscillator: \( h^2/(2m) \rightarrow 2h^2 \), \( m\omega^2 \rightarrow \gamma^2(\gamma^2 - 1) \) and \( h\omega/2 \rightarrow -h\gamma\sqrt{\gamma^2 - 1} \). From this analogy one easily gets the ground state energy:

\[
E_{g.s.} = \frac{1}{2\gamma} + \frac{\gamma}{2} + h\sqrt{\gamma^2 - 1}.
\]

This approximation turns out to be very reasonable as it can be seen in Fig. 3 by comparing the g.s. energies obtained using Eq. (16) and the ones obtained by solving numerically the pseudo-Schrödinger Eq. (12). The approximation is particularly good for large \( N \) (small \( h = 1/N \), and \( \gamma \) not too close to the bifurcation point, \( \gamma = -1 \), as shown in the inset of the figure.

For our analysis we assume that the harmonic oscillator estimate of the ground state is accurate enough and that the shape of \( \psi(z) \) around \( z_m \) (and also \(-z_m\)) is that of the g.s. harmonic oscillator, i.e. gaussian with the parameters also determined from Eq. (16). These normalized solutions will be denoted \( |\mathcal{L}R\rangle \) of \( \Psi_{\mathcal{L}}^{(h.o.)}(z) \), and \( |\mathcal{L}L\rangle \) or \( \Psi_{\mathcal{L}}^{(h.o.)}(z) \). They correspond to the clockwise and counter-clockwise rotor solutions to the pendulum in the language of Ref. [4]. They form the “two-mode” basis for the model to be described below. Notice also that these two modes are built in the Fock space, they are useful to describe the system during the bifurcation and in the self-trapping regime. In fact, the model works soon after the bifurcation starts, once the overlap \( \langle \mathcal{L}|R\rangle \) is small enough. This overlap is given by, \( \exp[2(\gamma^2 - 1)^{1/2}/(\gamma h)] \). As can be seen in panel (a) of Fig. 4 this overlap (black dot-dashed line) is essentially zero for \( \gamma \lesssim -1.05 \) and \( N = 50 \). For these basis vectors, \( \langle \mathcal{L}|z|\mathcal{L}\rangle = -z_m \) and \( \langle R|z|\mathcal{R}\rangle = z_m \). In this two-mode model, an approximate solution can be written as:

\[
|\psi\rangle = \cos \alpha |\mathcal{L}\rangle + \sin \alpha |\mathcal{R}\rangle.
\]

In the absence of bias the ground state is the symmetric combination, and therefore \( \alpha = \pi/4 \). The expectation value of \( z \) in the state (17) is easily calculated, \( \langle z \rangle = z_m (\cos^2 \alpha - \sin^2 \alpha) = -z_m \cos(2\alpha) \). The dispersion of \( z \), \( \sigma_z^2 \equiv \langle |z|^2 \rangle - \langle z \rangle^2 \), can also be readily computed. Retaining up to order \( h \),

\[
\sigma_z^2 = z_m^2 \sin^2 \gamma - h/(\gamma \sqrt{\gamma^2 - 1}).
\]

When no bias is present, \( \langle z \rangle = 0 \) and \( \sigma_z^2 = z_m^2 - \gamma - 1 \). The large values of \( \sigma_z^2 \) are due to the fact that the ground state is cat-like, that is, the wavefunction has two peaks in \( z \).
When a finite but small bias, $|\varepsilon| \ll 1$, is considered, $\alpha$ is determined by the balance between the tunneling across the middle barrier of $V$ and the bias term. In the absence of tunneling, $|\psi\rangle$ will consist only of $|L\rangle$ or of $|R\rangle$ depending on the sign of the bias constant, $\varepsilon$. In the latter situation the main contributor to $\sigma_z$ is the otherwise small $-\hbar/(\gamma \sqrt{\gamma^2 - 1})$ term, as the $\sin^2 2\alpha$ becomes negligible.

To take into account both effects, the tunneling across the Fock space barrier and the bias term, we write an effective Hamiltonian for this two-mode model

$$\mathcal{H} = \left( \frac{\varepsilon z_m/2}{-t} \right).$$

(19)

The eigenvalues of $\mathcal{H}$ are $E_S = -\sqrt{t^2 + \varepsilon^2 z_m^2} = -E_A$. Thus, one way to obtain the value of the tunneling constant, $t > 0$, is by computing the energy splitting between the symmetric and anti-symmetric states in the double well in the absence of bias, $t = (1/2)\Delta E_{AS} \equiv (1/2)(E_A - E_S)$.

To estimate this energy splitting in the double-well we will neglect the $z$ dependence of the effective mass. This brings our problem to a Schrödinger-like equation and we can make use of the WKB approximation as developed in Razavy’s book, [17]. The energy splitting is written in Eq. (3.109) of that book:

$$\Delta E_{AS} = \frac{\hbar \omega}{\pi} \exp \left( -\int_{z_m}^{z_{+}} \sqrt{(2m) / \hbar^2} (V(z) - E) dz \right).$$

(20)

In our case we use the equivalences given above Eq. (16) to assign values to $\hbar^2/(2m)$ and $\hbar \omega$. The value of $E$ corresponds to the ground-state energy and is taken from the harmonic oscillator approximation defined in Eq. (15). To compute the tunneling integral, and obtain analytic results, we will approximate $V(z)$ by an inverted parabola, $V(z) \simeq -1 + \frac{\gamma}{2} (\gamma + 1) z^2$, see Fig. 2. This gives an energy splitting,

$$\Delta E_{AS} = -\frac{2h\gamma}{\pi} \sqrt{\gamma^2 - 1} \exp \left( -\frac{\pi}{2h} \frac{|E| - 1}{\sqrt{|E| - 1}} \right).$$

(21)

This estimate of the splitting in absence of bias, is used to extract the value of $t$ and it is in very good quantitative agreement with the exact energy splitting obtained by solving Eq. (12) in absence of bias or as will be discussed later, when the bias is not dominant. It is an important improvement on the estimate given in Ref. 8 (cf. Eq. (31)). The value of $2t$ is plotted (red dot-dashed line) in panel (c) of Fig. 4.

From the two mode Hamiltonian (Eq. (15)) we find that the predicted “full” (including the bias) symmetric-antisymmetric energy splitting is

$$\Delta E_{AS}^{(sm)} = 2\sqrt{\left(\varepsilon z_m/2\right)^2 + t^2}$$

(22)

with two well-defined limits, $2t$ and $\varepsilon z_m$ (red dot-dashed and red dashed lines of panel (c) of Fig. 4 respectively), depending on whether tunneling or bias is the dominant contribution. The ground state can be readily computed, $\mathcal{H}\psi_S = E_S\psi_S$, with $\psi_S = (\cos \alpha, \sin \alpha)$ and $\tan \alpha = \xi + \sqrt{\xi^2 + 1}$, where, $\xi \equiv (\varepsilon z_m/2t)$.

The one body density matrix for the Bose-Hubbard Hamiltonian can be written as,

$$\hat{\rho} = \frac{1}{N} \left( \langle a_1^\dagger a_1 \rangle \langle a_2^\dagger a_2 \rangle \right),$$

(23)

with $\text{Tr}\hat{\rho} = 1$ and $\langle f(z) \rangle = \int dz |\Psi(z)|^2$. In the large-N
model we have, $a^\dagger_1 a_1 = (1+z)/2, a^\dagger_2 a_2 = (1-z)/2, a^\dagger_1 a_2 = a^\dagger_2 a_1 = \sqrt{1-z^2}/2$. In the two mode model retaining up to order $h^1$ we get,

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 1 + z_m \cos 2\alpha & \sqrt{1-z_m^2} \\ \sqrt{1-z_m^2} & 1 - z_m \cos 2\alpha \end{pmatrix}$$

(24)

with eigenvalues,

$$n_{\pm} = \frac{1}{2} \left( 1 \pm \sqrt{1 - z_m^2 \sin^2(2\alpha)} \right) = \frac{1}{2} \left( 1 \pm \sqrt{1 - \sigma_z^2} \right) + \mathcal{O}(h).$$

(25)

The last equality directly relates the appearance of fragmentation and the quantum fluctuations of the population imbalance measured by $\sigma_z$, and holds also in the transition region. Denoting the corresponding eigenvectors by: $\varphi_{\pm} = (\cos \theta_{\pm}/2, \sin \theta_{\pm}/2)$ one finds

$$\tan \frac{\theta_{\pm}}{2} = -\frac{z_m \cos 2\alpha + \sqrt{1 - z_m^2 \sin^2(2\alpha)}}{\sqrt{1-z_m^2}}.$$

(26)

B. Results

The quantitative predictions of the analytical model are presented in Fig. 1. The model provides a simple and yet deep understanding of the problem. For $\gamma < -1.5$, region (i), the ground state of the system is completely asymmetric (see the left upper smaller plot of Fig. 1), with a large population imbalance, i.e. it is localized on the well promoted by the bias ($|\mathcal{L}|$ for $\varepsilon < 0$). The location of the wells in the Fock space is measured by $z_m$. The blue thin line in panel (a) shows $z_m$, which is a decreasing function of $\gamma$ and reaches zero at the bifurcation point, $\gamma = -1$. In this regime, the bias dominates completely the hamiltonian of Eq. (19), which therefore is essentially diagonal with eigenvectors $|\mathcal{L}\rangle$ and $|\mathcal{R}\rangle$. In these cases, $\sigma_z$ is small and given by the spread of the occupied mode. In this region, the system is fully condensed. Correspondingly, as shown in the panel (b), the eigenvalues of the one-body density matrix of the ground state, are 1 and 0. In the panel (c), it is clearly shown that $2t$ is very small compared with $\varepsilon z_m$, and the splitting $E_{A,S}^{(tm)}$ (Eq. 23) in this region is given by $\varepsilon z_m$.

In region (ii) both the bias term $\varepsilon z_m$ and the tunneling matrix element, $t$, are of comparable size (see panel (c)). In that region the ground state is an asymmetric cat-like state (see the central upper smaller plot). The value of $\langle z \rangle$ is decreasing and has large fluctuations, shown in the region (ii) of panel (a), mostly due to having both modes populated simultaneously. The system is fragmented into two condensates, i.e the eigenvalues of the one-body density matrix are both different than zero, being $\varphi_+$ more populated, see panel (b) of the figure. The macro-occupied state, $\varphi_+$, varies from close to $|1\rangle$ to $(1/\sqrt{2})(|1\rangle + |2\rangle)$ as can be seen from the behavior of the mixing angle $\theta_+/2$ (blue dashed line in panel (b)).

The tunneling term, $t$, grows exponentially and is responsible for the abrupt decrease of $z$ as one crosses into the region, (iii). There, the two mode Hamiltonian is dominated by the tunneling matrix element, and the wave function becomes symmetric-cat-like, as shown in the right upper smaller plot. The cat like nature of the state reflects in a small value of the imbalance and a sizeable $\sigma_z$. Notice that when $\gamma$ approaches -1, the two-mode approximation is not valid anymore, because the $\langle \mathcal{L} | \mathcal{R} \rangle$, shown by the black-dot-dashed line in panel (a) is not longer close to zero.

The simplifications of the two mode model capture to a very large extent the features of the initial large-N model, Eq. (12), as can be seen from the comparison of the exact splitting (blue empty circles) between the ground and first excited state and the two-mode one (black solid line), shown in the last panel of the figure.

III. CONCLUSIONS

For attractive interactions, we have discussed here the appearance and properties of the cat states in the transition from the tunneling to the interaction dominated regimes. The semiclassical approach shows that at some critical value of the ratio of atom-atom to tunneling energies, $\gamma$, a bifurcation appears. We have constructed an effective “two mode model” built from the solutions corresponding to the branches of the bifurcation. And have shown that it is quite successful in describing not only the average imbalances in the presence of bias but also the quantum fluctuations. The model includes the main quantal effects since its predictions are in good agreement with exact solutions of the Bose Hubbard hamiltonian.

Our starting point is an already developed large-N model [6, 8] which gives accurate numerical predictions for $N \gtrsim 30$. We have managed to obtain analytic expressions valid on the transition region from self-trapped (bias-dominated) to the symmetric cat-like region (dominated by the tunneling term). The main feature is the sharp change of the population imbalance as $\gamma$ is decreased. It is due to the delicate interplay between the bias and an effective tunneling term with a sharp dependence on $\gamma$.

The fact that Eq. (12) captures most of the non-linear dynamics of the original Bose-Hubbard hamiltonian implies that the complex dynamics of systems governed by non-linear terms can be studied very conveniently with pseudo-Schrodinger equations governing the dynamics in Fock space. In these equations the main effects of non-linearities are mapped into exponentially varying magnitudes in linear systems. We have exploited this advantage to introduce further approximations and construct a very simple effective two-mode model to reproduce and
explain the main properties of the transition.

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