Spontaneous symmetry breaking and collapse in bosonic Josephson junctions

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We investigate an attractive atomic Bose-Einstein condensate (BEC) trapped by a double-well potential in the axial direction and by a harmonic potential in the transverse directions. We obtain numerically, for the first time, a quantum phase diagram which includes all the three relevant phases of the system: Josephson, spontaneous symmetry breaking (SSB), and collapse. We consider also the coherent dynamics of the BEC and calculate the frequency of population-imbalance mode in the Josephson phase and in the SSB phase up to the collapse. We show that these phases can be observed by using ultracold vapors of $^7\text{Li}$ atoms in a magneto-optical trap.

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In many experiments atomic Bose-Einstein condensates (BECs) are cigar-shaped due to a strong harmonic trapping potential in the cylindrical radial plane; these BECs can be separated in two parts by means of a double-well potential in the cylindrical axial direction\textsuperscript{1}. This kind of geometry is the ideal setup to study the Josephson effect, a macroscopic coherent phenomenon which has been observed in systems as diverse as superconductors\textsuperscript{2}, superfluid Helium\textsuperscript{3} and, recently, also BECs in trapped ultracold atomic gases\textsuperscript{4}. The observed coherent dynamics of the atomic BEC in the double-well potential (bosonic Josephson junction)\textsuperscript{1,4} is efficiently described by nonlinear Josephson equations (JEs)\textsuperscript{5}, which are based on a two-mode approximation of the Gross-Pitaevskii equation (GPE)\textsuperscript{6}. These JEs are fully symmetric by changing the sign of the inter-atomic scattering length and do not predict the collapse of the BEC. The collapse of an attractive BEC of $^7\text{Li}$ atoms or $^{85}\text{Rb}$ atoms has been observed by various experimental groups\textsuperscript{7} and theoretically analyzed by many authors: in a single-well potential\textsuperscript{8}, in a potential without axial confinement\textsuperscript{9}, in a toroidal confinement\textsuperscript{10}, in a double-well potential\textsuperscript{11}, and in a periodic potential\textsuperscript{12}.

In this paper, by correctly taking into account the dimensional reduction of GPE from 3D to 1D, i.e. by using the so-called 1D nonpolynomial Schrödinger equation (1D NPSE)\textsuperscript{13}, we show that for an attractive BEC (negative inter-atomic scattering length) the JEs are not reliable in the presence of strong coupling. By numerically solving the 1D NPSE we obtain, for the first time, a quantum phase diagram of the three relevant regimes of the attractive BEC in a double-well: the Josephson phase, where the metastable state of lowest finite energy has a balanced population\textsuperscript{2}, the spontaneous symmetry breaking (SSB) phase, where the metastable state has an unbalanced population\textsuperscript{1,3}, and the phase of collapse, where the system reaches the collapsed ground-state with energy equal to minus infinity. Note that the problem of BEC collapse in an axial double well potential has been investigated by Sakellari, Proukakis, and Adams\textsuperscript{11}, but they have not derived the quantum phase diagram of the attractive BEC. Instead, very recently the collapse region in a quantum phase diagram has been obtained for a pair of cigar-shaped traps coupled by tunneling of atoms\textsuperscript{14}. We also study the coherent dynamics of the system and calculate the frequency of the population imbalance both in the Josephson regime and in the SSB regime. In the SSB phase this frequency reaches its maximum value at the coupling strength where there is the collapse of the BEC. In addition, from the 1D NPSE we obtain generalized Josephson equations, which we call nonpolynomial Josephson equations (NPJEs)\textsuperscript{3} for the fractional imbalance and relative phase of the bosonic Josephson junction. These new NPJEs reduce to the familiar JEs in the weak-coupling limit, but show a better agreement with the numerical results of the 1D NPSE (and 3D GPE) for strong couplings (for both positive and negative scattering length). Finally, we suggest that our predictions can be observed experimentally by using an ultracold vapor of $^7\text{Li}$ atoms and tuning the $s$-wave scattering length.

Let us consider a dilute interacting BEC at zero temperature confined by a trapping potential $V_{\text{trap}}(\mathbf{r})$. This potential is taken to be the superposition of an isotropic harmonic confinement in the the transverse radial plane and a double-well potential $V_{\text{DW}}(x)$ in the axial direction $x$. Then, $V_{\text{trap}}(\mathbf{r})$ is given by

$$V_{\text{trap}}(\mathbf{r}) = V_{\text{DW}}(x) + \frac{m\omega_\perp^2}{2} r^2,$$

where $\rho$ is the cylindric radial coordinate, $m$ is the mass of the atom, and $\omega_\perp$ is the trapping frequency in the radial plane. The macroscopic wave function $\Psi(\mathbf{r}, t)$ describing the above system with $N$ atoms is governed by the 3D
where $a_s$ is the s-wave boson-boson scattering length and $\Psi(r, t)$ is normalized to 1. The 3D GPE captures the main properties of collapse threshold and, as shown by using a reliable nonlocal potential, the collapsed state is actually a state of very high density which decays due to inelastic two- and three-body collisions \[15,16\]. By following Ref. \[13\], we choose the wave function $\Psi(x, t)$ as the product of an axial complex wave function $f(x, t)$ and a Gaussian transverse wave function of radial width $\sigma$, where $\sigma$ depends on the axial wave function $f(x, t)$, i.e. $\sigma = \sigma(f(x, t))$. By expressing lengths in units of $a_\perp = \sqrt{\hbar/m\omega_\perp}$, times in units of $\omega_\perp^{-1}$, and energies in units of $\hbar\omega_\perp$, it is easy to show that the fields $f(x, t)$ and $\sigma(x, t)$ satisfy the following equations \[13\]

\[
\frac{\partial f}{\partial t} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V_{DW}(x) + \frac{1}{2} \left( \frac{1}{\sigma^2} + \sigma^2 \right) + \frac{\Gamma}{2} \frac{|f|^2}{\sigma^2} \right] f, \tag{3}
\]

\[
\sigma^4 = 1 + \Gamma |f|^2, \tag{4}
\]

where $\Gamma = 2a_sN/a_\perp$ and $f(x, t)$ is normalized to 1. Inserting Eq. (4) into Eq. (3) one gets the so-called 1D NPSE \[13\], which is extremely accurate in reproducing the properties of the full 3D GPE with transverse harmonic confinement \[13\].

\[\begin{align*}
\text{FIG. 1: (color online). Axial probability density } |f(x)|^2 \text{ of the metastable attractive BEC in the symmetric double-well potential } V_{DW}(x) \text{ where the two minima are at } x = \pm x_0 \text{ with } x_0 = 2 \text{ and the energy height is } U_0 = 0.8. \Gamma = 2Na_s/a_\perp \text{ is the interaction strength. Results obtained by using 1D NPSE, Eqs. (3) and (4). Length } x \text{ in units of } a_\perp = \sqrt{\hbar/m\omega_\perp}, \text{ density } |f|^2 \text{ in units of } a_\perp^{-1}, \text{ and energy in units of } \hbar\omega_\perp.
\end{align*}\]

We have solved the 1D NPSE by using a finite-difference Crank-Nicolson code with imaginary time \[16,17\] to obtain the ground-state of BEC in the symmetric double-well trap. In the numerical analysis the double-well potential $V_{DW}(x)$ is given by the combination of two Pöschl-Teller potentials with the energy barrier of height $U_0 = 0.8\hbar\omega_\perp$ and the local minima at $-x_0 = -2a_\perp$ and $x_0 = 2a_\perp$ (for details see Refs. \[18,19\]). It is important to stress that with $\Gamma < 0$ the ground-state is always the collapsed state with energy equal to minus infinity. Thus, for $\Gamma < 0$ we are actually looking for the metastable state of lowest finite energy. We find that this metastable state is symmetric for $\Gamma_{SSB} < \Gamma < 0$ (Josephson phase), it has a broken symmetry for $\Gamma_C < \Gamma < \Gamma_{SSB}$ (SSB phase), and it becomes the collapsed ground-state for $\Gamma < \Gamma_C$ (collapsed phase). In Fig. 1 we plot the axial probability density $|f(x)|^2$ of the metastable state obtained by solving the 1D NPSE with imaginary time. We start with a slightly asymmetric initial condition and proceed up to the convergence to a stable configuration. The figure shows that for $\Gamma = -0.2$ the profile of the (meta-)stable state is symmetric, while for $\Gamma = -0.3$ it is not. For $\Gamma = -0.8$ the BEC is practically localized only in the right well. In addition, we find that for $\Gamma < -1.2$ there is the collapse.

\[\begin{align*}
\text{FIG. 2: (color online). Quantum phase diagram } (U_0, \Gamma) \text{ of the attractive BEC in the symmetric double-well potential } V_{DW}(x) \text{. The two minima are at } x = \pm x_0 \text{ with } x_0 = 2, U_0 \text{ is height of the central barrier of } V_{DW}(x) \text{ and } \Gamma = 2Na_s/a_\perp \text{ is the interaction strength. There are three phases: Josephson (J), spontaneous symmetry breaking (SSB), and collapse (C). Solid lines are obtained with 1D NPSE, Eqs. (3) and (4). Length } x \text{ in units of } a_\perp = \sqrt{\hbar/m\omega_\perp}, \text{ density } |f|^2 \text{ in units of } a_\perp^{-1}, \text{ and energy in units of } \hbar\omega_\perp.
\end{align*}\]

\[\begin{align*}
\text{It is very interesting to analyze the quantum phases of the attractive BEC as a function of the height } U_0 \text{ of the energy barrier. We have performed a systematic investigation by changing both } U_0 \text{ and } \Gamma. \text{ The results are shown in Fig. 2 where we plot the quantum phase diagram in the plane } (U_0, \Gamma). \text{ To our knowledge, this is the first time that this kind of phase diagram is obtained for an attractive BEC in a symmetric double-well potential. In the figure, the solid lines are obtained from the 1D NPSE, Eqs. (3) and (4). The interaction strength } |\Gamma_{SSB}| \text{ of the SSB transition strongly decreases by increasing the height } U_0 \text{ of the energy barrier, while the}
\end{align*}\]
critical strength \( |\Gamma_C| \) to get the collapse slightly decreases by increasing \( U_0 \). To check the accuracy of the NPSE we have also solved the 3D GPE, Eq. \((3)\), by using a cylindric-symmetry finite-difference Crank-Nicolson code with imaginary time \([\ddot{1}]\). In Fig. \(2\) the collapse points predicted by 3D GPE are shown as filled circles, while the SSB points of 3D GPE are filled squares. As expected \([\ddot{1}]\), the agreement between 1D NPSE and 3D GPE is quite good. We stress, however, that both 3D GPE and 1D NPSE are based on a zero-range inter-atomic potential \([\ddot{1}, \ddot{1}3]\). A more accurate description of interaction might lead to a slightly different transition between the SSB and the collapse phase in Fig. \(2\).

Let us now consider this two-mode approximation of the 1D NPSE. Under the condition that the central barrier \( U_0 \) of the double-well potential \( V_{DW}(x) \) is sufficiently high - corresponding to a weak link between its left and right sides - the field \( f(x, t) \) can be decomposed by using the two-mode approximation

\[
f(x, t) = f_L(t)\phi_L(x) + f_R(t)\phi_R(x) .
\]

The functions \( \phi_L(x) \) and \( \phi_R(x) \), which are orthonormal, are localized in the left and right well, respectively. We assume that the above functions are real and use the ansatz \([\ddot{1}]\) in the NPSE. We multiply the resulting equation by \( \phi_\alpha(x) \) (\( \alpha = L, R \)), and integrate over \( x \). Then, by taking into account the overlaps between \( \phi_\alpha \)'s localized in the same well and neglecting those ones between \( \phi_\alpha \)'s localized in different wells, we obtain

\[
\frac{\partial f_\alpha}{\partial t} = \left[ \frac{1}{2} \left( \frac{1}{\sigma_\alpha^2} + \sigma_\alpha^2 \right) + \frac{g}{\sigma_\alpha^2} |f_\alpha|^2 + \epsilon \right] f_\alpha - K f_\beta ,
\]

or

\[
\sigma_\alpha^4 = 1 + g |f_\alpha|^2 ,
\]

where the parameters \( \epsilon \), \( K \) and \( g \) are given by

\[
\epsilon = \int_{-\infty}^{+\infty} dx \phi_\alpha(x) \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V_{DW}(x) \right] \phi_\alpha(x)
\]

\[
K = \int_{-\infty}^{+\infty} dx \phi_\beta(x) \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V_{DW}(x) \right] \phi_\alpha(x)
\]

\[
g = \Gamma \int_{-\infty}^{+\infty} dx(x_\alpha(x))^4 .
\]

Finally, we write the time-dependent amplitudes \( f_\alpha(t) \) as \( f_\alpha(t) = \sqrt{N_\alpha(t)} e^{i\theta_\alpha(t)} \), with \( N_\alpha(t) \) being the fraction of bosons in the \( \alpha \)-th well and \( \theta_\alpha(t) \) the corresponding phase. Then, Eqs. \((6)\) and \((7)\) give rise to the following system of coupled ordinary differential equations for the fractional imbalance \( z(t) = N_L(t) - N_R(t) \) (here \( N_L(t) + N_R(t) = 1 \)) and the relative phase \( \theta(t) = \theta_R(t) - \theta_L(t) \):

\[
\frac{\dot{z}}{\sqrt{1 - z^2}} = -2K \sqrt{1 - z^2} \sin \theta ,
\]

\[
\frac{\dot{\theta}}{\sqrt{1 - z^2}} = 2K \frac{z \cos \theta + g \sqrt{1 + z} (1 + z)}{\sqrt{2} \sqrt{1 + z} \sqrt{2 + g (1 + z)}} - \frac{\sqrt{1 - z} (4 + 3g (1 - z))}{2 \sqrt{2} \sqrt{1 - z} \sqrt{2 + g (1 - z)}} .
\]

We call these equations "nonpolynomial Josephson equations" (NPJEs) because they are derived from the NPSE. NPJEs describe the dynamics of the fractional imbalance \( z(t) \) and relative phase \( \theta(t) \) of the bosonic Josephson junction taking into account transverse-size effects. It is clearly much easier to solve numerically these NPJEs than the full 3D GPE or the 1D NPSE. When the coupling strength \( g \) is much smaller than one our NPJEs become

\[
\dot{z} = -2K \frac{z \sin \theta}{\sqrt{1 - z^2}} ,
\]

\[
\dot{\theta} = 2K \frac{z \cos \theta + g \sqrt{1 + z} (1 + z)}{\sqrt{2} \sqrt{1 + z} \sqrt{2 + g (1 + z)}} - \frac{\sqrt{1 - z} (4 + 3g (1 - z))}{2 \sqrt{2} \sqrt{1 - z} \sqrt{2 + g (1 - z)}} ,
\]

which are the familiar Josephson equations (JEs) for a BEC found in Ref. \([\ddot{1}]\). It is straightforward to verify that Eqs. \((11)\) and \((12)\) are invariant under the transformations \( \Gamma \rightarrow -\Gamma \) and \( \theta \rightarrow -\theta + \pi \). Instead, Eqs. \((11)\) and \((12)\) do not exhibit this invariance.

The stationary Josephson regime corresponds to the equilibrium points with \( z = 0 \) and \( \theta = 0 \) (balanced population). Both JEs and NPJEs show that this stationary phase exists only for \( \Gamma_{SSB} < \Gamma \), while \( \Gamma_{SSB} < 0 \). We have verified that the value of \( \Gamma_{SSB} \) predicted by JEs is always very close to the value obtained with NPJEs. The points below \( \Gamma_{SSB} \) correspond to SSB phase. This phase, according to the JEs, exists for any \( \Gamma_{SSB} < \Gamma \); while, according to the NPJEs, the SSB phase does not exist anymore at the collapse strength \( \Gamma_C \). Thus NPJEs predict a collapse phase while JEs do not.

\[ \Gamma = -1.05 \]

\[ \Gamma = -0.25 \]

\[ \Gamma = 0.25 \]

FIG. 3: (color online). Fractional imbalance \( z \) as a function of the time. Upper panel: \( \Gamma = -1.05 \). Middle panel: \( \Gamma = -0.25 \). Lower panel: \( \Gamma = 0.25 \). The solid lines are obtained with 1D NPSE, Eqs. \((5)\) and \((6)\). The dashed lines are obtained with NPJEs, Eqs. \((11)\) and \((12)\). The dot-dashed line are obtained with JEs, Eqs. \((13)\) and \((14)\). Initial conditions: \( z(0) = 0.2 \) and \( \theta(0) = 0 \). Parameters of the double-well potential \( V_{DW}(x) \): energy barrier height \( U_0 = 0.86 \) and location of the two minima at \( x = \pm x_0 \) with \( x_0 = 2 \). Lengths in units of \( a_\perp \), time in units of \( \omega_\perp^{-1} \), energies in units of \( h\omega_\perp \).

To compare NPJEs with JEs we plot in Fig. \(3\) the population imbalance \( z(t) \) for three values of \( \Gamma \), choosing
as initial conditions $z(0) = 0.2$ and $\theta(0) = 0$. The figure shows that the NPJE curves (dashed lines) are always closer to the NPSE results (solid lines) than the JE ones (dot-dashed lines). Nevertheless, for a sufficiently strong (and negative) $\Gamma$ the predictions NPJEs are no longer reliable. Notice that while for $\Gamma = 0.25$ the system displays Josephson oscillations, i.e. coherent oscillations around $z = 0$, for $\Gamma = 0.25$ and $\Gamma = -1.05$ there are SSB oscillations, i.e coherent oscillations around $z = z_{SSB} \neq 0$.

![Fig. 4](color online). Left panel: spontaneous symmetry breaking oscillation frequency $\omega_{SSB}$ around ($z = z_{SSB}, \theta = 0$) vs. $\Gamma$. Right panel: Josephson oscillation frequency $\omega_J$ around ($z = 0, \theta = 0$) vs. $\Gamma$. Filled squares are obtained with 1D NPSE, Eqs. (3) and (4). The dashed lines are obtained with NPJEs, Eqs. (13)-(14). The dot-dashed line are obtained with JEs, Eqs. (11) and (12). Parameters of the double well and units as in Fig. 3.

We investigate in detail these coherent oscillations by looking for the stationary points and calculating the frequency of small oscillations around these points. In the case of NPJEs and JEs we diagonalize the Jacobian matrices associated, respectively, to the NPJEs (13)-(14) and JEs (11)-(12). In general, the $2 \times 2$ Jacobian matrix has two complex eigenvalues, $\lambda_{1,2}$, and the stationary point is stable when $\lambda_{1,2} = \mp i \omega$ with $\omega > 0$ the frequency of stable oscillations.

We consider first the Josephson regime and thus we study oscillations around the equilibrium points with $z = 0$ and $\theta = 0$ (balanced population). Notice that for $\Gamma = 0$ the oscillation frequency $\omega_J$ reduces to the Rabi frequency, i.e. $\omega_J = 2K/\hbar$. In the right panel of Fig. 4 we report the frequency $\omega_J$ of coherent oscillations around $z = 0$ as a function of $\Gamma$. From the plots of Fig. 4 one can see the differences between the behavior of $\omega_J$ predicted by 1D NPSE (dots), NPJEs (dashed line), and JEs (dot-dashed lines). Among the three sets of data obviously NPSE ones are the more reliable. The softening of $\omega_J$ as $\Gamma < 0$ approaches $\Gamma_{SSB} = -0.21$ is reproduced extremely well by both NPJEs and JEs, while there are differences in correspondence of the hardening of $\omega_J$ for large positive values of $\Gamma$. At $\Gamma = 1.5$ the relative error in the determination of $\omega_J$ between NPSE and NPJEs results is about 15%.

We now analyze the oscillations in the SSB regime. As previously stressed to this regime is associated a symmetry breaking of the fractional population imbalance $z$, i.e. the stationary configuration has $\theta = 0$ but $z = z_{SSB} \neq 0$. In the left panel of Fig. 4 we plot the SSB oscillation frequency $\omega_{SSB}$ around the stationary $z_{SSB} \neq 0$ (with $\theta(0) = 0$) as a function of $\Gamma$. From these plots one can see that when $\Gamma$ is small enough the behavior of $\omega_{SSB}$ predicted by NPJEs and JEs are quite similar, but NPJEs results are slightly better than JEs ones. $\omega_{SSB}$ is equal to zero at $\Gamma_{SSB}$ and it increases by decreasing $\Gamma < 0$. As $\Gamma$ approaches the collapse strength $\Gamma_c = -1.1$ of 1D NPSE the relative error in the determination of $\omega_{SSB}$ between NPSE and NPJEs results becomes quite large: it is about 50% at $\Gamma = -1.1$. We have verified that, in contrast with JEs, NPJEs predict the BEC collapse but at a critical strength much smaller (in modulus much larger) than the one obtained by using the NPSE.

It is important to stress that it is possible to achieve the so-called “self-trapping regime” in correspondence of initial conditions ($z(0), \theta(0)$) which are not stationary points of JEs [8]. This regime is characterized by population imbalance ($z(t) \neq 0$) and a running phase during the time evolution. By solving our NPJEs we find this dynamical self-trapping for $\Gamma_c < \Gamma < \Gamma_{(ST, -)} < 0$ or $\Gamma > \Gamma_{(ST, +)} > 0$ with the thresholds $\Gamma_{(ST, \mp)}$ depending on the initial conditions $z(0)$ and $\theta(0)$. Note that by solving JEs one finds $\Gamma_c = 0$ and also $\Gamma_{ST, -} = -\Gamma_{ST, +}$.

In conclusion, we observe that the results obtained so far, can be used to describe concrete systems. For instance, by considering an attractive Bose-Einstein condensate made of $^7$Li atoms, and choosing the transverse confining frequency as $\omega_\perp \simeq 2 \pi \times 100$ Hz, we have a typical value of the transverse length $a_L \simeq 4 \mu m$, while the parameters of the double-well potential read: $U_0 \simeq 6 \times 10^{-32} J$ and $x_0 \simeq 8 \mu m$ [1]. The natural scattering length of $^7$Li atoms is $a_s = -1.45$ nm but it can be modified with an external constant magnetic field by means of a Feshbach resonance [7]. Working with $N \simeq 10^4$ condensed atoms in the trap, it is possible to observe experimentally the behavior of Josephson frequency $\omega_J$ and of the SSB frequency $\omega_{SSB}$ by tuning the scattering length $a_s$ from positive values to the collapse point at $a_s = \Gamma_c a_L/(2N) \simeq -0.2$ nm. Finally, we stress that with the above values the condition $|g|/K \ll N^2$ is fully satisfied, and the system is always in the coherent regime [8, 18, 19].

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