Exotic two-dimensional breathers in trapped Bose-Einstein condensates

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Abstract: A study of exotic breathers of two-dimensional Bose-Einstein condensates is presented to verify symmetries associated with the evolution of trapped condensates in harmonic oscillator potentials. We also study if these symmetries are also present in atom mixtures. We perform numerical simulations to investigate the dynamics of the potential energy and particle density of condensates trapped in harmonic oscillator potentials. The exotic breathers studied involve geometrical shapes that reappear periodically, even though they do not present clear spatial symmetries related to the harmonic oscillator.

I. INTRODUCTION

Bose-Einstein condensation of atomic vapors was first observed in 1995 with atoms of ^{87}Rb[1], ^{7}Li[2] and ^{23}Na[3] and prompted a Nobel Prize in Physics for the achievement [4]. Since then, the rise of experimental techniques in ultra-cold atomic systems has allowed for the study of new geometries and configurations of Bose-Einstein condensates (BECs) with great precision, even allowing the observation of 2D and quasi-1D condensates [5].

One phenomenon of special interest are breathers. We consider a breather to be a wave function, in this case of a Bose-Einstein condensate, that undergoes a periodic evolution. Motivated by the recent results reported in [6] in two dimensional BECs, we focus on periodicities associated with the potential energy and particle density, which spark great interest in the hidden symmetries these systems may have.

In this work we study through numerical simulations a symmetry unique to the two dimensional Gross-Pitaevskii equation and show how this symmetry appears in different geometries. We also study the behavior of mixtures of BECs, which can also be obtained experimentally by exploiting the hyperfine structure of ^{87}Rb atoms [7].

In Sec. II we characterize the system in the mean-field theory and discuss two theorems associated with the ground state and evolution of BECs. We then present a numerical method for solving the evolution of the system in Sec. III. Finally, we analyze the results of some exotic breathers for both single and two-component systems in section Sec. IV and Sec. V.

II. THEORETICAL BACKGROUND

The evolution of weakly interacting BECs is well described in mean-field theory by the Gross-Pitaevskii (GP) equation,

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}} + g|\Psi|^2\right)\Psi, \tag{1}$$

where V_{ext} is any external trapping potential and $g = \hbar^2\tilde{g}N/m$ where $\tilde{g}$ is a dimensionless parameter that characterizes the interaction strength. The wave function Ψ is normalized to unity. We focus on the particular case where the external potential is an harmonic oscillator $V(\vec{r}) = m\omega^2 r^2/2$. The potential energy of the condensate in this case reads

$$E_{\text{pot}} = \frac{N}{2}m\omega^2\int r^2|\Psi(\vec{r})|^2 d^2\vec{r}. \tag{2}$$

The kinetic and interaction energy can also be obtained from the GP equation,

$$E_{\text{kin}} = \frac{N\hbar^2}{2m}\int|\vec{\nabla}\Psi(\vec{r})|^2 d^2\vec{r}, \tag{3}$$

$$E_{\text{int}} = \frac{N\hbar^2}{2m}\tilde{g}\int|\Psi(\vec{r})|^4 d^2\vec{r}. \tag{4}$$

The total energy, $E_{\text{tot}} = E_{\text{kin}} + E_{\text{pot}} + E_{\text{int}}$, is conserved during the evolution.

A. Virial Theorem

The virial theorem relates the different contributions to the total energy of the system depending on the scaling of these different contributions. The virial theorem for a ground state in an harmonic oscillator trap takes the form [8],

$$E_{\text{kin}} - E_{\text{pot}} + E_{\text{int}} = 0. \tag{5}$$

This result is useful for checking the accuracy of numerical methods that compute ground states.

B. Dynamical SO(2,1) symmetry theorem

A remarkable theorem which applies to the evolution of any initial wave function trapped in an harmonic oscillator potential was presented by Pitaevskii [9]. Let us now consider an arbitrary interaction potential between the particles of the condensate of the form $V_{\rm int}(\vec{r}_{ij}) = C r_{ij}^n$ where $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$ and $\vec{r}_i$ the position of the ith particle and $\vec{r}_j$ the position of the jth. Consider too the quantity $I = \sum_i r_i^2$ which quantically would be equivalent to the r^2 operator. Classically we can write $\partial_t I = 2\sum_i \vec{r}_i\vec{p}_i/m$ which results in,

$$\partial_t \sum_i \vec{r}_i\vec{p}_i = \sum_i (\partial_t \vec{r}_i)\vec{p}_i + \sum_i \vec{r}_i(\partial_t \vec{p}_i). \tag{6}$$

We can associate the first term with two times the kinetic energy and the second one with the gradient of the potential energies,

$$\partial_t \sum_i \vec{r}_i\vec{p}_i = 2E_{\rm kin} - \sum_i \vec{r}_i\vec{\nabla}_i V_{\rm pot}(\vec{r}_i) - \sum_{i<j} \vec{r}_i\vec{\nabla}_i V_{\rm int}(\vec{r}_{ij}).$$

For the particular case of the harmonic oscillator the second term takes the form $2E_{\rm pot} + nE_{\rm int}$ which reduces the equation to

$$\partial_t \sum_i \vec{r}_i\vec{p}_i = 2E_{\rm kin} - 2E_{\rm pot} - nE_{\rm int}. \tag{7}$$

In the specific case where $n = -2$ we can use energy conservation to express the right hand side as $2E - 2m\omega^2 I$. Knowing that $E_{\rm pot} = \frac{1}{2}m\omega^2 I$ then Eq. (7) can be rewritten in terms of $E_{\rm pot}$,

$$\partial_t^2 E_{\rm pot} = -4\omega^2 E_{\rm pot} + 2\omega^2 E, \tag{8}$$

with the solution

$$E_{\rm pot} = A\frac{\omega^2}{2m}\cos(2\omega t + \gamma) + \frac{E}{2}. \tag{9}$$

It can be shown that $\gamma = 0$ when there are no currents in the initial state [10], e.g. when the initial state is real. We can now rewrite Eq. (9) in a simpler form knowing the energies of the initial state,

$$E_{\rm pot} = \Delta E\cos(2\omega t) + \frac{E}{2}, \tag{10}$$

with $\Delta E = \frac{1}{2}[E_{\rm pot}(0) - E_{\rm kin}(0) - E_{\rm int}(0)]$.

This result shows that the potential energy associated with the harmonic oscillator trap is periodic with frequency twice the one of the trap, regardless of the initial state. Our only assumption for this result is that the interaction potential scales as $n = -2$ which in 3D is only achieved by a $1/r^2$ potential. But in 2D the GP equation, which uses the contact potential $\delta^{(2)}(\vec{r})$, also scales in this manner. This is due to the property $x\delta'(x) = -\delta(x)$ which for the two dimensional Dirac delta produces an $n = -2$ scaling.

This means that this oscillation is a general result for the GP equation of the harmonic oscillator in two dimensions. This oscillation is associated with the two-dimensional Lorentz group SO(2,1) symmetry of the GP equation [9]. The SO(2,1) encompasses time translations, dilations and expansions, which is why this system is considered scale invariant [6].

C. Generalization to two components

Let us now consider two BECs that interact between them. This system can be described with two coupled GP equations,

$$\begin{aligned} i\hbar\frac{\partial\Psi_1}{\partial t} &= \left(-\frac{\hbar^2}{2m_1}\nabla^2 + V_{\rm ext} + g_{11}|\Psi_1|^2 + g_{12}|\Psi_2|^2\right)\Psi_1, \\ i\hbar\frac{\partial\Psi_2}{\partial t} &= \left(-\frac{\hbar^2}{2m_2}\nabla^2 + V_{\rm ext} + g_{22}|\Psi_2|^2 + g_{12}|\Psi_1|^2\right)\Psi_2. \end{aligned} \tag{11}$$

Where g_{11} and g_{22} are the coupling constants of each of the components and g_{12} the coupling constant for the interaction between them. We consider a simpler case where $g_{11} = g_{22} \equiv g$ and $m_1 = m_2 \equiv m$. In particular we set $N_1 = N_2 \equiv N$ and $\tilde{g}_1 = \tilde{g}_2 \equiv \tilde{g}$. We now have both intra and inter-species interaction energies. The intra-species one, $E_{\rm intra}$, is presented in Eq. (4) while the inter-species reads

$$E_{\rm inter} = \frac{N\hbar^2}{m}\tilde{g}_{12}\int |\Psi_1(\vec{r})|^2|\Psi_2(\vec{r})|^2 d^2\vec{r}. \tag{12}$$

One can check that the virial theorem can now be written with an extra term,

$$E_{\rm kin} - E_{\rm pot} + E_{\rm intra} + E_{\rm inter} = 0. \tag{13}$$

In Sec. V we check via numerical simulation if the dynamical symmetry theorem is also valid for mixtures of BECs for a specific configuration. Considering that the inter-species interaction potential is of the same form as the intra-species one we suspect that this may be the case.

III. NUMERICAL METHOD

We now solve numerically the GP equation. Formally one could try to solve the GP equation computing the time evolution operator,

$$\Psi(\vec{r}, t) = e^{-iHt/\hbar}\Psi(\vec{r}, t = 0), \tag{14}$$

with H being

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 + g|\Psi(\vec{r}, t)|^2. \tag{15}$$

As we can see, H is the sum of different parts parts $H = H_1 + H_2 + H_3$. The difficulty of solving Eq. (14) is that $[H_i, H_j] \neq 0$, so we cannot expand the exponential as a product of exponentials. The Trotter-Suzuki expansion [11, 12] can be expressed as

$$e^{A+B} = \lim_{n\to\infty}\left[e^{A/n}e^{B/n}\right]^n. \tag{16}$$

If we discretize time in elements of Δt and apply the expansion two times we can write

$$e^{-i(H_1+H_2+H_3)\Delta t/\hbar} = \lim_{\Delta t\to 0} e^{-iH_1\Delta t/\hbar}e^{-iH_2\Delta t/\hbar}e^{-iH_3\Delta t/\hbar}.$$

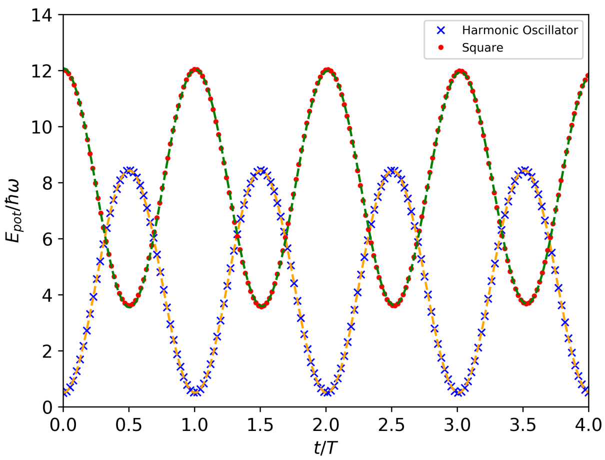

FIG. 1: Real time evolution of the potential energy per particle of a 2D ^{87}Rb condensate for an initial H.O. ground state (crosses) and square (dots). The H.O. ground state is trapped in a harmonic trap of frequency $\omega/2\pi = 232.6$ Hz while the square is trapped in an harmonic trap of frequency $\omega/2\pi = 744.3$ Hz. Each set of data has a cosine function fit (dashed lines) which produces frequencies of 231.974(1) Hz ($R^2 = 0.999997$) and 738.28(2) Hz ($R^2 = 0.9997$) respectively.

By taking $\Delta t \ll 1$ we can approximate this expansion as

$$e^{-iH\Delta t/\hbar} \approx e^{-iH_1\Delta t/\hbar} e^{-iH_2\Delta t/\hbar} e^{-iH_3\Delta t/\hbar}. \tag{17}$$

The error in this approximation scales as $(\Delta t)^2$ and is proportional to the commutators of the operators H_i (if all operators commute, this is an exact expansion). By discretizing space we can compute the exponentials in Eq. (17) easily, as the potential and interaction operators are diagonal and, if we approximate the laplacian with three points, the kinetic operator is tridiagonal. The method has been implemented in an extremely efficient way in [13]. This code allows for both real and imaginary time evolution, so we can use the latter to compute the ground state of different geometries. It is also capable of simulating two-component systems, which we will use in Sec. V.

A. Accuracy test of imaginary time evolution

To test the accuracy of imaginary time evolution of this numerical method, we compute the ground state of the system at different values of g and check if the virial theorem is fulfilled, which is usually not trivial in numerical simulations.

We compute the ground state of a condensate in an harmonic trap of frequency $\omega/2\pi = 232.6$ Hz for values of g ranging from $gm/\hbar^2 = 0$ to $gm/\hbar^2 = 1000$. We consider that the state has converged when the total energy between consecutive iterations is of less than $5 \times 10^{-4}\,\hbar\omega$.

The quantity $E_{\text{kin}} - E_{\text{pot}} + E_{\text{int}}$ was less than 0.7% of the total energy in all cases. Notably, the case without interaction presented a total energy which was in agreement with the known solution of the harmonic oscillator ($E/\hbar\omega = 1$) to a 99.99998%, which gives confidence in the accuracy of the numerical method with imaginary time evolution

IV. TWO-DIMENSIONAL BREATHERS OF SINGLE COMPONENT BECS

We now study the evolution of trapped BECs in different initial geometries with the aim of verifying the theorem presented in section II B. The geometries include an harmonic oscillator (H.O.) ground state, a square and a triangle. The latter are particularly interesting because while the triangle presents a breather, the square does not [6].

The evolution is performed using the method mentioned in the previous section. We consider a similar configuration as the one reported in [6]. In all cases the atoms of the condensate are ^{87}Rb atoms due to their popularity in the experiments. The condensate is confined in a $20\,\mu\text{m} \times 20\,\mu\text{m}$ box dicretized with 512×512 points. The time discretization step is of $\Delta t = 1.37 \times 10^{-5}$ ms.

A. Harmonic oscillator ground state breather

The first configuration we consider is that of a sudden increase of the interaction strength. We start by preparing the system in the non-interacting ground state of an harmonic oscillator trap. Then, we suddenly change the interaction strength to $gm/\hbar^2 = 4350$ and perform real time evolution for ~ 4 oscillations in the same harmonic trap. The results of the potential energy are presented in Fig. 1. The fitted frequency is compatible with the dynamical symmetry theorem to 0.3%. The standard deviation of the total energy is of less than 0.1%.

B. Square condensate

We study next the evolution of a BEC in an initial square-shaped state. The generality of the theorem presented in Sec. II B means that the evolution of the potential energy should show the same oscillations as the ones presented in Sec. IV A, even if it is very different from the eigenstates of the system.

We begin by obtaining the initial state. We perform imaginary time evolution on a condensate of $gm/\hbar^2 = 1000$ with very high barriers that form a square of side $5\,\mu$m, the ground state of this potential is similar to a square, see first frame of top row of Fig. 3. We consider that the imaginary time evolution method has converged when the difference in total energy of the system between iterations is less than $1.6 \times 10^{-6}\,\hbar\omega$. After finding the

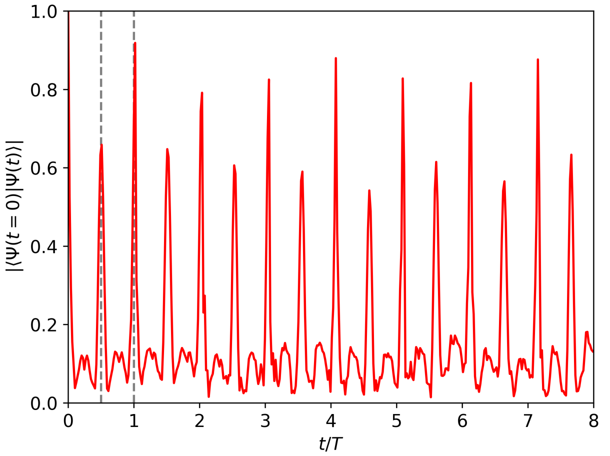

FIG. 2: Real time evolution of the projections of a 2D ^{87}Rb condensate on to initial triangle state. The condensate is on a harmonic trap of frequency $\omega/2\pi = 744.3$ Hz. Times $t/T = 0.5$ and $t/T = 1$ are marked with dashed vertical lines.

ground state we remove the square barriers and perform real time evolution for ~ 4 oscillations in an harmonic trap. The results are presented in Fig. 1. The fitted frequency is compatible with the dynamical symmetry theorem to 0.3%. The standard deviation of the total energy is of less than 0.1%.

C. Triangle breather

Another notable case is the evolution of a BEC in an initial triangle-shaped state. Unlike the square, this initial state also presents an oscillation in the particle density of the same period as the potential energy oscillations (see Fig. 3).

We proceed in the same manner than in the square. First, we perform imaginary time evolution on a condensate of $gm/\hbar^2 = 14500$ with very high barriers in an equilateral triangle shape of side $10\,\mu$m, see first frame of bottom row of Fig. 3. The criterion of convergence is the same as in the square. Then we remove the triangle walls and perform real time evolution for about 8 oscillations on an harmonic oscillator.

We can also fit a cosine to the potential energy to confirm the dynamical symmetry theorem. In this case the fitted cosine yielded a frequency of 728.1(3) Hz ($R^2 = 0.96$). This result is compatible with the dynamical symmetry theorem to 2.2%. The standard deviation of the total energy is of less than 0.1%.

Additionally to the oscillations in the potential energy, the system also presents a breather with the same period as the potential energy oscillations, see bottom row in Fig. 3. To study this in more detail we computed the scalar product of the initial condensate and the condensate at a certain time, $|\langle\Psi(t=0)|\Psi(t)\rangle|$. The closer

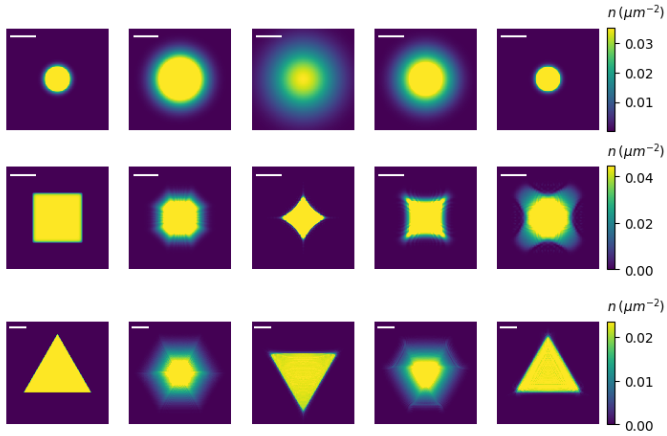

FIG. 3: Particle densities of ^{87}Rb condensates in harmonic trapping potentials at times $t/T = 0, 0.25, 0.5, 0.75, 1$, increasing in time from left to right. From top to bottom: initial harmonic oscillator ground state, initial square-shaped state and initial triangle-shaped state. The boxes shown for the H.O. ground state and square are of $10\,\mu$m $\times$ $10\,\mu$m and for the triangle of $15\,\mu\mathrm{m} \times 15\,\mu\mathrm{m}$. The white lines in all represent $2.5\,\mu$m.

this quantity is to 1, the more similar is the condensate to the initial triangle-shaped state. The projections are showed in Fig. 2 and show maximums at $t/T = 1, 2, 3\ldots$. Additionally one can observe smaller maximums at half periods.

The oscillation appears to have a smaller frequency than predicted, which is reflected in both the fitted cosine and in the projections, where the maximums do not appear at the predicted times and instead get slightly delayed.

D. Comparison between the square and triangle breathers

As we have seen, both the initial square-shaped and triangle-shaped states have oscillations in the potential energy whose frequency is directly related with the harmonic trapping potential. However, an interesting distinction was reported in [6] when comparing the particle density evolution. The square shape does not present a clear periodicity while the triangle shape does. To illustrate this, in Fig. 3 we show the particle densities in the initial states and at 4 different times in the first period of evolution.

Focusing on the triangle (bottom row), it can be seen that after a period it has recovered its initial shape (last frame). The harmonic oscillator (top row) also recovers its initial shape but the square (middle row) does not. It is also worth noticing that the triangle experiences a vertical inversion at half a period (bottom row, third frame). This is not reproduced in either the harmonic oscillator nor the square, which have shapes that cannot

FIG. 4: Particle densities of two ^{87}Rb condensates in a harmonic trap of frequency $\omega/2\pi = 744.3$ Hz at times $t/T = 0, 0.25, 0.5, 0.75, 1$. The initial state is triangle shaped divided vertically such that each half is filled by one component. The box is shown is of $20\,\mu\text{m} \times 20\,\mu\text{m}$ and the white lines represent $5\,\mu$m

be related to their initial states.

Additionally, the states at $t/T = 0.25$ and $t/T = 0.75$ (second and third frames of each row) are also interesting, in the harmonic oscillator and square the shape at $t/T = 0.25$ appears to be different to the shape in $t/T = 0.75$. This is not the case for the triangle, where the shapes appear to be vertical mirrors of each other.

These behaviors indicate that a condensate in a triangle shape is unique in its evolution in an harmonic trap, at least when described by the GP equation.

V. TWO-DIMENSIONAL BREATHERS IN TWO COMPONENT BECS

We now extend the study to the case of two component BEC systems with the aim of analyzing the fate of similar triangle-shaped breathers and verifying if the dynamical symmetry theorem also holds in this case. We focus in particular on a breather similar to the triangle one we saw in the previous section but the initial triangle is divided vertically in two halves, which are filled each with a component of our system. We set $gm/\hbar^2 = 14500$ and, to avoid the mixing of the species, $g_{12}m/\hbar^2 = 25000$ so that $g/g_{12} = 0.58$. Other parameters take the same values as in the single component simulations.

We perform imaginary time evolution with the same criteria as in the previous cases but now the triangle barriers have an additional barrier that restricts the first component of the system to the left half of the box and the second component to the right half. The ground state of this system has a collective shape of an equilateral triangle of side 10 μm, see Fig. 4. We then remove the barriers and place the condensates on an harmonic trap and perform real time evolution for about 8 oscillations. The evolution of the first period can be seen in Fig. 4

The evolution in this case is similar to the single component evolution but with an increased expansion at $T/2$ due to the additional repulsion between the species. However at $t = T$ the initial triangle shape is recovered like with a single component. A cosine fit to the potential energy of both components yields a frequency of 724.0(2) Hz ($R^2 = 0.98$), which has a discrepancy with of 2.7% with the theoretical predictions. The standard deviation of the total energy in this case was of 0.6%, on account of the increased complexity of the system.

This confirms that under certain conditions the exotic breather produced by the triangle shape in an harmonic trap can be reproduced for mixtures of BECs, which has not been checked experimentally yet.

VI. CONCLUSIONS

In this work we have investigated the consequences of the symmetries of the GP equation and how they reflect on some exotic breathers which present clear oscillations on their potential energy as they evolve. By means of direct numerical simulations of the GP equation we confirmed that the triangle in particular presents a unique periodic motion in contrast to the square. Reportedly, other geometries like pentagons and hexagons did not present the same kind of evolution as the triangle [6], although the cause of these behaviors is still an open issue.

We have extended the study to the case of two component BECs, observing a similar behavior for breathers where the two components do not mix due to the repulsive inter-species interaction. This fact opens up a lot of uncharted phenomena regarding mixtures of BECs and could shed some light on the cause of these exotic breathers. The breather we have considered can be readily studied in state-of-art laboratories worldwide.

Acknowledgments

I would like to thank Dr. Bruno Juliá and Dr. Artur Polls for their advice and outstanding support during this project.

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