Collapse of triaxial bright solitons in atomic Bose-Einstein condensates

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We study triaxial bright solitons made of attractive Bose-condensed atoms characterized by the absence of confinement in the longitudinal axial direction but trapped by an anisotropic harmonic potential in the transverse plane. By numerically solving the three-dimensional Gross-Pitaevskii equation we investigate the effect of the transverse trap anisotropy on the critical interaction strength above which there is the collapse of the condensate. The comparison with previous predictions [Phys. Rev. A 66, 043619 (2002)] shows significant differences for large anisotropies.

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The experimental achievement of quantum degeneracy with ultracold alkali-metal atoms $^1$, $^2$ has opened the possibility of studying various topological configurations of the Bose-Einstein condensate (BEC) with repulsive or attractive inter-atomic interaction $^3$. Dark solitons in repulsive BECs have been experimentally achieved ten years ago $^4$, while bright solitons have been detected only more recently in two different experiments $^5$, $^6$ involving attractive BECs of $^7$Li vapors. In these latter experiments, an optical red-detuned laser beam generated along the axial direction of the sample is used to trap the attractive BEC by a cylindric isotropic transverse confinement; the BEC propagates along the longitudinal axis of the cylinder without relevant spreadings. Recently, also $^{85}$Rb atoms have been used to achieve the Bose-Einstein condensation and investigate the formation of bright matter-wave solitons during the collapse $^7$.

Many theoretical works have been devoted to the study of cigar-shaped and axially symmetric bright-soliton configurations, also in presence of an axial periodic potential $^8$, $^9$, $^{10}$, $^{11}$, $^{12}$, $^{13}$, $^{14}$, $^{15}$, $^{16}$, $^{17}$, $^{18}$, $^{19}$. The transverse confinement produced by the isotropic harmonic potential in the cylindric radial direction plays a crucial role in giving rise to single $^{10}$, $^{11}$, $^{12}$, $^{13}$, $^{14}$ or multiple $^{13}$, $^{14}$ metastable bright solitons, which collapse above a critical number of particles $^{10}$, $^{11}$, $^{12}$, $^{13}$. These theoretical investigations showed that increasing the inter-atomic strength, e.g. by Fano-Feshbach resonances, makes the bright soliton less cigar-shaped. In particular, a quasi-spherical shape is achieved only when the interaction strength approaches the critical value that signs the collapse $^{10}$, $^{12}$.

In this paper we study an attractive BEC trapped by an anisotropic harmonic potential in the transverse plane and without confinement in the axial direction. Under this trapping condition the BEC admits stable bright-soliton configurations, which are generally triaxial. The deformation of the transverse anisotropic confinement can be described by two independent parameters $^{18}$, or by a unique quantity, the ellipticity $^{19}$. In both cases, by using the numerical integration of the three-dimensional Gross-Pitaevskii equation, we investigate as a function of the transverse trap anisotropy the critical interaction strength above which the triaxial soliton collapses, i.e. it shrinks to the zero-size ground-state of infinite negative energy. We compare our results with previous numerical predictions $^{11}$ and find that our stability domain is significantly smaller.

Let us consider an attractive BEC without confinement in the axial direction $z$ and confined in the transverse plane $(x, y)$ by the anisotropic harmonic potential

$$U(x, y) = \frac{m}{2} (\omega_1^2 x^2 + \omega_2^2 y^2) , \quad (1)$$

where $m$ is the mass of a Bose-condensed atom, and $\omega_1$, $\omega_2$ are the two frequencies of the harmonic confinement. With the aim of working in scaled units we set

$$\omega_1 = \lambda_1 \omega_\perp , \quad \omega_2 = \lambda_2 \omega_\perp . \quad (2)$$

In particular, if $a_\perp = (\hbar/(m\omega_\perp))^{1/2}$ is used as characteristic harmonic length of the system, then lengths may be measured in units of $a_\perp$ and energies in units of $\hbar \omega_\perp$.

The dynamics of an attractive BEC can be accurately described by the adimensional time-dependent 3D Gross-Pitaevskii equation (3D GPE), given by

$$i \hbar \frac{\partial}{\partial t} \Psi = \left[ -\frac{1}{2} \nabla^2 + \frac{1}{2} (\lambda_1^2 x^2 + \lambda_2^2 y^2) - 2\pi g |\Psi|^2 \right] \Psi , \quad (3)$$

where $\Psi(r, t)$ is the macroscopic wave function of the condensate and

$$g = \frac{2 N |a_s|}{a_\perp} . \quad (4)$$
is the interaction strength, with $N$ the number of atoms and $a_s < 0$ the $s$-wave scattering length of the inter-atomic potential. Setting

$$
\Psi(r, t) = \psi(r) e^{-i\mu t},
$$

from Eq. (5) one finds the stationary 3D GPE

$$
\left[-\frac{1}{2} \nabla^2 + \frac{1}{2} \left(\lambda_1^2 x^2 + \lambda_2^2 y^2\right) - 2\pi g|\psi|^2\right] \psi = \mu \psi,
$$

where the chemical potential $\mu$ is fixed by the normalization

$$
\int |\psi(r)|^2 \, d^3r = 1.
$$

Stable solutions of Eq. (6) are called bright solitons [8, 9, 10, 11, 12]. They correspond to an attractive BEC with a self-confinement along the $z$ axis.

To determine the solutions of Eq. (6) we solve Eq. (3) by using a finite-difference Crank-Nicolson algorithm with imaginary time [21] and a spatial mesh of $160 \times 160 \times 160$ points (for details see the Appendix). In this way we determine the wave function $\psi(r)$ of the metastable bright soliton and we can also calculate the integrated density profiles of the triaxial bright soliton along the three spatial directions, given by

$$
\rho(x) = \int |\psi(r)|^2 \, dy \, dz,
$$

$$
\rho(y) = \int |\psi(r)|^2 \, dx \, dz,
$$

$$
\rho(z) = \int |\psi(r)|^2 \, dx \, dy.
$$

To study the critical strength above which there is the collapse, we consider first the simpler case of elliptic transverse confinement. As explained by Jamaludin et al. [19], it is possible to consider an elliptic transverse harmonic confinement and consequently to parametrize the transverse anisotropy of the harmonic confining potential
by using a unique parameter, the trap ellipticity $\epsilon$. In terms of the ellipticity $\epsilon$, the scaled harmonic frequencies are written as

$$\lambda_1 = \sqrt{1 - \epsilon}, \quad \lambda_2 = \sqrt{1 + \epsilon},$$

with $\epsilon$ restricted to the interval $[-1,1]$. Clearly $\epsilon = 0$ corresponds to the isotropic transverse confinement, while $\epsilon = \pm 1$ implies the absence of confinement along the $x$ axis ($\epsilon = 1$) or along the $y$ axis ($\epsilon = -1$).

As an example, in Fig. 1 we plot the density profiles of the bright soliton choosing the interaction-strength $g = 1.2$ and an elliptic transverse confinement with ellipticity $\epsilon = 0.4$. The shape of the bright soliton strongly depends on the ellipticity $\epsilon$ of the transverse potential and the interaction strength $g$. By varying $\epsilon$ and $g$ the bright soliton can be spherical-shaped, cigar-shaped, disk-shaped, but also fully triaxial.

Our numerical investigation shows that under the condition $\epsilon \geq 0$ the width $\sigma_x$ of the soliton along the $x$ axis is always close to 1 (in units of $a_\perp$). The width $\sigma_y$ of the soliton along the $y$ axis is equal to $\sigma_x$ only for $\epsilon = 0$; moreover $\sigma_y$ becomes extremely large as $\epsilon \rightarrow 1$. Obviously, with $\epsilon < 0$ the behaviors of $\sigma_x$ and $\sigma_y$ are interchanged. The width $\sigma_z$ along the $z$ axis is instead controlled by the interaction strength $g$: a small $g$ implies a very large $\sigma_z$, while when $g$ is sufficiently large the width $\sigma_z$ is around 1. In addition it exists a critical strength $g_c$ above which there is no solution, i.e. the wave function of the metastable soliton collapses to the zero-size ground-state of infinite negative energy.

In Fig. 2 we plot this critical strength $g_c$ as a function of the ellipticity $\epsilon$ of the transverse trap. Our numerical results based on the integration of the 3D GPE are displayed as filled circles. The figure shows that when the trap...
FIG. 4: Critical strength $g_c$ as a function of the scaled frequency $\lambda_2$ with $\lambda_1 = 1$. The interaction strength is $g = 2N|a_+|a_-$. Filled circles: numerical results obtained with the 3D GPE. Dashed line: prediction of Eq. (12).

is perfectly symmetric ($\epsilon = 0$) the critical strength $g_c$ reaches its minimum value, $g_c = 1.35$. Instead, as $|\epsilon| \to 1^-$ the critical strength has its maximum value given by $g_c = 1.66$. We notice that when $|\epsilon| \to 1^-$, the frequency of confinement along one of the two transverse directions goes to zero, but only at $\epsilon = \pm 1$ the triaxial bright soliton becomes unbounded.

It is interesting to compare our results with previous predictions based on numerical calculations and scaling [11]. According to these predictions [11] the critical strength $g_c$ is simply given by the formula

$$g_c = \frac{1.352}{(\lambda_1 \lambda_2)^{1/4}}. \tag{12}$$

In Fig. 2 the dashed line is obtained with Eq. (12) and the scaled frequencies given by Eq. (11). The figure shows that there are relevant differences between our numerical results (filled circles) and Eq. (12) for $|\epsilon|$ close to 1. In fact, Eq. (12) implies that $g_c \to +\infty$ for $|\epsilon| \to 1^-$. Actually, Eq. (12) is based on the hypothesis of an attractive BEC with triaxial harmonic confinement of frequencies $\lambda_1$, $\lambda_2$, and $\lambda_3$ under the conditions $\lambda_1, \lambda_2 \gg \lambda_3$ and $\lambda_3 \to 0$ [11], but these conditions on the harmonic frequencies break down for $|\epsilon| \to 1$. As previously discussed, our numerical results suggest instead a finite value of $g_c$ for $|\epsilon| \to 1^-$, as confirmed also by a fully Gaussian variational approach [18].

An important issue is the dynamical stability of the triaxial bright solitons we have found. According to the Vachitov-Kolokolov criterion [22], the fundamental solitons are stable if they satisfy the condition $d\mu/dg < 0$. We have verified that up to the collapse this condition is always satisfied by our bright solitons. For completeness, in Fig. 3 we show the calculated chemical potential $\mu$ versus the interaction strength $g$ for the triaxial bright solitons with ellipticity $\epsilon = 0.8$.

Let us now investigate the general case where $\lambda_1$ and $\lambda_2$ are independent. Keeping fixed one of the two harmonic frequencies, e.g. $\lambda_1$, we may independently tune the other, $\lambda_2$. Without loss of generality we fix $\lambda_1 = 1$. We find that the critical strength $g_c$ approaches a maximum finite value when the trapping frequency $\lambda_2$ tends to zero. This effect is shown in Fig. 4, where we plot the critical strength $g_c$ as a function of $\lambda_2$ with $\lambda_1 = 1$. Instead, for large values of $\lambda_2$ the critical strength $g_c$ becomes smaller. By using a Gaussian variational approach [18] we have indeed verified that $g_c \to 0$ as $\lambda_2 \to +\infty$. For the sake of completeness, in Fig. 4 we have included also the prediction of Eq. (12) with $\lambda_1 = 1$. Remarkably, there are deviations not only for small values of $\lambda_2$ but also for large values of $\lambda_2$.

In conclusion, in this work we have investigated the collapse of triaxial bright solitons in Bose-condensed atoms under transverse anisotropic harmonic confinement by using the 3D Gross-Pitaevskii equation. Our predictions on the stability domain of these triaxial bright solitons can be useful for future experimental investigations with deformed atomic waveguides.

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Appendix: Numerical method

The numerical integration of the time dependent GPE, in Eq. (5), is obtained by using a finite-difference Crank-Nicolson scheme modified with a split operator technique, adapted to the integration of a Schrödinger equation [21]. This approach has been successfully applied in various problems and configurations [14, 15].

First, we write Eq. (3) in the form
\[
i\hbar \frac{\partial}{\partial t} \Psi(r, t) = \left( H_1(r, t) + H_2(r, t) + H_3(r, t) \right) \Psi(r, t),
\]
(13)
where
\[
H_\alpha(r, t) \equiv -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_{\alpha}^2} + U(x_{\alpha}) - \frac{1}{3} g |\Psi(r, t)|^2,
\]
(14)
with \( \alpha = 1, 2, 3 \) and \( x_1 = x, x_2 = y, x_3 = z \). Here we have used the fact that the external potential is separable: \( U(x, y, z) = U(x) + U(y) + U(z) \). In this way we split the full Hamiltonian in three sub-Hamiltonians, so that at each time we have to write the Laplacian with respect to one coordinate only, leading to the solution of a tridiagonal system, and to huge savings in computer memory.

Equation (13) is integrated using the splitted Crank-Nicolson scheme
\[
\Psi(r, t + \delta_t) = \frac{1}{1 + A_2(t)/2} \left( 1 - A_1(t)/2 \right) \times \frac{1}{1 + A_3(t)/2} \left( 1 - A_2(t)/2 \right) \times \frac{1}{1 + A_1(t)/2} \left( 1 - A_3(t)/2 \right) \Psi(r, t).
\]
(15)
where \( \delta_t \) is the integration time step, and \( A_\alpha(t) \equiv \imath \delta_t H_\alpha(r, t)/\hbar \). The splitting is carried out so that the commutators are exact up to the order \( \delta_t^2 \) included. There is obviously a problem with the nonlinear term \( g|\Psi(r, t)|^2 \), because we should really use a \( \Psi \) somehow averaged over the time step \( \delta_t \), not a \( \Psi \) evaluated at the beginning of the time step. To circumvent this problem, we use a predictor-corrector step, where each integration step is really done in two times: going from the time \( t \) to the time \( t + \delta_t \), the first time we used \( \Psi(r, t) \) in the nonlinear term, obtaining a “predicted” \( \Psi(r, t + \delta_t) \); we then repeated the integration step, starting again from \( \Psi(r, t) \), but using \( \frac{1}{2} \left( \Psi(r, t) + \Psi(r, t + \delta_t) \right) \) in the nonlinear term.

In our numerical method the wave function is discretized in the following way
\[
\Psi(r, t) = \Psi(x^i, y^j, z^k, t^s)
\]
(16)
where \( x^i = x_0 + i \delta_x, y^j = y_0 + j \delta_y, z^k = z_0 + k \delta_z \), and \( t^s = s \delta_t \), with \( i, j, k, s \) integer numbers. Second derivatives are approximated by finite-difference formulas. For instance, along the \( x \) axis we use
\[
\frac{\partial^2}{\partial x^2} \Psi(x^i, y^j, z^k, t^s) = \frac{\Psi(x^{i+1}, y^j, z^k, t^s) - 2\Psi(x^i, y^j, z^k, t^s) + \Psi(x^{i-1}, y^j, z^k, t^s)}{\delta_x^2}.
\]
(17)

In the upper panel of Fig. 5 we show the typical behavior of the energy \( E \) of the triaxial bright soliton as a function of the imaginary time \( t \). We use a triaxial Gaussian as initial trial wave function \( \Psi(r, t = 0) = \Psi_{\text{initial}}(r) \), normalizing to one the norm of \( \Psi(r, t) \) at each time step. The energy \( E \) of the system, given by
\[
E = \int \Psi^* (r, t) \left[ \frac{-\hbar^2}{2m} \nabla^2 + \left( \lambda_1^2 x^2 + \lambda_2^2 y^2 \right) - \frac{1}{2} (2\pi g)|\Psi(r, t)|^2 \right] \Psi(r, t) \, d^3r,
\]
(18)
decreases during the (imaginary-)time evolution and eventually reaches its asymptotic value \( E_{\text{final}} \). We find that the asymptotic value \( E_{\text{final}} \) depends of the number \( N_x \times N_y \times N_z \) of points in the spatial mesh. Nevertheless, as shown in the lower panel of Fig. 5 for sufficiently large values of \( N_x \) the energy \( E_{\text{final}} \) saturates to the exact value. As a final check, we have verified that smaller values of the time step \( \delta_t \), with respect to the one we use (\( \delta_t = 0.05 \)), do not modify the final results within the third digit. Moreover, we have checked that the final energy \( E_{\text{final}} \) and the final wave function \( \Psi_{\text{final}}(r) \) do not depend on the initial trial wavefunction \( \Psi_{\text{initial}}(r) \). \( \Psi_{\text{final}}(r) \) is the wave function of triaxial bright soliton. In the case of collapse, we find that the final energy is \( E_{\text{final}} = -\infty \) and the final wave function is a Dirac delta peak, centered at \( r = 0 \).
FIG. 5: Triaxial bright soliton with $g = 1.2$ and $\epsilon = 0.8$. Upper panel: energy $E$ of the bright soliton as a function of the imaginary time $t$ for 3 values of $N_s$. The spatial mesh has $N_s \times N_s \times N_s$ points. Lower panel: asymptotic energy $E_{\text{final}}$ of the bright soliton as a function of $N_s$.

A very recent and complete review of numerical methods used to solve the Gross-Pitaevskii equation has been written by Muruganandam and Adhikari [23]. In this paper the finite-difference Crank-Nicolson scheme we have used is explained with many details.

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