Critical numbers of attractive Bose-condensed atoms in asymmetric traps

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The recent Bose-Einstein condensation of ultracold atoms with attractive interactions led us to consider the novel possibility to probe the stability of its ground state in arbitrary three-dimensional harmonic traps. We performed a quantitative analysis of the critical number of atoms through a full numerical solution of the mean field Gross-Pitaevskii equation. Characteristic limits are obtained for reductions from three to two and one dimensions, in perfect cylindrical symmetries as well as in deformed ones.

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The predicted collapsing behavior of the condensed systems with attractive two-body atomic interactions\(^{[4]}\), first observed in experiments with \(^{7}\)Li\(^{[3]}\), was recently tested in experiments with \(^{85}\)Rb\(^{[3]}\). In the experiments described in Ref. \(^{[3]}\), and more recently in \(^{[1]}\), by means of Feshbach resonance techniques\(^{[3]}\), the two-body interaction was tuned from positive to negative values. Besides the fact that the experimental results qualitatively agree with the theory, and confirm results of previous variational treatments\(^{[1]}\), they also show a consistent quantitative deviation of about 20\% from the mean-field predicted critical number of atoms, \(N_c\). The asymmetry of the trap was shown in Ref. \(^{[2]}\) to be responsible for about 4\% of the observed deviation.

In this respect, it is relevant to obtain precise and reliable numerical results for the mean-field calculations, in order to probe their consistency and possible limitations. The actual experimental atomic traps are in general harmonic and non-symmetric. Extreme asymmetric traps have been recently employed in experimental investigations with condensates constrained to quasi-one (1D)\(^{[1]}\) or quasi-two dimensions (2D)\(^{[1]}\), exploring theoretical analysis considered by several authors\(^{[1]}\). A non symmetric three-dimensional (3D) trap is reported in Ref.\(^{[2]}\), with the frequencies given by \(2\omega_1 = 2\omega_2 = 2\omega_3 = 2\pi \times 33\text{Hz}\).

Considering the general non-symmetric traps that have been employed, the accuracy of the comparison between experiments and the results of mean-field approximation relies in precise calculations using arbitrary three-dimensional traps. In case of attractive two-body interaction, the maximum critical number of atoms for a stable system is one of the interesting observables to study, which is also related to the collapse of the wave-function of the system. In these cases, where the two-body scattering length is negative and the kinetic energy cannot be considered to be a small perturbation, the Gross-Pitaevskii mean field approximation has been applied, given reliable results in explaining the observations in the stable (non-collapsing) conditions\(^{[2]}\).

Before presenting the mean-field equation for an arbitrary 3D case, let us analyze qualitatively the collapse phenomenon for asymmetric traps. The interaction energy is proportional to the square of the density, varying with the negative two-body scattering length. For traps with cylindrical (or almost cylindrical) shapes, there are two quite different situations: one, pancake-like, with the frequencies in the transverse directions being smaller than the frequency in the longitudinal direction; the other, cigar-like (quasi-1D), with the frequency in the longitudinal direction smaller than the frequencies in the perpendicular directions. For a true 1D system, one does not expect the collapse of the system with increasing number of atoms\(^{[2]}\). However, it happens that a realistic 1D limit is not a true 1D system, with the density of particles still increasing due to the strong restoring forces in the perpendicular directions\(^{[6]}\).

The relevance of the quasi-1D trap have been pointed out in Ref.\(^{[6]}\), to control the condensate motion. But, as we are going to see, the critical number of particles in the quasi-1D limit is smaller than the critical number of particles in the 2D limit, if we just exchange the longitudinal and perpendicular frequencies. The physical reason for that behavior is the increase of the average density in the cigar-like configuration relative to the pancake like one for the same number of atoms, implying in a strong collapsing force in the first case and consequently the cigar-like geometry is a more unstable configuration compared to the pancake like one. This conclusion is in apparent contradiction with the remark made in section IV of Ref.\(^{[6]}\), saying that, considering the better collapse-avoiding properties, “the cigar-shaped trap is the optimal one”. We are going to discuss this problem in detail and clarify this issue.

In the following, we revise the Gross-Pitaevskii (GP) formalism, for an atomic system with arbitrary non-spherically symmetric harmonic trap. The Bose-Einstein condensate, at zero temperature, in the GP mean-field approximation is given by

\[
\text{i} \hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \frac{m}{2} \left( \omega_1^2 r_1^2 + \omega_2^2 r_2^2 + \omega_3^2 r_3^2 \right) \right] \Psi(\vec{r}, t)
\]
\( + \frac{4\pi\hbar^2}{m} |\Psi(\vec{r},t)|^2 \)  \( \Psi(\vec{r},t) = \mu\Psi(\vec{r},t), \) \( \) (1)

where \( r = \sqrt{r_1^2 + r_2^2 + r_3^2} \), \( m \) is the mass of the atom, \( \mu \) is the chemical potential, and the wave-function \( \Psi \equiv \Psi(\vec{r},t) = \Psi(\vec{r},0)\exp(-i\mu t/\hbar) \) is normalized to the number of particles \( N \). The arbitrary geometry of the trap is parameterized by three different frequencies \( \omega_1, \omega_2 \) and \( \omega_3 \). For convenience, it is appropriate to define the frequencies according to their magnitude, such that, in the present work we assume \( \omega_1 \leq \omega_2 \leq \omega_3 \).

Here we will be concerned only with systems that have attractive two-body interactions \( [a = -|a|] \), in Eq. (1). In this case, it was first shown numerically, in Ref. [1], that the system becomes unstable if a maximum critical number of atoms, \( N_c \), is achieved. We present precise results for a critical parameter \( k \), directly related to the maximum number of atoms, in a general non-symmetric configuration of the trap.

By rewriting Eq. (1) in dimensionless units:

\[
\frac{\partial \phi}{\partial \tau} = \left[ \frac{1}{2} \sum_i \left( -\frac{\partial^2}{\partial x_i^2} + \frac{\omega_i^2 x_i^2}{\omega^2} \right) - |\phi|^2 \right] \phi, \tag{2}
\]

where \( \tau \equiv \omega t, r_i \equiv l_0 x_i \) and \( \phi \equiv l_0 \sqrt{4\pi|a|} \Psi \), with

\[
\int d^3x |\phi|^2 = 4\pi \frac{N|a|}{l_0} \tag{3}
\]

The oscillator length \( l_0 \) is defined in terms of \( \omega \), which is taken as the geometrical mean value of the frequencies:

\[
l_0 = \sqrt{\frac{\hbar}{m\omega}}, \quad \text{with} \quad \omega \equiv (\omega_1\omega_2\omega_3)^{1/3}. \tag{4}
\]

For strong non-symmetric cases, particularly when comparing the two extreme cylindrical-shape geometries, \( \omega_1 \sim \omega_2 << \omega_3 \) (pancake-shape) and \( \omega_1 << \omega_2 \sim \omega_3 \) (cigar-shape), it is expected a noticeable difference between the corresponding critical number of particles.

We define a parameter \( k \), related to the critical number of trapped atoms \( N_c \) as in Ref. [13]:

\[
k = \frac{N_c|a|}{l_0}. \tag{5}
\]

This parameter is a maximum critical limit for stable solutions of the dimensionless Eq. (3). It will depend only on the ratio of the frequencies of the trap. Within the precision given in Ref. [23], \( k_s = 0.5740 \), where \( k_s \) is \( k \) for spherically symmetric traps. In Ref. [24], the critical number was calculated for a nonsymmetrical geometry, but in a case that the frequency ratio is not too far from the unity \( (\omega_1/\omega_{\perp} = 0.72) \), giving a result for the number of atoms almost equal to the spherical one.

In the experiments with \(^{85}\text{Rb} \)[1], they have considered an almost cylindrical “cigar-type” symmetry, with the three frequencies given by 17.47 Hz, 17.24 Hz and 6.80 Hz. With this symmetry, they have obtained \( k = 0.459 \pm 0.012 \) (statistical) \( \pm 0.054 \) (systematic). In Ref. [22], assuming the cylindrical symmetry \( \omega_1 = 2\pi \times 6.80 \) Hz \( \omega_2 = \omega_3 = 2\pi \times 17.35 \) Hz, it was obtained \( k = 0.55 \), a value about 4% lower than \( k_s \).

In our numerical approach, the calculation is performed by evolving the nonlinear equation (3) through imaginary time [24]. The evolution is performed for an initial value of the normalization (3) until the wave function relaxes to the ground state. The wave function is renormalized after each time step. The process is repeated systematically for larger values of the renormalization, until a critical limit is reached. At this critical limit the ground state becomes unstable. The time evolution is done with a semi-implicit second order finite difference algorithm. An alternating scheme is used in the \( x_1 \) and \( x_2 \) direction, with a split step in the \( x_3 \) direction. This procedure is done only for \( x_3 \geq 0 \), taking advantage of the reflection symmetry of the ground state. We consider \( 100^3 \) grid points and time step equal to \( \Delta \tau = 0.001 \), verifying that the algorithm is stable for long time evolution. As we increment the renormalization, approaching the critical limit, the wave function starts to shrink. So, in order to maintain the precision, we introduce an automatic reduction of the grid sizes, \( \Delta x_1, \Delta x_2, \) and \( \Delta x_3 \), gauged by the respective root mean-square-radius in each direction.

In Fig. 1 we show our main results for the critical constant \( k \), covering many different geometries. We plot \( k/k_s \) (and \( k \) in the rhs \( y \)-axis) as a function of \( \lambda \), which is defined by

\[
\lambda \equiv \frac{\omega_1\omega_3}{\omega_2^2} = \left( \frac{\omega}{\omega_2} \right)^3, \quad \text{with} \quad \omega_3 \geq \omega_2 \geq \omega_1. \tag{6}
\]

FIG. 1. Critical constant \( k = N_c|a|(m\omega_3/\hbar)^{1/2} \), calculated for an arbitrary \( \omega_3 \geq \omega_2 \geq \omega_1 \). The ratio \( \omega_3/\omega_1 \) is shown below each corresponding curve. The dotted-lines correspond to cylindrical (\( \eta = 1 \)) and deformed cylindrical (\( \eta \), 0.459 ± 0.012 (statistical) ±0.054 (systematic). In Ref. [22], assuming the cylindrical symmetry \( \omega_1 = 2\pi \times 6.80 \) Hz \( \omega_2 = \omega_3 = 2\pi \times 17.35 \) Hz, it was obtained \( k = 0.55 \), a value about 4% lower than \( k_s \).

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We show several curves in which we kept constant the ratio \( \omega_3/\omega_1 \) (solid-lines). The values of \( \omega_3/\omega_1 \) are indicated inside the figure, just below the corresponding plot. The dashed and dotted-lines correspond to cylindrical \((\eta = 1)\) and deformed cylindrical \((\eta = 1.144)\) symmetries for the trap, where \( \eta \) is the deformation parameter, as it will be explained. In the left-hand-side (lhs) of these plots we have \( \omega_3 = \eta \omega_2 > \omega_1 \) (cigar-shape); and, in the right-hand-side, \( \omega_3 > \omega_2 = \eta \omega_1 \) (pancake-shape). \( k \) can be determined for any symmetry that was not shown, by interpolating the already given results. The results for the complete non-symmetric case are consistent with the previously obtained values in cylindrical symmetry \([12]\). The maximum value for the critical number \( k \) is obtained for the spherically symmetric case \((\omega_1 = \omega_2 = \omega_3)\).

As already observed, Fig. 1 includes previous calculations in the limit of the quasi 1D (cigar-shape) and quasi 2D (pancake-shape) symmetries (see dashed-line). However, for the sake of comparison with previous results obtained by several authors, we also present in Fig. 2 the cylindrical pancake-type \((\omega_\perp = \omega_1 = \omega_2 < < \omega_3)\) and cigar-type \((\omega_\perp = \omega_3 = \omega_2 > \omega_1)\) results. In Fig. 2, for cylindrical geometries, we compare our exact results, for \( k_3 = N_c |a| (m\omega_3/\hbar)^{1/2} \) as a function of \( \lambda \), with the corresponding variational ones of Refs. \([7,15]\). The variational results (dashed-lines) are consistently a bit higher than the exact ones. For \( \lambda \to 0 \) \((\omega_1 < < \omega_2 = \omega_3 = \omega_\perp)\), the exact and variational results for the critical constant are \( N_c |a| (m\omega_3/\hbar)^{1/2} = 0.676 \) and 0.776, respectively. They are consistent with the quasi-1D limits given in Refs. \([12,16]\). When \( \omega_3 > > \omega_2 = \omega_1 \), the variational 2D limit \( \sqrt{\pi/2} \) of Ref. \([1]\) is comparable with our exact result \( k_3 = 0.931 \sqrt{\pi/2} \). In this case, the quasi-2D limit coincide with the true 2D limit \([23,13,22,26]\).

![Graph showing the relationship between \( k_3 \) and \( \lambda \) for different \( \omega_3/\omega_1 \) ratios (solid and dotted lines)].

Considering the present analysis, we observe that \( N_c \) in a cigar-like (quasi-1D) trap is smaller than \( N_c \) in a pancake-like (quasi-2D) trap. And, as we deform a cigar-like trap, \( N_c \) also increases. We need to clarify this matter, which is the subject of the next four paragraphs, because such result is apparently contradicting a remark made in Ref. \([16]\), saying that “the cigar-shaped trap is the optimal one”.

As shown in Ref. \([12]\) and also in the present calculation, in a deformed cylindrical symmetry, the cigar shape (with one of the frequencies smaller than the other two) is more favorable to obtain a larger value of \( k \) than the pancake-shape symmetry (with one of the frequencies larger than the other two). See, for example, in Fig. 1, the two extreme points of the curve with \( 2\omega_3/\omega_1 = 100 \). This results from the definition of \( k \), Eq. \([7]\), in terms of the averaged oscillator length \( l_0 \). However, the maximum value of \( k \) can only be directly related with the maximum value of \( N_c \) in case that \( \omega \) is kept fixed. And, with \( l_0 \) fixed, \( N_c \) is maximized for \( \lambda = 1 \), corresponding to the spherically symmetric case \((k = k_3)\). If we fix \( l_0 \) and \( \omega_3/\omega_1 \), \( N_c \) is maximized for a deformed cylindrical symmetry with \( \lambda < 1 \), as one can see from Fig. 1.

Considering exact cylindrical traps, by exchanging the frequencies (which, obviously, does not keep constant the averaged frequency \( \omega \)), it is valid the following ratio that was obtained in Ref. \([12]\):

\[
R(\lambda) \equiv \frac{N_c(\lambda)}{N_c(1/\lambda)} = \lambda^{1/6} \frac{k(\lambda)}{k(1/\lambda)} \quad (7)
\]

This result favors the pancake-like symmetry \((\lambda = \omega_3/\omega_1 = \omega_3/\omega_\perp > 1)\), to obtain a larger value for \( N_c \). Consider, for example, a cylindrical pancake-type trap with \( \lambda = 100 \), in comparison with a cigar-type trap with \( \lambda = 1/100 \). We notice that, in this case, \( R(\lambda = 100) \approx 1.6 \), implying that with such pancake-like trap \((\omega_3 = 100\omega_\perp)\) one can obtain about 60% more particles than with the corresponding cigar-like trap \((\omega_3 = \omega_\perp = 100\omega_1)\). Let us consider the recent experiment with quasi-1D (cigar-like) trap used in the formation and propagation of matter wave solitons, with \(^7\)Li \([4]\). In this case, it was used axial and radial frequencies, respectively, equal to 3.2 Hz and \( \sim 625 \) Hz \([22,23]\) or, \( \omega_\perp = \omega_3 = 2\pi \times 625 \) Hz, \( \omega_1 = 2\pi \times 3.2 \) Hz and \( \lambda = \omega_1/\omega_3 = 0.00513 \). So, as shown in Fig.2, we are practically in the limit \( \lambda = 0 \), which gives \( N_c^{1D}[a]/\sqrt{\hbar/(m\omega_\perp)} \approx 0.675 \). Considering that the scattering length was tuned to \( a = -3a_0 \) \((a_0\) is the Bohr radius), the maximum number of atoms in this quasi-1D trap is \( N_c^{1D} \approx 6400 \). If we exchange the radial and axial frequencies in this experiment, going from a cigar-like to a pancake-like trap, \( \omega_\perp = 2\pi \times 3.2 \) Hz, \( \omega_3 = 2\pi \times 625 \) Hz and \( \lambda = \omega_1/\omega_3 = 195.3 \). In this case, \( N_c^{2D}[a]/\sqrt{\hbar/(m\omega_3)} \approx 1.12 \). So, the critical number in the quasi-2D limit is about 60% larger than the corresponding number of atoms in the quasi-1D limit \( N_c^{1D} \approx 6400 \).

The discussion about the best way to distribute the frequencies to obtain the maximum number of atoms was first considered in Ref. \([6]\), arriving that the best is to do a spherical trap, for achieving maximum density. (In
their almost spherical trap they have obtained from \( \sim 600 \) to \( \sim 1300 \) atoms, in an overall agreement with theoretical predictions [2] (with \( \eta \) such that we still have \( \omega_2 >> \omega_1 \)). The 1D solid line given in Fig.2 is also applied to deformed cigar-shaped symmetries if we replace \( k_3 \) by \( k_3\eta^{-1/4} \) in the \( y \)-axis. This result may be relevant for deformed waveguide propagation as one can deform the cigar-type symmetry and control the collapsing condition. From Eq. (3) we observe that the maximum critical number \( N_c \) will increase when deforming the cigar-like symmetry by a factor proportional to \( (\omega_3/\omega_2)^{1/4} \).

Now, let us see the effect of deformation in the same example of the cigar-shaped geometry used in Ref. [1], with \( ^7 \)Li gas. We use the same value of \( a = -3a_0 \), with \( \omega_3 = 2\pi \times 625 \) s\(^{-1} \), and take \( \omega_2 = \omega_3/\eta \). As given in Eq. (8), we go from \( N_c = 6392 \) (\( \eta = 1 \)) to \( N_c = 6970 \) (\( \eta = \sqrt{2} \)) or \( N_c = 7601 \) (\( \eta = 2 \)). It means, an increase of \( \sim 9\% \) when \( \eta = \sqrt{2} \); and \( \sim 19\% \) when \( \eta = 2 \). In case, \( \eta > 1 \), the approximation considered in the wave-function separation, as given in [1], is not valid. In such case we are reaching the other deformed pancake-like symmetry, where \( \omega_3 >> \omega_2 \sim \omega_1 \). However, in the pancake geometry, the effect of deformation in \( N_c \) is negligible. By comparing the quasi pancake-like geometry with the quasi cigar-like geometry, the number \( N_c \) in the cigar-like geometry is much more sensitive to deformations.

We have also studied the behavior of the root mean square radius for the case \( \omega_3 = \sqrt{2} \omega_2 = 2\omega_1 \). We verified that, as the system approaches the critical point (or collapse), the wave function tends to be more “spherical”,

\[
N_c|a|\left(\frac{m\sqrt{\omega_2\omega_3}}{\hbar}\right)^{1/2} = \frac{N_c|a|}{\eta^{1/4}} \sqrt{\frac{m\omega_3}{\hbar}} = 0.676. \tag{8}
\]

This generalizes the cigar-shape quasi-1D results of [14] to the \( \eta \)-dependence for any number of particles.
confirming earlier conclusion made with a Gaussian variational approximation [30]. In Fig. 3, we show the corresponding results, for the three components of the mean-square-radius, \( \langle r_i^2 \rangle = \frac{\hbar^2}{2m} \langle x_i^2 \rangle \) \( (i = 1, 2, 3) \). As shown, when \( N = 0 \), we have \( \langle r_1^2 \rangle / \langle r_2^2 \rangle = \langle r_2^2 \rangle / \langle r_3^2 \rangle = \sqrt{2} \); and, when \( N \approx N_c \) such ratio is drastically reduced.

In summary, we have calculated systematically the critical number of particles, in systems that have negative two-body interactions, for traps with arbitrary geometries. The maximum critical number of particles, in systems that have negative two-body interactions, for traps with arbitrary geometries, is again pancake-like. We show that the trap. The results are shown in Figs. 1 and 2. The value of \( k \), for any symmetry non explicitly given, can be easily derived from Fig. 1, by interpolation. It is also pointed out that the results shown in Fig. 2, in the 1D cigar-like case, can be extended for slightly deformed cylindrical symmetries, by replacing the \( y \)-axis label \( k_3 \) by \( k_3 \eta^{-1/4} \).

Our main results in the present work are: (i) The maximum number of particles, \( N_c \), for arbitrary 3D trap geometries is given through the results shown in Fig.1. (ii) The optimal trap configuration, to avoid the collapse with minimum \( N_c \), is found to be strongly dependent on the constraints of the frequencies of the trap. If we initially fix one of the frequencies, the best configuration of the trap is pancake-like, with the other two frequencies going to zero. Analogously, if we initially fix two equal frequencies, the best configuration of the trap is cigar-like, with the third frequency close to zero. If we initially fix two different frequencies and try to vary the third frequency between the fixed ones, the best configuration is again pancake-like. We show that \( N_c \) is much more sensitive to deformations of the trap in a cigar-like geometry than in a pancake-like geometry. Finally, for small deformations \( \eta \) of the cigar-like traps, where \( \eta \geq 1 \), releasing the longitudinal direction, the solitonic solutions, obtained in Ref. [16], will be rescaled by the deformation. \( N_c \) will be rescaled by a factor \( \eta^{1/4} \), generalizing the findings of Ref. [16].

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