Bosons in a toroidal trap: Ground state and vortices

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We study the Bose-Einstein condensate (BEC) in a three-dimensional toroidal sombrero-shaped trap. By changing the parameters of the potential, or the number of bosons, it is possible to modify strongly the density profile of the BEC. We consider the ground-state properties for positive and negative scattering length and calculate the spectrum elementary excitations. We also discuss the macroscopic phase coherence and superfluidity of the BEC by analyzing vortex states and their stability. [S1050-2947(99)06804-3]

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I. INTRODUCTION

Recent spectacular experiments with alkali-metal vapors ^{87}Rb,^{23}Na, and ^{7}Li confined in magnetic traps and cooled down to a temperature of the order of 100 nK [1–3] have renewed the interest in the Bose-Einstein condensation. Theoretical studies of the Bose-Einstein condensate (BEC) in harmonic traps have been performed for the ground state [4–7], collective low-energy surface excitations [8,9], and vortex states [6]. The presence of vortex states is a signature of the macroscopic phase coherence of the system (the existence of a macroscopic quantum phase has been recently demonstrated [10]). Moreover, vortices are important to characterize the superfluid properties of Bose systems [11]. It has been found that the BEC in monotonically increasing potentials cannot support stable vortices in the absence of an externally imposed rotation [12]. Instead, stable vortices of Bose condensates can be obtained in one-dimensional (1D) [13] and quasi-2D [14] toroidal traps: such Bose condensates are superfluid [11].

In this paper we study a 3D toroidal trap given by a quartic sombrero potential along the cylindrical radius and a harmonic potential along the z axis. The resulting trapping potential is very flexible and it is possible to modify considerably the density profile of the BEC by changing the parameters of the potential or the number of bosons. We analyze the ground-state properties and the vortex stability of the condensate for both positive and negative scattering length and calculate also the spectrum of the Bogoliubov elementary excitations. In particular, we consider ^{87}Rb and ^{7}Li atoms.

The Gross-Pitaevskii energy functional [15] of the BEC reads

$$\frac{E}{N}=\int d^3\mathbf{r}\frac{\hbar^2}{2m}|\nabla\Psi(\mathbf{r})|^2+V_0(\mathbf{r})|\Psi(\mathbf{r})|^2+\frac{gN}{2}|\Psi(\mathbf{r})|^4, \tag{1}$$

where $\Psi(\mathbf{r})$ is the wave function of the condensate normalized to unity, $V_0(\mathbf{r})$ is the external potential of the trap, and the interatomic potential is represented by a local pseudopotential so that $g=4\pi\hbar^2 a_s/m$ is the scattering amplitude (a_s is the s-wave scattering length). N is the number of bosons of the condensate and m is the atomic mass. The scattering length a_s is supposed to be positive for ^{87}Rb and ^{23}Na, but negative for ^{7}Li. It means that for ^{87}Rb and ^{23}Na the interatomic interaction is repulsive while for ^{7}Li the atom-atom interaction is effectively attractive. The extremum condition for the energy functional gives the Gross-Pitaevskii (GP) equation [15]

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V_0(\mathbf{r})+gN|\Psi(\mathbf{r})|^2\right)\Psi(\mathbf{r})=\mu\Psi(\mathbf{r}), \tag{2}$$

where μ is the chemical potential. This equation has the form of a nonlinear stationary Schrödinger equation.

We study the BEC in an external sombrero potential with cylindrical symmetry, which is given by

$$V_0(\mathbf{r})=\frac{\lambda}{4}(\rho^2-\rho_0^2)^2+\frac{m\omega_z^2}{2}z^2, \tag{3}$$

where $\rho=\sqrt{x^2+y^2}$ and z are the cylindrical coordinates. This potential is harmonic along the z axis and quartic along the cylindrical radius ρ. $V_0(\mathbf{r})$ is minimum along the circle of radius $\rho=\rho_0$ at $z=0$ and $V_0(\mathbf{r})$ has a local maximum at the origin in the (x,y) plane. Small oscillations in the (x,y) plane around ρ_0 have a frequency $\omega_\perp=\rho_0(2\lambda/m)^{1/2}$.

First, let us consider the Thomas-Fermi (TF) approximation: i.e., neglect the kinetic energy. It is easy to show that the kinetic energy is negligible if $N\gg(\hbar^2/2m)(\lambda\rho_0^2+m\omega_z^2/2)/\mu_0^2$, where $\mu_0=(2/\pi^2)(\lambda/4)^{1/4}(m\omega_z^2/2)^{1/4}g^{1/2}$ is the bare chemical potential. This condition is satisfied for $\lambda^2\rho_0^8\gg 16\hbar^2(\lambda\rho_0^2+m\omega_z^2/2)/(2m)$. In the TF approximation we have

$$\Psi(\mathbf{r})=\left(\frac{1}{gN}[\mu-V_0(\mathbf{r})]\right)^{1/2}\Theta[\mu-V_0(\mathbf{r})], \tag{4}$$

where $\Theta(x)$ is the step function. For our system we obtain that (a) the wave function has its maximum value at $\rho=\rho_0$

and $z=0$; (b) for $\mu<\lambda\rho_0^4/4$ the wave function has a toroidal shape; (c) for $\mu>\lambda\rho_0^4/4$ the wave function has a local minimum at $\rho=z=0$; (d) the chemical potential scales as $\mu \sim \mu_0 N^{1/2}$. It is important to note that the TF approximation neglects tunneling effects: to include these processes, it is necessary to analyze the full GP problem.

II. GROUND-STATE PROPERTIES AND ELEMENTARY EXCITATIONS

We perform the numerical minimization of the GP functional by using the steepest descent method [16]. It consists of projecting onto the minimum of the functional an initial trial state by propagating it in imaginary time. In practice one chooses a time step $\Delta\tau$ and iterates the equation

$$\Psi(\mathbf{r},\tau+\Delta\tau)=\Psi(\mathbf{r},\tau)-\Delta\tau\hat{H}\Psi(\mathbf{r},\tau) \tag{5}$$

by normalizing Ψ to 1 at each iteration.

We discretize the space with a grid of points taking advantage of the cylindrical symmetry of the problem. At each time step the matrix elements entering the Hamiltonian are evaluated by means of finite-difference approximants. We use grids up to 200×200 points verifying that the results do not depend on the discretization parameters. The number of iterations in imaginary time depends on the degree of convergence required and the goodness of the initial trial wave function. We found that strict convergence criteria have to be required on the wave function in order to obtain accurate estimates of the wave function.

In our calculations we use the z-harmonic oscillator units. We write ρ_0 in units $a_z=[\hbar/(m\omega_z)]^{1/2}=1$ μm, λ in units $(\hbar\omega_z)a_z^{-4}=0.477(5.92)$ peV/μm^4, and the energy in units $\hbar\omega_z=0.477(5.92)$ peV for ^{87}Rb(^{7}Li). Moreover, we use the following values for the scattering length: $a_s=50$ (-13) Å for ^{87}Rb(^{7}Li) [1,3].

We have to distinguish two possibilities: positive or negative scattering length. In the case of positive scattering length we can control the density profile of the BEC by modifying the parameters of the potential and also the number of particles. In Fig. 1 we show the ground-state density profile of the ^{87}Rb condensate for several numbers of atoms. For a small number of particles the condensate is essentially confined along the minimum of $V_0(\mathbf{r})$; there is a very small probability of finding particles in the center of the trap so that the system is effectively multiply connected. As N increases, the center of the trap starts to fill up and the system becomes simply connected. The value of N for which there is a crossover between the two regimes increases with the value of λ and of ρ_0 and, within the Thomas-Fermi (TF) approximation, scales like $\lambda^{3/2}\rho_0^8$. In Table I we show the energy per particle, the chemical potential, and the average transverse and vertical size for the trapping potential characterized by the parameters $\rho_0=2$ and $\lambda=4$ in the z-harmonic oscillator units. As expected, the energy per particle and the chemical potential grow by increasing the number of particles but they do not scale as $N^{1/2}$ because, with this trapping potential, the TF approximation is valid for $N\gg10^4$. It is instead interesting to observe that $\sqrt{\langle x^2\rangle}=\sqrt{\langle y^2\rangle}$ grows less than $\sqrt{\langle z^2\rangle}$ due to the presence of a steep (quartic) potential along the transverse direction $\rho=\sqrt{x^2+y^2}$ and a softer (quadratic) barrier along the vertical direction z.

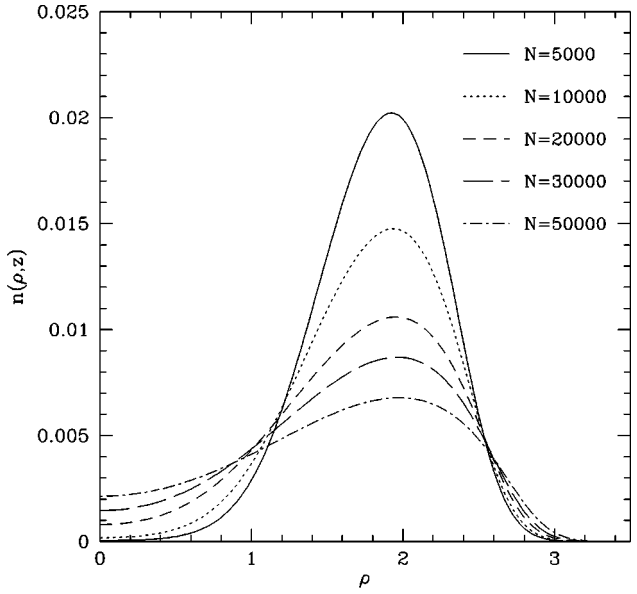

FIG. 1. Particle probability density in the ground state of ^{87}Rb atoms as a function of the cylindrical radius at $z=0$ (symmetry plane). The curves correspond to different numbers of atoms: from 5000 to 50 000. Parameters of the external potential: $\rho_0=2$ and $\lambda=4$. Lengths are in units of $a_z=1$ μm and λ in units of $(\hbar\omega_z)a_z^{-4}=0.477$ peV/μm^4.

In the case of negative scattering length, it is well known that for the BEC in harmonic potential there is a critical number of bosons N_c, beyond which there is the collapse of the wave function [7]. We obtain the same qualitative behavior for the ^{7}Li condensate in our sombrero potential. However, in cylindrical symmetry, the collapse occurs along the line which characterizes the minima of the external potential, i.e., at $\rho=\rho_0$ and $z=0$. The numerical results are shown in Fig. 2. We notice that, for a fixed ρ_0, the critical number of bosons N_c is only weakly dependent on the height of the barrier of the Sombrero potential. These results suggest that we cannot use toroidal traps to significantly enhance the metastability of the BEC with negative scattering length.

To calculate the energy and wave function of the elementary excitations, one must solve the so-called Bogoliubov–de Gennes (BdG) equations [18,19]. The BdG equations can be obtained from the linearized time-dependent GP equation.

TABLE I. Ground state of ^{87}Rb atoms in the toroidal trap with $\rho_0=2$ and $\lambda=4$. Chemical potential and energy are in units of $\hbar\omega_z=0.477$ peV($\omega_z=0.729$ kHz). Lengths are in units of $a_z=1$ μm.

N	E/N	μ	$\sqrt{\langle\rho^2\rangle}$	$\sqrt{\langle z^2\rangle}$
5000	5.85	7.71	1.96	1.41
10000	7.45	10.26	1.97	1.70
20000	9.84	14.00	1.97	2.05
30000	11.73	16.94	1.97	2.29
40000	13.36	19.47	1.98	2.48
50000	14.81	21.74	1.99	2.63

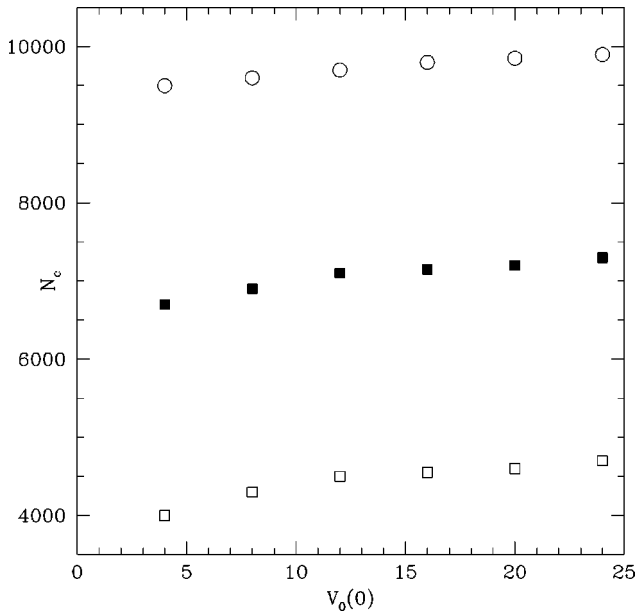

FIG. 2. Critical number N_c of ^{7}Li atoms vs the potential barrier at the origin: $V_0(0)=\lambda\rho_0^4/4$. Open squares, $\rho_0=2$; full squares, $\rho_0=3$; open circles, $\rho_0=4$. Energy is in units of $\hbar\omega_z=5.92$ peV($\omega_z=9.03$ kHz) and length in units of $a_z=1$ μm.

Namely, one can look for zero angular momentum solutions of the form

$$\Psi(\mathbf{r},t)=e^{-(i/\hbar)\mu t}[\psi(\rho,z)+u(\rho,z)e^{-i\omega t}+v^*(\rho,z)e^{i\omega t}], \tag{6}$$

corresponding to small oscillations of the wave function around the ground-state solution ψ. By keeping terms linear in the complex functions u and v, one finds the following BdG equations:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{\partial^2}{\partial z^2}\right)+V_0(\rho,z)-\mu+2gN\left|\psi(\rho,z)\right|^2\right]u(\rho,z)+gN|\psi(\rho,z)|^2v(\rho,z)=\hbar\omega u(\rho,z), \tag{7}$$

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{\partial^2}{\partial z^2}\right)+V_0(\rho,z)-\mu+2gN\left|\psi(\rho,z)\right|^2\right]v(\rho,z)+gN|\psi(\rho,z)|^2u(\rho,z)=-\hbar\omega v(\rho,z). \tag{8}$$

The BdG equations allow one to calculate the eigenfrequencies ω and hence the energies $\hbar\omega$ of the elementary excitations. This procedure is equivalent to the diagonalization of the N-body Hamiltonian of the system in the Bogoliubov approximation [17]. The excitations can be classified according to their parity with respect to the symmetry $z\rightarrow -z$.

We have solved the two BdG eigenvalue equations by finite-difference discretization with a lattice of 40×40 points in the (ρ,z) plane. In this way, the eigenvalue problem reduces to the diagonalization of a 3200×3200 real matrix.

TABLE II. Lowest elementary excitations of the Bogoliubov spectrum for the ground state of ^{87}Rb atoms in the toroidal trap with $\rho_0=2$ and $\lambda=4$. Units are as in Table I.

N	$\hbar\omega_1$	$\hbar\omega_2$	$\hbar\omega_3$	$\hbar\omega_4$
1	1.00	1.98	2.97	3.96
5000	1.00	1.70	2.43	3.19
10000	1.00	1.68	2.37	3.08
20000	1.00	1.66	2.32	3.00
30000	1.00	1.66	2.30	2.96
40000	1.00	1.66	2.30	2.95
50000	1.00	1.66	2.30	2.95

We have tested our program in simple models by comparing numerical results with the analytical solution and verified that a 40×40 mesh already gives reliable results for the lowest part of the spectrum. In Table II we show the lowest elementary excitations of the Bogoliubov spectrum for the ground state of the system. One observes the presence of an odd collective excitation at energy quite close to $\hbar\omega=1$ (in units $\hbar\omega_z$). This mode is related to the oscillations of the center of mass of the condensate which, due to the harmonic confinement along the z-axis, is an exact eigenmode of the problem characterized by the frequency ω_z, independently of the strength of the interaction. For large N the lowest elementary excitations saturate, suggesting that the Thomas-Fermi asymptotic limit is reached.

In the case of negative scattering length we verified that, quite close to the critical number of bosons N_c, an even mode softens driving the transition towards a collapsed state.

III. VORTICES AND THEIR METASTABILITY

Let us consider states having a vortex line along the z axis and all bosons flowing around it with quantized circulation. The observation of these states would be a signature of macroscopic phase coherence of trapped BEC. The axially symmetric condensate wave function can be written as

$$\Psi_k(\mathbf{r})=\psi_k(\rho,z)e^{ik\theta}, \tag{9}$$

where θ is the angle around the z axis and k is the integer quantum number of circulation. The resulting GP functional (1), representing the energy per particle, can be written in terms of $\psi_k(\mathbf{r})$ by taking advantage of the cylindrical symmetry of the problem:

$$\frac{E}{N}=\int\rho d\rho dz d\theta\frac{\hbar^2}{2m}\left(\left|\frac{\partial\psi_k(\rho,z)}{\partial\rho}\right|^2+\left|\frac{\partial\psi_k(\rho,z)}{\partial z}\right|^2\right)+\left(\frac{\hbar^2k^2}{2m\rho^2}+V_0(\rho,z)\right)|\psi_k(\rho,z)|^2+\frac{gN}{2}|\psi_k(\rho,z)|^4. \tag{10}$$

Due to the presence of the centrifugal term, the solution of this equation for $k\neq 0$ has to vanish on the z axis providing a signature of the vortex state.

Vortex states are important to characterize the macroscopic quantum phase coherence and also superfluid properties of Bose systems [11]. It is easy to calculate the critical

TABLE III. Vortex states and excitation energies of ^{87}Rb atoms with $k=1$ in the toroidal trap with $\rho_0=2$ and $\lambda=4$ within the Hartree-Fock approximation. Units are as in Table I.

N	E_1/N	μ_1	ϵ	$\hbar\Omega_c$
5000	6.00	7.87	9.56	0.15
10000	7.61	10.44	12.46	0.16
20000	10.02	14.22	16.60	0.18
30000	11.93	17.20	19.80	0.20
40000	13.57	19.75	22.54	0.21
50000	15.04	22.04	25.09	0.23

frequency Ω_c at which a vortex can be produced. One has to compare the energy of a vortex state in a frame rotating with angular frequency Ω, that is $E-\Omega L_z$, with the energy of the ground state with no vortices. Since the angular momentum per particle is $\hbar k$, the critical frequency is given by $\hbar\Omega_c=(E_k/N-E_0/N)/k$, where E_k/N is the energy per particle of the vortex with quantum number k. In Table III we show some results for vortices of ^{87}Rb. The critical frequency turns out to increase slightly with the number of atoms. This corresponds to a moderate lowering of the momentum of inertia per unit mass of the condensate when N grows.

For ^{7}Li we calculate the critical number N_c of bosons for which there is the collapse of the vortex wave function. We find that N_c has a rather weak dependence on the quantum number of circulation k. Note that, in the case of a harmonic external potential, there is an enhancement of N_c by increasing k because in that case rotation strongly reduces the density in the neighborhood of the origin, where the external potential has its minimum [6].

Once a vortex has been produced, the BEC is superfluid if the circulating flow persists, in a metastable state, in the absence of an externally imposed rotation [11]. As discussed previously, vortex solutions centered in harmonic traps have been found [6], but such states turn out to be unstable to single-particle excitations out of the condensate. To study the metastability of the vortex we first analyze the following Hartree-Fock equation [12]:

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V_0(\mathbf{r})+2gN\left|\psi_k(\mathbf{r})\right|^2\right)\phi(\mathbf{r})=\epsilon\phi(\mathbf{r}), \quad (11)$$

which describes, in the weak coupling limit, one particle transferred from the vortex state $\Psi_k(\mathbf{r})$ to an orthogonal single-particle state $\phi(\mathbf{r})$. Quasiparticle motion is governed by an effective Hartree potential $v_{\rm eff}(\mathbf{r})=V_0(\mathbf{r})+2g|\psi_k(\mathbf{r})|^2$, which combines the effects of the trap with a mean repulsion by the condensate. Figure 3 shows $v_{\rm eff}(\rho,z)$ for $N=5000$ and 50 000. The repulsion induced by the underlying condensate is quite evident near $\rho=\rho_0$. Let μ_k be the chemical potential of the vortex state characterized by a circulation quantum number k, then the vortex is metastable if $\epsilon>\mu_k$ and unstable if $\epsilon<\mu_k$ [12]. As shown in Table III, for our 3D system all the studied vortices are metastable and so the BEC can support persistent currents, thus it is superfluid. Contrary to what may be inferred by means of semiclassical arguments [12], the wave function describing the excitation $\phi(\mathbf{r})$ is not localized near the symmetry axis even for rather large numbers of atoms. A bound state at $\rho=z=0$ should pay a large kinetic energy cost due to the strong localization of the particle induced by the effective potential. Instead, it is more convenient to place the excited particle on top of the Bose condensate, i.e., at $\rho=\rho_0$ and $z\neq 0$ as shown in Fig. 4.

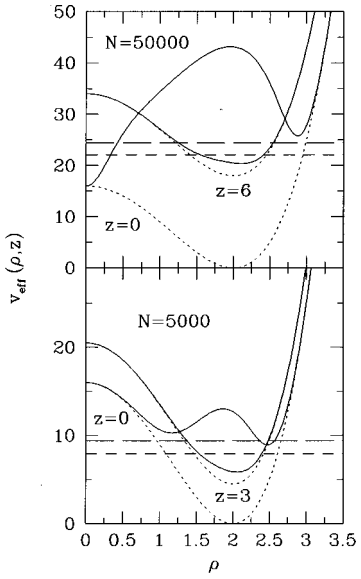

FIG. 3. Effective potential $v_{\rm eff}(\rho,z)$ appearing in the eigenvalue equation for the single-particle excitation Eq. (8). Two sections at $z=0$ and $z=3(z=6)$ are shown for $N=5000$ ($N=50\,000$) atoms in panel (a) [(b)]. $z=0$ corresponds to the symmetry plane. The dotted line represents the external potential. The chemical potential of the vortex state is marked by a short dashed line, the excitation energy by a long dashed line. Parameters of the external potential: $\rho_0=2$ and $\lambda=4$. Units as in Fig. 1 with $\hbar\omega_z=0.477$ peV($\omega_z=0.729$ kHz).

It is well known that the Hartree-Fock approximation describes only single-particle excitations [17]. To have the

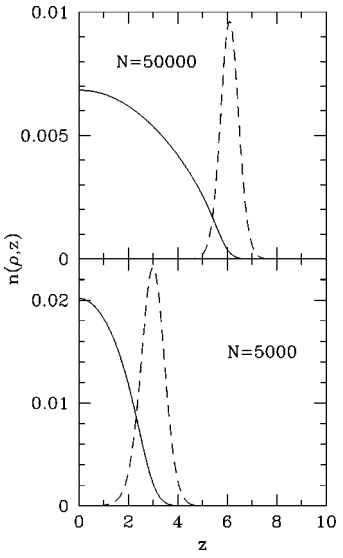

FIG. 4. Particle probability density of the $k=1$ vortex state (solid line) and square of the excitation wave function (dashed line) at the radial distance $\rho=\rho_0=2$, i.e., where both the wave functions peak. Curves are for $N=5000$ ($N=50\,000$) atoms in panel (a) [(b)]. Units and parameters as in Fig. 3.

TABLE IV. Bogoliubov vs Hartree-Fock lowest elementary excitation for a vortex state of ^{87}Rb atoms with $k=1$ in the toroidal trap with $\rho_0=2$ and $\lambda=4$. Units are as in Table I.

N	$\hbar\omega$	$\epsilon-\mu_1$
5000	1.22	1.69
10000	1.48	2.02
20000	1.73	2.38
30000	1.88	2.60
40000	1.99	2.79
50000	2.08	3.05

complete spectrum, including collective excitations, one must solve the BdG equations [18,19]. One must look for solutions of the form

$$\Psi_k(\mathbf{r},t)=e^{-(i/\hbar)\mu_k t}[\psi_k(\rho,z)e^{ik\theta}+u(\rho,z)e^{i(k+q)\theta} \times e^{-i\omega t}+v^*(\rho,z)e^{i(k-q)\theta}e^{i\omega t}]. \quad (12)$$

Here q represents the quantum number of circulation of the elementary excitation. We have solved the two BdG eigenvalue equations by finite-difference discretization using the same method described in Sec. II. We have checked that a 40×40 mesh gives the correct excitation energies within the Hartree-Fock approximation. Therefore, for the purpose of determining the stability of the vortex state, this rather coarse mesh is sufficiently accurate. The results are shown in Table IV: The lowest Bogoliubov excitation is positive and always lower than the lowest Hartree-Fock one. Moreover, by increasing the number of particles, their difference increases as expected for collective excitations. We have also verified that vortex states become unstable by strongly reducing either density (down to about one hundred bosons in our model trap) or scattering length.

Therefore, the behavior of the 3D trap we have analyzed closely resembles the simplified 1D model studied in Ref. [13], which represents the limit of a deep trapping potential. Also in that case the Bogoliubov approximation has been used to evaluate the spectrum of elementary excitations showing that vortices are stabilized by strong repulsive interparticle interactions (or equivalently by high density). The 1D model, however, should be taken with caution because other branches of low energy collective excitations are present in such low-dimensional systems [20].

IV. CONCLUSIONS

We have studied the Bose-Einstein condensate in a 3D toroidal trap given by a quartic sombrero potential along the cylindrical radius and a harmonic potential along the z axis. We have shown that it is possible to modify strongly the density profile of the condensate by changing the parameters of the potential or the number of bosons. The properties of the condensate and its elementary excitations have been analyzed for both positive and negative scattering length by considering ^{87}Rb and ^{7}Li atoms. For ^{7}Li, which has negative scattering length, we have calculated the critical number of atoms for which there is the collapse of the wave function. The results have shown that a toroidal trap does not enhance the metastability of the ground state of the condensate. On the other hand, in the case of a harmonic external potential, we have recently shown [21,22] that, when a realistic nonlocal (finite range) effective interaction is taken into account, a new stable branch of Bose condensate appears for ^{7}Li at higher density. Presumably a similar state can be found also in the presence of a toroidal external trap for a sufficiently large number of particles when nonlocality effects are included.

A superfluid is characterized by the presence of persistent currents in the absence of an externally imposed rotation. In order to investigate this peculiar sign of the macroscopic phase coherence of the condensate, we have also studied vortex states. Our results suggest that vortices can support persistent currents in 3D toroidal traps with fairly large numbers of atoms. This feature essentially depends on the toroidal geometry of the trap and should be independent of other details of the confining potential.

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