Bosons in anisotropic traps: Ground state and vortices

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We solve the Gross-Pitaevskii equations for a dilute atomic gas in a magnetic trap, modeled by an anisotropic harmonic potential. We evaluate the wave function and the energy of the Bose-Einstein condensate as a function of the particle number, both for positive and negative scattering length. The results for the transverse and the vertical size of the cloud of atoms, as well as for the kinetic and potential energy per particle, are compared with the predictions of approximated models. We also compare the aspect ratio of the velocity distribution with experimental estimates available for ^{87}Rb. Vortex states are considered and the critical angular velocity for production of vortices is calculated. We show that the presence of vortices significantly increases the stability of the condensate in the case of attractive interactions.

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I. INTRODUCTION

Recent experiments support the existence of a Bose-Einstein condensate in vapors of alkali atoms, such as rubidium [1], litium [2] and sodium [3], confined in magnetic traps and cooled down to temperature of the order of 100 nK. This important discovery opens new interesting perspectives in the field of many-body physics (for a comprehensive review on Bose-Einstein condensation see, for instance, Ref. [4]).

The vapors of alkali atoms used in the experiments are very dilute, i.e., the average distance among the atoms is much larger than the range of the interaction. So the physics is expected to be dominated by two-body collisions, well accounted for by the knowledge of the s-wave scattering length. This also implies that the Gross-Pitaevskii theory [5] for weakly interacting bosons finds in these systems an ideal field of application. This theory has been already used to describe bosons confined in isotropic traps [6–8]. The anisotropic case has been recently discussed by Baym and Pethick [9], who have obtained approximate analytic solutions, thereby providing a qualitative insight into many interesting features of these systems. To make the analysis more quantitative one has to solve numerically the Gross-Pitaevskii equations.

In the present work we provide a complete set of solutions of the Gross-Pitaevskii equations applied to N alkali atoms in anisotropic traps. We calculate the condensate wave function at $T=0$ for bosons interacting through positive and negative scattering lengths. We explore the N dependence of relevant quantities, such as energy, chemical potential, and the aspect ratio of the velocity distribution. We also discuss vortex states, studying the density profile and the critical angular velocity.

The results of the numerical minimization of the energy functional are compared with the analytic solution of the noninteracting anisotropic harmonic oscillator as well as with approximated models available when the interaction is strongly repulsive (strongly repulsive limit). For instance, we will show that the surface structure of the condensate wave function, for which a sound treatment of the kinetic energy is needed, is relevant in determining the aspect ratio. Our results for the aspect ratio in ^{87}Rb, with N of the order of a few thousands, are in agreement with the experimental findings of Ref. [1]. An accurate determination of the particle distribution in the vapor cloud is also relevant in order to calculate the moment of inertia of the system, which is directly connected with the superfluid behavior [10].

We find instabilities in the solutions for negative scattering length when the number of atoms exceeds certain critical values, of the order of 1400 for ^{7}Li, in agreement with a previous analysis [7]. However, we find also that the stability of these systems is significantly increased when vortex states are considered. This happens because the vortex flow pushes the atoms away from the center of the trap decreasing the highest value of the local density. For ^{7}Li we find minima of the Gross-Pitaevskii functional corresponding to vortex states with quantum of circulation higher than 1 and having N of the order of 10 000.

The paper is organized as follows. In Sec. II we present the formalism of the Gross-Pitaevskii theory for anisotropic traps and discuss the solutions in two limits (the noninteracting and the strongly repulsive limit). We also discuss the generalization of the theory to include vortex states. In Sec. III we briefly introduce the numerical procedure, which is based on the steepest descent method for functional minimization. In Sec. IV we present the results for the two cases of positive (^{87}Rb) and negative (^{7}Li) scattering length. Finally, in Sec. V we summarize the main results.

II. GROSS-PITAEVSKII THEORY FOR TRAPPED BOSONS

In the Gross-Pitaevskii theory [5] the ground-state energy for condensed bosons of mass m is given by the functional

$$E[\psi]=\int d\mathbf{r}\left[\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r})|^2+\frac{m}{2}(\omega_\perp^2x^2+\omega_\perp^2y^2+\omega_z^2z^2)|\psi(\mathbf{r})|^2+\frac{2\pi\hbar^2a}{m}|\psi(\mathbf{r})|^4\right], \quad (1)$$

where $\psi(\mathbf{r})$ is the condensate wave function (order parameter), $\omega_\perp$ and ω_z are the two angular frequencies associated

with the external potential of the anisotropic trap, and a is the s-wave scattering length. The wave function is assumed to be normalized to the number of atoms in the condensate

$$\int d\mathbf{r}\,|\psi(\mathbf{r})|^2 = N. \tag{2}$$

In the $T \to 0$ limit considered in this work, N coincides with the total number of atoms in the trap. The explicit form of the ground-state wave function is obtained by minimizing the energy functional. One can also write explicitly the variation of the energy functional at first order, finding the Euler-Lagrange equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{m}{2}(\omega_\perp^2 x^2 + \omega_\perp^2 y^2 + \omega_z^2 z^2) + \frac{4\pi\hbar^2 a}{m}|\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) = \mu\psi(\mathbf{r}), \tag{3}$$

where μ is the chemical potential. This equation has the form of a nonlinear stationary Schrödinger equation. It has been recently solved for bosons in isotropic harmonic traps by Edwards and Burnett [6], by means of iterated Runge-Kutta integrations. An efficient numerical calculation of the ground state, which works well also in the case of anisotropic traps with and without vortices, consists of minimizing directly the energy functional (1) with a steepest descent method, as we will show in Sec. III.

The Gross-Pitaevskii theory is expected to be accurate when the system is dilute. If ρ is the density of bosons, the parameter that measures the applicability of the theory is the product $a^3\rho$, which should be much less then 1. This condition is largely satisfied by the samples of alkali atoms used in the recent experiments [1,2]. For instance, the central density of 10 000 atoms of ^{87}Rb in the trap of Ref. [1] is expected to be of the order of 10^{12}–10^{13} cm^{-3}, which yields $a^3\rho \simeq 10^{-6}$ or less. Even in the experiment of Ref. [3] on sodium, where the number of atoms in the condensate is much larger, the quantity $a^3\rho$ remains very small ($\simeq 10^{-5}$). The theory is also accurate for dilute systems of bosons having negative scattering length. In this case, however, one has to take care of the possible instability induced by the attractive interaction when N is large. When the system collapses, a more accurate theory is required in order to include short-range effects.

To simplify the formalism one can choose a slightly different notation, taking advantage of the fact that all distances and energies in the calculation scale as the typical length and energy of the harmonic external potential. So we introduce the standard lengths

$$a_\perp = \left(\frac{\hbar}{m\omega_\perp}\right)^{1/2}, \quad a_z = \left(\frac{\hbar}{m\omega_z}\right)^{1/2} \tag{4}$$

and we rescale the spatial coordinate, the energy, and the wave function as

$$\mathbf{r} = a_\perp \mathbf{r}_1, \tag{5}$$

$$E = \hbar\omega_\perp E_1, \tag{6}$$

$$\psi(\mathbf{r}) = \sqrt{N/a_\perp^3}\,\psi_1(\mathbf{r}_1). \tag{7}$$

The wave function ψ_1 is normalized to 1. Finally, we introduce the asymmetry parameter

$$\lambda = \omega_z/\omega_\perp \tag{8}$$

and define the quantity

$$u_1 = \frac{8\pi a N}{a_\perp}. \tag{9}$$

With these changes, the Gross-Pitaevskii energy functional takes the form

$$\frac{E_1}{N} = \int d\mathbf{r}_1 \left[|\nabla_1\psi_1(\mathbf{r}_1)|^2 + (x_1^2 + y_1^2 + \lambda^2 z_1^2)|\psi_1(\mathbf{r}_1)|^2 + \frac{u_1}{2}|\psi_1(\mathbf{r}_1)|^4 \right] \tag{10}$$

and the nonlinear Schrödinger equation becomes

$$[-\nabla_1^2 + x_1^2 + y_1^2 + \lambda^2 z_1^2 + u_1|\psi_1(\mathbf{r}_1)|^2]\psi_1(\mathbf{r}_1) = 2\mu_1\psi_1(\mathbf{r}_1), \tag{11}$$

where $\mu = \hbar\omega_\perp\mu_1$. The dimensionless quantity u_1, entering the left-hand side of Eq. (11), characterizes the effect of the interaction in the equation for the condensate. It is worth noting that even if the system is very dilute ($a^3\rho \ll 1$) the interactions can nevertheless play a crucial role in determining the solution of the Gross-Pitaevskii equations. In fact, the two conditions $a^3\rho \ll 1$ and $u_1 \simeq 1$ can be well satisfied for realistic values of the parameters of the problem, i.e., the scattering length, the oscillator frequencies, and the number of atoms in the trap. We now discuss briefly the two limiting cases of noninteracting particles and of strongly repulsive interactions, where the solution of Eq. (11) is available in an analytic way. We then show how the formalism can be extended to describe vortex states.

A. Noninteracting model

When the scattering length a vanishes, the problem reduces to the solution of the stationary Schrödinger equation for an anisotropic harmonic oscillator. The ground-state wave function is

$$\psi_1(\mathbf{r}_1) = \lambda^{1/4}\pi^{-3/4}\exp[-\tfrac{1}{2}(x_1^2 + y_1^2 + \lambda z_1^2)]. \tag{12}$$

The chemical potential coincides with the energy per particle, which turns out to be $(1+\lambda/2)$. The Gaussian has different transverse and vertical widths. In particular one has $\langle x_1^2\rangle = \langle y_1^2\rangle = 1/2$ and $\langle z_1^2\rangle = 1/(2\lambda)$. The mean values of the momentum operators p_x^2 and p_z^2 can also be easily calculated. In particular it is interesting to calculate the quantity

$$\sqrt{\langle p_z^2\rangle/\langle p_x^2\rangle} = \sqrt{\langle x_1^2\rangle/\langle z_1^2\rangle} = \sqrt{\lambda}. \tag{13}$$

In the following we consider the quantity $\sqrt{\langle p_z^2\rangle/\langle p_x^2\rangle}$ as a measure of the *aspect ratio*, which characterizes the anisotropy of the velocity distribution. This is a relevant quantity in the interpretation of the experimental results. Values of the

aspect ratio different from 1 reflect a peculiar and unique feature of Bose-Einstein condensation.

B. Strongly repulsive limit

The opposite limit is obtained when the interaction is so strong or the number of particles so large that the kinetic energy can be neglected in the energy functional. It corresponds to very large values of the parameter u_1 [see Eq. (9)]. This limit has been already discussed in Refs. [6,9]. The solution is easily obtained by dropping the kinetic energy term in Eq. (11). It has the form

$$\psi_1^2(\mathbf{r}_1)=\frac{1}{u_1}(2\mu_1-x_1^2-y_1^2-\lambda^2 z_1^2) \tag{14}$$

if the right-hand side is positive and $\psi_1=0$ elsewhere. The chemical potential is easily calculated by imposing the normalization condition $\int \psi_1^2 d\mathbf{r}_1=1$. One finds

$$2\mu_1=\left(\frac{15}{8\pi}\lambda u_1\right)^{2/5} \tag{15}$$

and $\mu=\hbar\omega_\perp\mu_1$. Using the definition of u_1 given in Eq. (9) and the relation $\mu=dE/dN$, one also gets the relationship $E/N=(5/7)\mu$. The cloud of atoms extends over a radius $R_1=\sqrt{2\mu_1}$ and a vertical size $Z_1=\lambda R_1$. One also finds the results

$$\langle x_1^2\rangle=\frac{2\mu_1}{7},\quad \langle z_1^2\rangle=\frac{2\mu_1}{7\lambda^2} \tag{16}$$

for the square radius $\langle x_1^2\rangle$ and $\langle z_1^2\rangle$. Due to the different scaling properties of the wave function with respect to the variable z [compare Eqs. (12) and (14)], the aspect ratio $\sqrt{\langle p_z^2\rangle/\langle p_x^2\rangle}$ in this case is equal to λ and not to $\sqrt{\lambda}$ as in the noninteracting case. The central density of the cloud is $\sqrt{2\mu_1/u_1}$. The wave function (14) is expected to approximate well the exact solution of the nonlinear Schrödinger equation (11) for large N, apart from the structure of the surface region where the exact wave function has to vanish smoothly. This fact has been already tested for isotropic traps in Ref. [6]. However, some relevant observables can be significantly affected by this surface structure even at large N, as we will see later.

C. Vortex states

The energy functional (10) is easily generalized to include vortex states. Indeed one of the primary motivations of the Gross-Pitaevskii theory was the study of vortex states in weakly interacting bosons [5]. Here we consider states having a vortex line along the z axis and all the atoms flowing around it with quantized circulation. One can write the axially symmetric condensate wave function in the form

$$\Psi(\mathbf{r})=\psi(\mathbf{r})\exp[iS(\mathbf{r})], \tag{17}$$

where $\psi(\mathbf{r})=\sqrt{\rho(\mathbf{r})}$ is the modulus, while the phase S acts as a velocity potential: $\mathbf{v}=(\hbar/m)\nabla S$. By choosing $S=\kappa\phi$, where ϕ is the angle around the z axis and κ is an integer, one has vortex states with tangential velocity

$$v=\frac{\hbar}{mr_\perp}\kappa, \tag{18}$$

with $r_\perp^2=x^2+y^2$. The number κ is the quantum of circulation and the angular momentum along z is $N\kappa\hbar$. Now, one has to put the complex wave function Ψ in place of ψ in the energy functional (1). Using the adimensional quantities defined in Eqs. (5)–(7) and $r_{1\perp}^2=x_1^2+y_1^2$, the resulting Gross-Pitaevskii functional becomes

$$\frac{E_1}{N}=\int d\mathbf{r}_1\Big[|\nabla_1\psi_1(\mathbf{r}_1)|^2+(\kappa^2 r_{1\perp}^{-2}+r_{1\perp}^2+\lambda^2 z_1^2)|\psi_1(\mathbf{r}_1)|^2 + \frac{u_1}{2}|\psi_1(\mathbf{r}_1)|^4\Big], \tag{19}$$

which differs from the functional (10) because of the centrifugal term. The corresponding nonlinear Schrödinger equation is

$$[-\nabla_1^2+\kappa^2 r_{1\perp}^{-2}+r_{1\perp}^2+\lambda^2 z_1^2+u_1|\psi_1(\mathbf{r}_1)|^2]\psi_1(\mathbf{r}_1) =2\mu_1\psi_1(\mathbf{r}_1). \tag{20}$$

Due to the presence of the centrifugal term, the solution of this equation for $\kappa\neq 0$ has to vanish on the z axis.

For noninteracting particles one falls again in the case of the stationary Schrödinger equation for the anisotropic harmonic potential. For instance, the $\kappa=1$ solution has the form

$$\psi_1(\mathbf{r}_1)\propto r_{1\perp}\exp[-\tfrac{1}{2}(r_{1\perp}^2+\lambda z_1^2)]. \tag{21}$$

The energy per particle of the $\kappa\neq 0$ states of the anisotropic harmonic oscillator is simply $\kappa\hbar\omega_\perp$ plus the ground-state energy. In our dimensionless notation $\mu_1=1+(\lambda/2)+\kappa$.

In the interacting case the kinetic energy cannot be neglected even for large N, since it determines the structure of the vortex core. In particular, the balance between the kinetic energy and the interaction energy fixes a typical distance over which the condensate wave function can heal. For a dilute Bose gas the *healing length* is given by [5]

$$\xi=(8\pi\rho a)^{-1/2}, \tag{22}$$

where ρ is the density of the system. In the case of a vortex it corresponds to the distance over which the wave function increases from zero, on the vortex axis, to the bulk density. For the trapped atoms in the $N\to\infty$ limit we have seen that the central density of the cloud is about $\sqrt{2\mu_1/u_1}$, where u_1 and μ_1 are given in Eqs. (9) and (15), so that the healing length (in units $a_\perp$) is $\xi_1\simeq(2\mu_1)^{-1/2}$. Since the radius R_1 of the cloud, in the same units, is of the order of $(2\mu_1)^{1/2}$, one has [9]

$$\frac{\xi_1}{R_1}=\frac{1}{2\mu_1}=\frac{1}{R_1^2} \tag{23}$$

or, equivalently,

$$\frac{\xi}{R}=\left(\frac{a_\perp}{R}\right)^2. \tag{24}$$

Thus the healing length is small compared with the size of the cloud if R is much larger than $a_\perp$.

Vortex states play an important role in characterizing the superfluid properties of Bose systems, as is well known in the case of superfluid helium [11]. The critical angular velocity required to produce vortex states is easily calculated once the energies of the states with and without vortices are known. One has to compare the energy of a vortex state in 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 $\kappa\hbar$, the critical angular velocity, in $\omega_\perp$ units, is

$$\Omega_c=\kappa^{-1}[(E_1/N)_\kappa-(E_1/N)_0]. \tag{25}$$

In the noninteracting case the difference of energy per particle is simply κ, so that $\Omega_c=1$; the critical angular velocity is just the angular frequency of the trap in the (x,y) plane.

III. NUMERICAL PROCEDURE

The main purpose of this work is the numerical minimization of the Gross-Pitaevskii functional (19) in order to calculate the properties of the ground state ($\kappa=0$) and of vortex states ($\kappa\neq 0$) for given values of the parameters $N,\lambda,a_\perp$, and a. A method of direct minimization is provided by the steepest descent approach. In brief, it consists of projecting onto the minimum of the functional an initial trial state by propagating it in imaginary time. A time-dependent wave function $\psi_1(\mathbf{r}_1,t)$, where t is a fictitious time variable, is evaluated at different time steps, starting from an arbitrary trial function and converging to the exact solution $\psi_1(\mathbf{r}_1,\infty)\equiv\psi_1(\mathbf{r}_1)$. The time evolution can be formulated in terms of the equation

$$\frac{\partial}{\partial t}\psi_1(\mathbf{r}_1,t)=-\frac{\bar{\delta}E_1/N}{\bar{\delta}\psi_1(\mathbf{r}_1,t)}, \tag{26}$$

where $\bar{\delta}$ indicates the constrained functional derivative that preserves the normalization. This equation defines a trajectory in the wave function space (and the fictitious time is just a label for different configurations) in which at each step one moves a little bit down the gradient $-\bar{\delta}E/\bar{\delta}\psi$. The constrained functional derivative is obtained by adding the normalization condition to the functional derivative

$$\frac{\delta E_1/N}{\delta\psi_1(\mathbf{r}_1,t)}=H\psi_1(\mathbf{r}_1,t), \tag{27}$$

where H depends nonlinearly on ψ_1. The end product is the self-consistent minimization of the energy, which corresponds to $(\partial\psi_1/\partial t)=0$ or, including the normalization, to the equation $H\psi_1=2\mu_1\psi_1$, which coincides with the nonlinear Schrödinger equation (20). In practice one chooses an arbitrary time step Δt and iterates the equation

$$\psi_1(\mathbf{r}_1,t+\Delta t)\simeq\psi_1(\mathbf{r}_1,t)-\Delta t\ H\psi_1(\mathbf{r}_1,t), \tag{28}$$

by normalizing ψ_1 to 1 at each iteration. The time step Δt controls the rate of convergence. Several methods have been proposed in the recent literature (see, for instance, Ref. [12] and references therein) to improve the steepest descent method of functional minimization; however, the Gross-Pitaevskii functional is much simpler than the typical functionals used in strongly correlated systems and the steepest descent method described above is efficient enough for our purposes.

In practice, one has to discretize the $(r_{1\perp},z)$ space with a two-dimensional grid of points, so that the wave function becomes a matrix. At each time step the matrix elements are changed as in Eq. (28), where the derivatives entering the Hamiltonian are evaluated by means of finite-difference formulas. The algorithm can be tested by comparing the results of the noninteracting case with the analytical solution of the anisotropic harmonic potential. In the interacting case, with large N, it is also possible to compare the numerical results with the analytic solution (14). Another test of accuracy is given by the virial theorem, which fixes rigorous relationships among the different contributions to the kinetic and the potential energy of the system at any value of N.

The system is sufficiently well described using a grid of 50×50 points in the range $0<r_{1\perp}<5$, and the same for z. The number of iterations in imaginary time depends on the degree of convergence required and the goodness of the initial trial wave function. The latter can be one of the two analytical limits already discussed, but the final results do not depend on the trial wave function. Typically we use 2000–10 000 iterations. Since the internal energy is a local functional, each iteration is very fast, so that the functional minimization takes no more than 2–3 min of CPU on a DEC-Alpha processor.

IV. RESULTS

A. Positive scattering length: ^{87}Rb

As an example of atoms with repulsive interaction we choose ^{87}Rb, as in the experiment of Ref. [1]. The s-wave triplet-spin scattering length is in the range $85a_0<a<140a_0$, where a_0 is the Bohr radius [13]. In our analysis we use $a=100a_0$. The asymmetry parameter of the experimental trap is $\lambda=\omega_z/\omega_\perp=\sqrt{8}$. The axial frequency $\omega_z/2\pi$ is taken to be 220 Hz [14]. The corresponding characteristic length is $a_\perp=1.222\times10^{-4}$ cm and the ratio between the scattering and the oscillator lengths is $a/a_\perp=4.33\times10^{-3}$.

We minimize the Gross-Pitaevskii functional in a wide range of particle number N. Results for the chemical potential and the energy per particle are shown in Table I. Both quantities are expressed in units of $\hbar\omega_\perp$ or of the equivalent temperature $\hbar\omega_\perp/k_B=3.73$ nK. The partial contributions to the energy per particle coming from the kinetic energy (kin), the harmonic oscillator potential (HO), and the internal potential energy (pot) are also given. The $N=1$ case coincides with the noninteracting anisotropic harmonic oscillator: in this case the internal potential energy vanishes, the kinetic energy and the harmonic oscillator potential energy are equal, and the chemical potential and the total energy per particle are both equal to the analytic value $(1+\lambda/2)=2.41$. When N increases the repulsion among atoms tends to lower the central density, expanding the cloud of atoms towards regions where the trapping potential is higher. This produces an increase of both the internal and the harmonic oscillator potential energy per particle. Conversely,

TABLE I. Results for the ground state of ^{87}Rb atoms in a trap with $\lambda=\sqrt{8}$. Chemical potential and energy are in units $\hbar\omega_\perp$, with $2\pi\omega_\perp=220$ Hz. Length is in units $a_\perp$.

N	μ_1	(E_1/N)	$(E_1/N)_{\rm kin}$	$(E_1/N)_{\rm HO}$	$(E_1/N)_{\rm pot}$	$\sqrt{\langle x_1^2\rangle}$	$\sqrt{\langle z_1^2\rangle}$
1	2.414	2.414	1.207	1.207	0.000	0.707	0.420
100	2.88	2.66	1.06	1.39	0.21	0.79	0.44
200	3.21	2.86	0.98	1.52	0.36	0.85	0.45
500	3.94	3.30	0.86	1.81	0.63	0.96	0.47
1000	4.77	3.84	0.76	2.15	0.93	1.08	0.50
2000	5.93	4.61	0.66	2.64	1.32	1.23	0.53
5000	8.14	6.12	0.54	3.57	2.02	1.47	0.59
10000	10.5	7.76	0.45	4.57	2.74	1.69	0.65
15000	12.2	8.98	0.41	5.31	3.26	1.84	0.70
20000	13.7	9.98	0.38	5.91	3.68	1.94	0.73

the kinetic energy per particle decreases because the density distribution is flattened. In the strongly repulsive limit, $N\to\infty$, one should find that the internal potential energy is much greater than the kinetic energy, which is the case discussed in Sec. II B. Indeed, the convergence towards this limit turns out to be rather slow. An approximate estimate of the kinetic energy per particle can be obtained, assuming the wave function to be a Gaussian, having a width of the order of the radius R of the cloud [9]. In this model the kinetic energy is of the order of $\hbar^2/(2mR^2)$, which is much smaller than the internal potential energy even for relatively small N. The discrepancy between the Gaussian approximation and the exact solution is well understood by looking at the effect of the surface structure of the cloud. In Fig. 1 we plot the profiles of the wave function along the x and the z axis for several values of N. The noninteracting case is shown as a dashed line. Increasing N, the central density is significantly lowered. The density in the cloud becomes almost flat and it is well approximated by the analytic solution (14), valid in the strongly repulsive limit. At the surface the wave function vanishes gradually, the typical decay length being almost independent of N. The contribution of the surface to the kinetic energy remains sizable even for large N, so that the kinetic energy is larger than the Gaussian estimate $\hbar^2/(2mR^2)$. A typical profile of the condensate wave function ψ_1 is plotted along the x axis for $N=5000$ in Fig. 2. The exact minimization of the Gross-Pitaevskii functional (solid line) is compared with the noninteracting case (dashed line) and the strongly repulsive limit (dot-dashed line).

Simple relationships among the different contributions to the total energy are obtained by means of the virial theorem. When applied to the anisotropic trap it gives the rigorous relation

$$\frac{\langle p_x^2\rangle}{2m}-\frac{m}{2}\omega_\perp\langle x^2\rangle+\frac{1}{2}E_{\rm pot}=0, \tag{29}$$

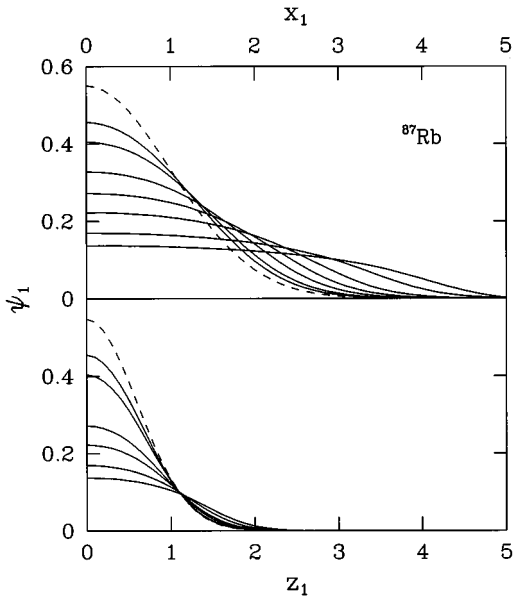

FIG. 1. Ground-state wave function for ^{87}Rb along the x axis (upper part) and along the z axis (lower part). Distances are in units $a_\perp$ [see Eq. (4)]. The dashed line is the noninteracting case; the solid lines corresponds to $N=100,200,500,1000,2000,5000,$ and 10 000, in descending order of central density.

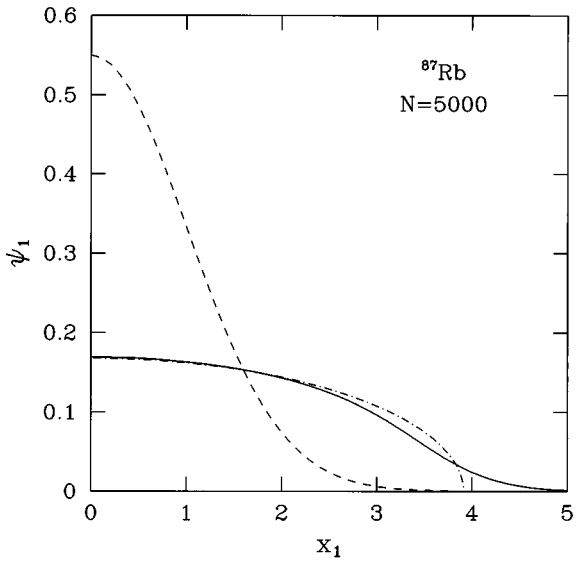

FIG. 2. Ground-state wave function for 5000 atoms of ^{87}Rb. Dashed line, noninteracting case (see Sec. II A); dot-dashed line, strongly repulsive limit (see Sec. II B); solid line, exact solution of the Gross-Pitaevskii functional.

TABLE II. Chemical potential (in units $\hbar\omega_\perp$) and average transverse and vertical size (in units $a_\perp$) in the strongly repulsive approximation (Sec. II B), for ^{87}Rb in the same trap as in Table I.

N	μ_1	$\sqrt{\langle x_1^2\rangle}$	$\sqrt{\langle z_1^2\rangle}$
100	1.60	0.68	0.24
500	3.05	0.94	0.33
1000	4.02	1.07	0.38
5000	7.66	1.48	0.52
10 000	10.1	1.70	0.60
20 000	13.3	1.94	0.69

and analogously for y and z. Summing over the three equations for x, y, and z one finds

$$2E_{\rm kin}-2E_{\rm HO}+3E_{\rm pot}=0. \tag{30}$$

One can easily see that the numerical results in Table I agree very well with this relation.

The average size of the cloud in both directions can be easily evaluated once the ground-state wave function is known. In the last two columns of Table I we report the quantities $\sqrt{\langle x_1^2\rangle}$ and $\sqrt{\langle z_1^2\rangle}$. When N increases the quantity $\langle x_1^2\rangle$ deviates rapidly from the noninteracting value 1/2, reflecting the spreading of the atom distribution in the direction of the softer trapping potential. The increase of $\langle z_1^2\rangle$ is slower, but never negligible. On can compare the results of the numerical solution of the Gross-Pitaevskii equations with the ones obtained in the strongly repulsive limit [see Eq. (16)]. In Table II we give the approximated chemical potential (15) and the average sizes (16), using the same input parameters (frequencies of the trap and scattering length). Comparing these values with the ones in Table I, one clearly sees that the strongly repulsive limit provides good estimates for the quantities $\langle x_1^2\rangle$ and $\langle z_1^2\rangle$. This means that the behavior of the surface structure, which is very different in the exact and approximated wave functions, does not affect significantly the average sizes of the cloud. Actually, the estimate of $\langle x_1^2\rangle$ is better than the one for $\langle z_1^2\rangle$, since the exact wave function approaches more rapidly the one of the strongly repulsive limit in the direction of the softer trapping potential. The approximated values of the chemical potential are close to the exact ones for N very large. The quality of the strongly repulsive approximation is improved in systems with greater values of the parameter u_1, as in the case of the sodium vapor used in the experiment of Ref. [3], where $N\simeq 10^5$ and u_1 is of the order of 10^3.

Another interesting quantity that can be easily calculated from the ground-state wave function is the aspect ratio of the velocity distribution, that is, the ratio $\sqrt{\langle p_z^2\rangle/\langle p_x^2\rangle}$. This quantity is equal to $\sqrt{\lambda}$ in the noninteracting case and should approach λ in the strongly repulsive limit. The numerical results, as a function of N, are shown in Fig. 3. The two limiting cases are shown as dashed lines. One clearly sees that the convergence to the value $2.828=\lambda$ is very slow; the aspect ratio remains well below the asymptotic value even for $N=20\,000$. The aspect ratio measured in Ref. [1] is estimated to be about 50% larger than the noninteracting value,

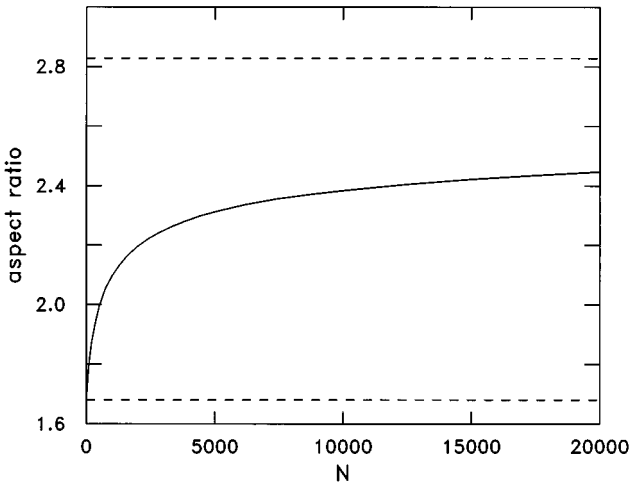

FIG. 3. Ratio of the axial to transverse average velocity as a function of N in ^{87}Rb. The lower and upper dashed lines correspond to $\sqrt{\lambda}$ and λ, respectively.

while the number of particles is of the order of 5000. The agreement with our results is good, even if one has to consider that the experimental estimate implicitly assumes a ballistic expansion of the atoms after switching off the external trap. The effects of the interaction on the expansion of the gas should be explicitly taken into account in order to draw more definitive conclusions.

Let us now consider the vortex states. In Fig. 4 we show the wave function of a cloud of 5000 atoms; the $\kappa=1$ wave function [Fig. 4(b)], which corresponds to atoms flowing around the z-axis with angular momentum $N\hbar$, is compared with the $\kappa=0$ ground state [Fig. 4(a)]. The atoms are pushed away from the axis forming a toroidal cloud. From the energy of the vortex states we calculate the critical angular velocity, through Eq. (25). The results for $\kappa=1$ are shown in Fig. 5. The critical angular velocity decreases rapidly with N. For $N>5000$ it is less than 40% of the noninteracting value, given by the transverse angular frequency $\omega_\perp$ of the trap. A rough estimate of the critical frequency in the large-N limit is given by [9] $\Omega_c/\omega_\perp\simeq(a_\perp/R)^2\ln(R/\xi)$, where R is the radius of the cloud. The *healing length* is the distance over which the wave function grows from zero to the *bulk* value. In the limit of large systems it can be approximated by Eq. (22) with ρ equal to the density in the central part of the toroidal distribution. The estimates of both ξ and Ω_c obtained in this way are in qualitative agreement with the behavior of the numerical solutions. One can also find solutions for $\kappa>1$. The critical velocity turns out to increase with κ. For instance, the critical frequency $\Omega_c/2\pi$ for the creation of vortices in a system of 10 000 atoms is 26, 35, and 41 Hz for $\kappa=1,2,$ and 3, respectively.

Finally, it is worth recalling that the dimensionless parameter characterizing the effects of the interactions in the Gross-Pitaevskii equations is given by $u_1=8\pi aN/a_\perp$ [see Eqs. (9) and (10)]. This implies that all the results obtained in the present work can be applied, with a proper rescaling of the variable N, to different choices for a and/or $a_\perp$. For instance, changing the axial frequency of the trap from 220 Hz to 120 Hz, so that $a_\perp$ increases by a factor $\sqrt{11/6}$, is

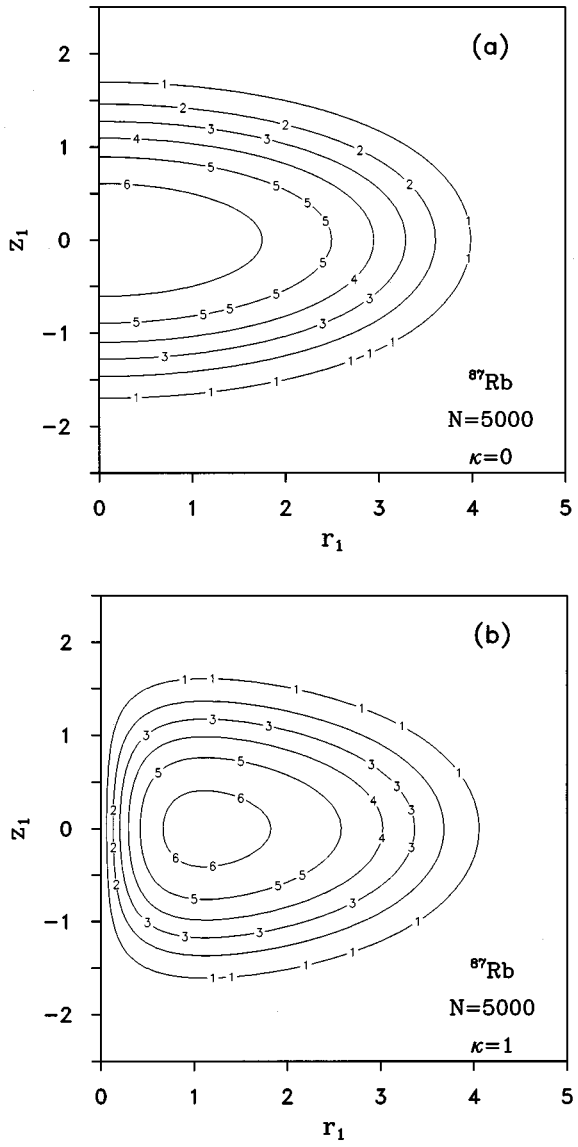

FIG. 4. Wave function, in arbitrary units, of 5000 ^{87}Rb atoms. (a) Ground state. (b) Vortex state with $\kappa=1$.

equivalent to keeping a and $a_\perp$ unchanged and reducing the number of atoms by the same factor $\sqrt{11/6}$.

B. Negative scattering length: ^{7}Li

As an example of atoms with attractive interaction we choose ^{7}Li, as in the experiment of Ref. [2]. The s-wave triplet-spin scattering length is $-27a_0$ [15]. The axial frequency reported in Ref. [2] is $\omega_z/2\pi=117$ Hz and the corresponding characteristic length is $a_\perp=2.972\times10^{-4}$ cm, thereby yielding a ratio $|a|/a_\perp=0.48\times10^{-3}$. The transverse frequency is $\omega_z/2\pi=163$ Hz, so that the asymmetry parameter is $\lambda=\omega_z/\omega_\perp=0.72$.

The first important point to stress is that Gross-Pitaevskii functional has no global minimum for a negative scattering length. This reflects the tendency of the system to collapse. For spatially inhomogeneous systems, however, the zero-point energy can exceed the attractive potential, producing local minima of the functional when the density of atoms is not too high. The nonlinear stationary Schrödinger equation

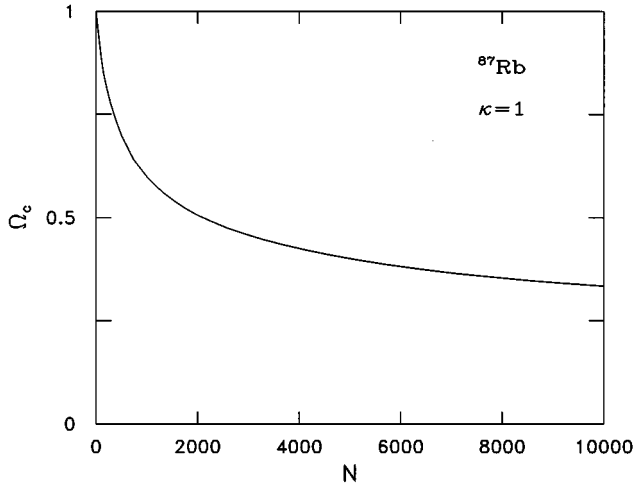

FIG. 5. Critical angular velocity, in units $\omega_\perp$, for the formation of $\kappa=1$ vortices in ^{87}Rb vapor as a function of N.

provides the solutions ψ for which $\delta E/\delta\psi=0$, but does not say anything about the stability of these solutions. A proper treatment of the stability requires a time-dependent theory [7,8]. The minimization of the Gross-Pitaevskii functional with the steepest descent method explores the configuration space with axial symmetry near the local minimum.

In Fig. 6 we show the results for the wave function along the x and the z axis for several values of N. As in Fig. 1 we plot the noninteracting case with a dashed line. Here the vapor extends more along z than along x, just because the external potential of the trap is softer in the axial direction ($\lambda<1$). Apart from this purely geometrical fact, the most striking difference with respect to the repulsive case is that

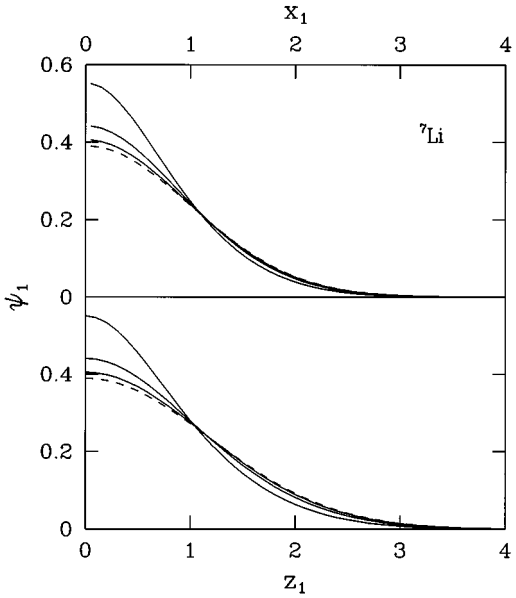

FIG. 6. Ground-state wave function for ^{7}Li along the x axis (upper part) and along the z axis (lower part). Distances are in units $a_\perp$ [see Eq. (4)]. The dashed line is the noninteracting case; the solid lines corresponds to $N=200$,500 and 1000, in ascending order of central density.

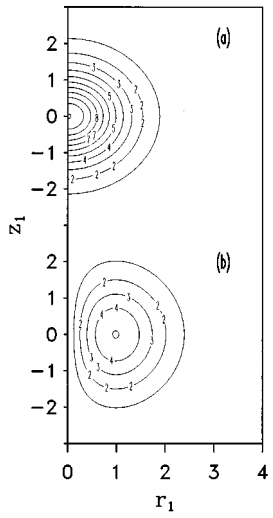

FIG. 7. Wave function, in arbitrary units, of 1000 ^{7}Li atoms. (a) Ground state. (b) Vortex state with $\kappa=1$.

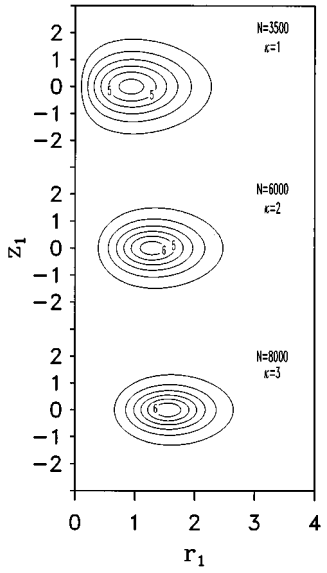

FIG. 8. Vortex-state wave functions, in arbitrary units, for different values of N and κ in ^{7}Li.

here the central density of the cloud increases rapidly with N. This is the effect of adding more and more attractive potential energy. When the central density reaches a certain critical limit the system collapses. In term of functional minimization this implies that the convergence towards the local minimum becomes slower and slower, until a critical N above which the energy falls down and does not converge anymore. In ^{7}Li, with the input parameters given above, the critical number N turns out to be about 1400.

Looking at Fig. 6, one also notices that the wave function changes its form in the same way along x and z. Both the average sizes $\sqrt{\langle x^2\rangle}$ and $\sqrt{\langle z^2\rangle}$ decrease slowly when N increases. For instance, for $N=1000$ one has $\sqrt{\langle x_1^2\rangle}=0.62$ and $\sqrt{\langle z_1^2\rangle}=0.69$, both values being about 15% smaller than the ones in the noninteracting case. The ratio $\sqrt{\langle x^2\rangle/\langle z^2\rangle}$ is practically independent of N. For instance, for $N=1$ it is equal to $\sqrt{\lambda}=0.85$, while for $N=1000$ it is 0.90, with an increase of only 5%. The aspect ratio of the velocity distribution, which is equal to $\sqrt{\lambda}$ in the noninteracting case, behaves in the same way. Even the energy per particle depends smoothly on N. In units $\hbar\omega_\perp$, it is equal to 1.36 and 1.15 for $N=1$ and $N=1000$, respectively.

Returning to the question of the stability, we notice that, when the local minimum associated with wave functions of the form shown in Fig. 6 disappears, nothing prevents *a priori* the existence of other local minima associated with different configurations. Such configurations should have local density lower than the critical one. A natural way to obtain a favorable situation is to move the atoms away from the z axis, conserving the total number of particles. This happens in the presence of a vortex. In Fig. 7 we show the wave function for 1000 ^{7}Li atoms with no vortices [Fig. 7(a)] and with an axial vortex of unit circulation [Fig. 7(b)]. We use the same units in both cases, so one can see that the maximum value of the wave function inside the toroidal distribution of the vortex is approximately a factor 2 lower than the central value in the state with no vorticity (the density is four times smaller). The critical angular frequency for the formation of the vortex state in Fig. 7 is 1.12 times the transverse angular frequency of the trap. In systems with an attractive interaction the critical angular velocity is larger than for noninteracting particles, while the opposite is true for repulsive interactions. This is because it costs internal potential energy to lower the average density, as the vortex does, for attractive interactions. However, once a vortex is created, the corresponding state is more stable than in the absence of vorticity: one can put more atoms inside the rotating cloud before reaching the critical density for the final collapse. Indeed we find local minima of the Gross-Pitaevskii functional for N much larger than 1400 if $\kappa>0$. We show three examples in Fig. 8. One notices that the maximum density of the $\kappa=1$ state slightly increases from the case $N=1000$ [Fig. 7(b)] to the case $N=3500$ (top of Fig. 8), however remaining well below the value of the central density in the state without vorticity [Fig. 7(a)]. The three vortices in Fig. 8 have almost the same peak density, but very different number of particles. They correspond to well defined local minima of the functional. If the number of particles is increased, one finds again critical values of N for which the minima disappear. For $\kappa=1$ we find a critical value of $N\simeq 4000$; for $\kappa=2$ and 3 we find critical values of 6500 and 8300, respectively. It is worth mentioning that the number of particles in the condensate reported in the experimental work of Ref. [2] is an order of magnitude higher than the critical value for the stability of the Gross-Pitaevskii solution without vorticity ($N\simeq 1400$). This discrepancy between the experimental finding of Ref. [2] and the predictions of the Gross-Pitaevskii theory could be significantly reduced if one assumes the existence of a vortex in the atomic cloud.

V. CONCLUSIONS

In this paper we have solved the Gross-Pitaevskii equations for a dilute gas of alkali atoms in anisotropic magnetic traps by numerical minimization of the total energy. The theory provides the condensate wave function at $T=0$ for states with and without vorticity. The comparison

with approximate models, such as the noninteracting gas and the strongly repulsive limit, has been carefully explored. We have explicitly discussed the results for ^{87}Rb (positive scattering length) and ^{7}Li (negative scattering length) since these elements have been used recently in the successful measurements of Bose-Einstein condensation [1,2]. We summarize here the main results of the present analysis.

(i) We have explored in a systematic way the density distribution and the energy systematics of the atomic clouds. The exact condensate wave function is flat in the interior and vanishes smoothly at the surface. The contribution of the surface to the kinetic energy per particle remains sizable even for relatively large N, differently from the predictions of approximated models recently proposed. This affects significantly the behavior of the aspect ratio of the velocity distribution. In the case of positive scattering length the aspect ratio is larger than the value $\sqrt{\lambda}$ given by the noninteracting model, but smaller than the value λ given by the strongly repulsive limit. The values calculated for ^{87}Rb are in agreement with the experimental findings of Ref. [1].

(ii) We have studied the properties of vortex states. For systems with repulsive interaction the critical angular velocity for the formation of vortices decreases rapidly with N with respect to the value of the noninteracting gas. Conversely, it increases with N in systems with attractive interaction. The most striking feature of vortex states is the tendency to lower the peak density in the cloud of atoms. This tendency has a dramatic effect for systems with an attractive interaction, where high values of the peak density can produce the disappearance of the local minimum of the functional, i.e., the collapse of the system. In ^{7}Li this happens for $N \simeq 1400$. It turns out that the presence of a vortex increases the stability of the system, in the sense that local minima with larger N can be found. We have shown the results up to $N = 8000$ with circulation number $\kappa = 3$. Higher values of N can be obtained by increasing κ. Axially symmetric vortices with circulation κ are natural candidates as metastable configurations for the condensed atoms in the traps here considered. In principle, other configurations could be possible, for instance, several separate vortices with unit circulation instead of a single vortex with circulation κ. The energetics of such states remains to be investigated.

Further work is planned in order to study in more detail the velocity distribution of the atomic vapor. Time-dependent calculations are also feasible within the same theoretical scheme.

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