Bose condensate in a double-well trap: Ground state and elementary excitations

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We study the Bose-Einstein condensate in the MIT double-well trap. We calculate the ground-state density profile of ^{23}Na atoms and the Bogoliubov spectrum of the elementary excitations as a function of the strength of the double-well barrier. In particular, we analyze the behavior of quantum-mechanical collective excitations. Finally, we discuss the observability criteria for macroscopic quantum tunneling and macroscopic quantum self-trapping. [S1050-2947(99)03411-3]

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Three years ago the Bose-Einstein condensation of alkali-metal vapors ^{87}Rb, ^{23}Na, and ^{7}Li has been achieved in magnetic harmonic traps at temperature of the order of 100 nK [1–3]. Theoretical studies of the Bose-Einstein condensate (BEC) in harmonic traps have been performed for the ground state [4–8], collective low-energy surface excitations [9–11], and vortex states [6,12].

In this paper we study the BEC in the MIT double-well trap given by a harmonic anisotropic potential plus a Gaussian barrier along the z axis, which models the effect of a laser beam perpendicular to the long axis of the condensate. In the MIT experiment [13], the macroscopic interference of two Bose condensates released from the double minimum potential has been demonstrated. Such phenomenon has been theoretically reproduced [14] by using the Gross-Pitaevskii (GP) equation [15]. Here, we concentrate on the ground-state properties of the condensate and calculate the spectrum of the Bogoliubov elementary excitations as a function of the intensity of the laser field. A comparison between our calculations and future experiments will clarify the accuracy of the GP equation and the role of correlations in Bose condensates with up to 4×10^6 particles.

By varying the strength of the barrier one can observe macroscopic quantum effects, like the formation of two Bose condensates, the collective oscillations, and the quantum tunneling [16,17].

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

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

where $\Psi(\mathbf{r})$ is the wave function of the condensate normalized to unity, $V_{ext}(\mathbf{r})$ 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 extremum condition for the energy functional gives the GP equation

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

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

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

$$V_{ext}(\mathbf{r})=\frac{m\omega_\rho^2}{2}\rho^2+\frac{m\omega_z^2}{2}z^2+U_0\exp\left(\frac{-z^2}{2\sigma^2}\right), \tag{3}$$

where $\rho=\sqrt{x^2+y^2}$, z and the angle θ are the cylindrical coordinates. The parameter values appropriate for Ref. [13] are $\omega_\rho=2\pi\times250$ Hz, $\omega_z=2\pi\times19$ Hz, and $\sigma=6$ μm. The anisotropic harmonic trap implies a cigar-shaped condensate ($\lambda=\omega_z/\omega_\rho=15/250<1$), where z is the long axis, and the Gaussian barrier of strength U_0 creates a double-well potential.

We perform the numerical minimization of the GP functional by using the steepest descent method [18]. It consists of projecting onto the minimum of the functional an initial trial state by propagating it in imaginary time. At each time step the matrix elements entering the Hamiltonian are evaluated by means of finite-difference approximants using a grid of 200×800 points. In our calculations we use the z harmonic-oscillator units. For ^{23}Na atoms, the harmonic length is $a_z=[\hbar/(m\omega_z)]^{1/2}=4.63$ μm and the energy is $\hbar\omega_z=0.78$ peV. Moreover, we use the following value for the scattering length: $a_s=3$ nm [3]. Most of our computations have been performed for $N=5\times10^6$ atoms, a value typical of the MIT experiment [13].

In Fig. 1 we show the ground-state density profile of the ^{23}Na condensate for different values of the strength of the barrier. By increasing the strength, the fraction of ^{23}Na atoms decreases in the central region and the Bose condensate separates in two condensates. As shown in Table I, the condensate slightly expands in the z direction due to the barrier potential at the origin. The numerically calculated density profiles are in good agreement with the phase-contrast images of the MIT experiment [13] and with the Thomas-Fermi (TF) approximation, which neglects the kinetic term in the GP equation. Due to the large number of atoms involved ($N=5\times10^6$), only near the borders of the wave function are there small deviations from the TF approximation. Note that the potential barrier U_0 can be written as $U_c/k_B=(37\mu K)P/\sigma^2$ (μm^2/mW), where P is the total power of

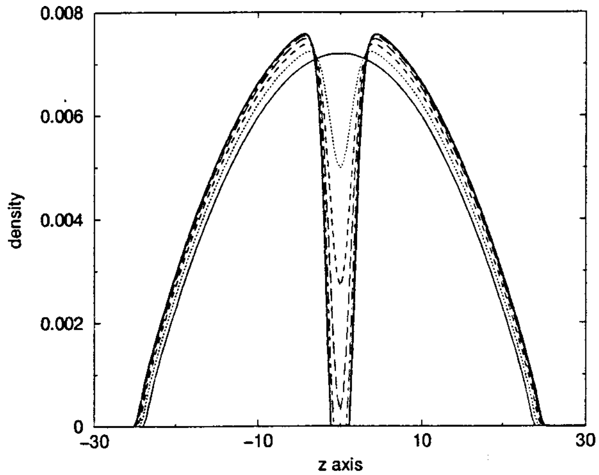

FIG. 1. Particle probability density in the ground state of $N = 5\times10^6$ ^{23}Na atoms as a function of the z axis at $r=0$ (symmetry plane). The curves correspond to increasing values of the strength U_0 of the barrier (from 0 to 500), in units of $\hbar\omega_z = 0.78$ peV. The laser power is given by the conversion formula $P = 0.09\times U_0$ mW. Lengths are in units of $a_z = 4.63$ μm.

the laser beam perpendicular to the long axis of the condensate and $\sigma = 6$ μm is the beam radius [19]. The conversion factor is 0.09 mW/($\hbar\omega_z$), such that $U_0 = 100$ (in $\hbar\omega_z$ units) gives a laser power $P = 9$ mW.

Another important property of the BEC is the spectrum of elementary excitations. To calculate the energy and wave function of the elementary excitations, one must solve the so-called Bogoliubov–de Gennes (BdG) equations [20–22]. The BdG equations can be obtained from the linearized time-dependent GP equation. Namely, one can look for q angular momentum solutions of the form

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

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:

$$H_{eff}u(\rho,z) + gN|\psi(\rho,z)|^2 v(\rho,z) = \hbar\omega u(\rho,z),$$
$$H_{eff}v(\rho,z) + gN|\psi(\rho,z)|^2 u(\rho,z) = -\hbar\omega v(\rho,z), \tag{4}$$

TABLE I. Ground state of $N = 5\times10^6$ ^{23}Na atoms. Energies are in units of $\hbar\omega_z = 0.78$ peV ($\omega_z = 2\pi\times19$ Hz). Lengths are in units of $a_z = 4.63$ μm. The laser power is given by the conversion formula $P = 0.09\times U_0$ mW.

U_0	E/N	μ	$\sqrt{\langle\rho^2\rangle}$	$\sqrt{\langle z^2\rangle}$
0	211.142	294.909	0.989	9.145
100	221.334	303.910	0.982	9.635
200	227.467	310.705	0.986	10.011
300	230.852	315.297	0.993	10.268
400	232.855	317.952	0.997	10.417
500	234.283	319.763	0.999	10.518

TABLE II. Lowest elementary excitations of the $q=0$ BdG spectrum for the ground state of $N = 5\times10^6$ ^{23}Na atoms. $^{(-)}$ and $^{(+)}$ mean odd and even z parity, respectively. Units as in Table I.

U_0	$\hbar\omega_1^{(-)}$	$\hbar\omega_2^{(+)}$	$\hbar\omega_3^{(-)}$	$\hbar\omega_4^{(+)}$	$\hbar\omega_5^{(-)}$
0	1.000	1.580	2.120	2.645	3.164
100	0.939	1.596	2.022	2.640	3.004
200	0.799	1.624	1.886	2.711	2.916
300	0.311	1.643	1.672	2.724	2.744
400	0.003	1.655	1.655	2.730	2.730
500	10^{-4}	1.663	1.663	2.744	2.744

where

$$H_{eff} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2}\right) + \frac{\hbar^2 q^2}{2m\rho^2} + V_{ext}(\rho,z) - \mu + 2gN|\psi(\rho,z)|^2.$$

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 [22]. The excitations can be classified according to their parity with respect to the symmetry $z\to -z$.

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. We have tested our program in simple models by comparing numerical results with analytical solutions and verified that a 40×40 mesh already gives reliable results for the lowest part of the spectrum [12].

In Table II we show the $q=0$ lowest elementary excitations of the Bogoliubov spectrum for the ground state of the system. When the Gaussian barrier is switched off, one observes the presence of an odd excitation at energy quite close to $\hbar\omega = 1$ (in units $\hbar\omega_z$). This mode is related to the oscillation of the center of mass of the condensate along the z axis, due to the harmonic confinement. This collective oscillation is an exact eigenmode of the problem characterized by the frequency ω_z, independently of the strength of the interaction. The inclusion of the Gaussian barrier modifies the harmonic confinement along the z axis and this odd collective mode decreases by increasing the strength of the barrier (see Fig. 2).

In cylindrical coordinates, the other collective mode of the center of mass, due to the harmonic confinement along the radial axis, is an off-axial oscillation with angular quantum number $q=1$. Such oscillation is the lowest even mode for $q=1$ and in the absence of a Gaussian barrier, it is exactly equal to the radial frequency ω_ρ ($\hbar\omega_\rho = 250/19 = 13.158$, in $\hbar\omega_z$ units). One expects that this mode is only weakly affected by the Gaussian barrier along the z axis. In Table III are reported the first elementary excitations for $q=1$. The lowest $q=1$ excitation ($\hbar\omega = 13.132$) remains constant and differs by less than 2.5% from the theoretical prediction. Also when the BEC separates in two condensates, each condensate has the same off-axial ($q=1$) collective oscillation of the center of mass.

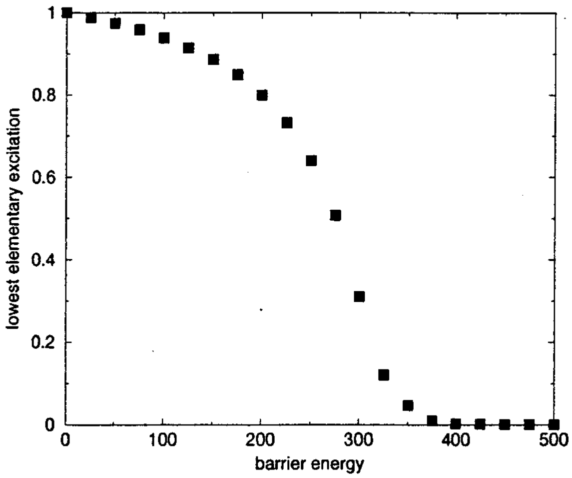

FIG. 2. Lowest elementary excitation $\hbar\omega_1^{(-)}$ with $q=0$ vs barrier energy U_0 for $N=5\times10^6$ ^{23}Na atoms. Units as in Fig. 1.

As shown both in Tables II and III, for large values of the Gaussian barrier, i.e., when the BEC separates in two condensates, we find quasidegenerate pairs of elementary excitations (even-odd). The lowest $q=0$ mode and the ground state of the GP equation constitute one of such pairs and get closer and closer as the barrier is increased. This is not surprising because in the infinite barrier limit we have two equal and independent Bose condensates with the same energy spectrum.

An interesting aspect of BEC in double-well traps is the possibility to detect the macroscopic quantum tunneling (MQT). The MQT has been recently investigated by Smerzi *et al.* [16,23]. They have found that the time-dependent behavior of the condensate in the tunneling energy range can be described by the two-mode equations

$$\dot{z}=-\sqrt{1-z^2}\sin\phi, \quad \dot{\phi}=\Lambda z+\frac{z}{\sqrt{1-z^2}}\cos\phi, \tag{5}$$

where $z=(N_1-N_2)/N$ is the fractional population imbalance of the condensate in the two wells, $\phi=\phi_1-\phi_2$ is the relative phase (which can be initially zero), and $\Lambda=4E^{int}/\Delta E^0$. E^{int} is the interaction energy of the condensate and ΔE^0 is the kinetic+potential energy splitting between the ground state and the quasidegenerate odd first excited state of the GP equation. For a fixed Λ ($\Lambda>2$), there exists a critical $z_c=2\sqrt{\Lambda-1}/\Lambda$ such that for $0<z\ll z_c$ there are Josephson-like oscillations of the condensate with period $\tau=\tau_0/\sqrt{1+\Lambda}$, where $\tau_0=2\pi\hbar/\Delta E^0$. But for $z_c<z\leqslant1$ there is macroscopic quantum self-trapping (MQST) of the condensate: even if the populations of the two wells are initially set in an asymmetric state ($z\neq0$) they maintain the original population imbalance without transferring particles through the barrier as expected for a free Bose gas. This two-mode approximation seems quite reliable. In fact, we have compared the predictions of the two-mode equations with the numerical solutions of the one-dimensional (1D) time-dependent GP equation in different regimes, finding a very good agreement (relative difference in the period of the Josephson-like oscillations less than 1%. By using the 1D time-dependent GP equation, we have studied the dynamics of the condensate also outside the tunneling region, i.e., when the chemical potential is higher than the Gaussian barrier and the two-mode equations do not hold. In such a case, starting, for example, with the condensate in one well, it does not oscillate nor remain self-trapped but instead spreads over the two wells.

TABLE III. Lowest elementary excitations of the $q=1$ BdG spectrum for the ground state of $N=5\times10^6$ ^{23}Na atoms. $^{(+)}$ and $^{(-)}$ mean even and odd z parity, respectively. Units as in Table I.

U_0	$\hbar\omega_1^{(+)}$	$\hbar\omega_2^{(-)}$	$\hbar\omega_3^{(+)}$	$\hbar\omega_4^{(-)}$
0	13.132	13.165	13.214	13.278
100	13.132	13.158	13.218	13.260
200	13.132	13.145	13.222	13.236
300	13.132	13.133	13.225	13.225
400	13.132	13.132	13.226	13.226
500	13.132	13.132	13.227	13.227

TABLE IV. Parameters of the MQT for different values of the scattering length a_s with $a_s^{\mathrm{Na}}=3$ nm and $\tau_0=2\pi\hbar/\Delta E^0$. Condensate with $N=5\times10^3$ atoms. Barrier with $U_0=20$ and $\sigma=1.5$ μm. Unit of U_0 as in Table I.

a_s/a_s^{Na}	Λ	τ_0 (sec)	z_c
10^{-1}	1108.337	14.583	0.060
10^{-2}	133.643	13.887	0.173
10^{-3}	1.390	13.842	none
10^{-4}	0.103	10.253	none

By solving the stationary GP equation in the MIT double-well trap with ^{23}Na, we find that the parameter Λ is larger than 10^4 also when few particles are present. Nevertheless, we can control the dynamics of the condensate by reducing the scattering length a_s and the thickness σ of the laser beam. In Table IV it is shown that, as expected, the parameter Λ scales linearly with a_s. This is an important point because recently it was confirmed experimentally that it is now possible to control the two-body scattering length by placing atoms in an external field [24]. This fact opens the way to a direct observation of a macroscopic quantum tunneling of thousands of atoms through a potential barrier.

Note also that the geometry and the dimensions of the trap play an important role. In fact, if the condensate is less cigar-shaped (greater $\lambda=\omega_z/\omega_\rho$) the system has a lower chemical potential and weaker Gaussian barriers are requested to enter the tunneling regime. Moreover, because the strength of the nonlinear self-interaction scales as a_s/a_z, by increasing the dimensions of the trap we reduce the effect of the nonlinearity thereby favoring quantum tunneling.

In conclusion, we have shown that one can observe interesting macroscopic quantum-mechanical effects by studying the Bose-Einstein condensate in a double-well trap. We have accurately reproduced the formation of two Bose condensates observed by phase-contrast images at the MIT experiment [13]. Moreover, by using the Bogoliubov–de Gennes equations, we have analyzed the behavior of elementary excitations as a function of the strength of the double-well barrier. In particular, we have identified two collective excitations that have a different fate by increasing the strength of the barrier: an odd $q=0$ mode that asymptotically goes to zero and an even $q=1$ mode that remains constant also when the BEC separates in two condensates. We hope that our calculations will stimulate new, precise measurements of the excitation spectrum in this system in order to assess the validity of the theoretical framework adopted in the theoretical analysis. We have also considered the macroscopic quantum tunneling. Our calculations suggest that, in the tunneling region and with ^{23}Na atoms, one sees only the macroscopic quantum self-trapping (MQST) of the condensate also when a small laser-sheet thickness is applied. We have shown that to get outside the MQST regime it is necessary to strongly reduce the scattering length or to increase the dimensions of the trap. Note that at nonzero temperature, BEC depletion and thermal fluctuations will slightly modify the parameters of the tunneling and will dampen the coherent oscillations.

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