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 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.

Three years ago the Bose-Einstein condensation of alkali 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 $4 \times 10^6$ 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.

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

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

where $\Psi(r)$ is the wave function of the condensate normalized to unity, $V_{ext}(r)$ is the external potential of the trap, and the interatomic potential is represented by a local pseudopotential so that $g = 4\pi\hbar^2a_s/m$ 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

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

where $\mu$ 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

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

where $\rho = \sqrt{x^2 + y^2}$, $z$ and the angle $\theta$ are the cylindrical coordinates. The parameter values appropriate for Ref. [13] are $\omega_\rho = 2\pi \times 250$ Hz, $\omega_z = 2\pi \times 19$ Hz, and $\sigma = 6 \mu$m. 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 $200 \times 800$ points. In our calculations we use the $z$-harmonic oscillator units. For $^{23}$Na atoms, the harmonic length is $a_z = (\hbar/(m\omega_z))^{1/2} = 4.63 \mu$m 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 has been performed for $N = 5 \times 10^6$ atoms, a value typical of the MIT experiment [13].

In Figure 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 1, 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 ($N = 5 \times 10^6$), only near the borders of the wave function there are small deviations from the TF approximation. Note that the potential barrier can be classified according to their parity with respect to the Bogoliubov approximation [22]. The excitations can be written as $U_0$ can be written as $U_{\text{e}}/k_B = (37\mu K)P/\sigma^2$ (\mu m^2/mW), where $P$ is the total power of the laser beam perpendicular to the long linear in the complex functions $\Omega$. Note that the potential barrier $U_{\text{e}}$ 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 $\omega_z$, 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 Figure 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 $\omega_r$ ($\hbar\omega_r = 250/19 = 13.158$, in $\hbar\omega_z$ units). One expects that this mode is only weakly affected by the Gaussian barrier along the $z$-axis. In Table 3 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 $\sigma/\omega_0$ 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.

As shown both in Table 2 and Table 3, for large values of the Gaussian barrier, i.e., when the BEC separates in two condensates, we find quasi-degenerate 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. [23,24]. They have found that the time-dependent behavior of the condensate in the tunneling energy range can be described by the two-mode equations

$$
\dot{\phi} = \Omega - \frac{z}{\sqrt{1 - z^2}} \cos \phi, \quad \dot{z} = -\sqrt{1 - z^2} \sin \phi, \quad \phi = \Delta z + \frac{z}{\sqrt{1 - z^2}} \cos \phi,
$$

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 $\Delta = 4E^{\text{int}}/\Delta E^0$. $E^{\text{int}}$ is the interaction energy of the condensate and $\Delta E^0$ is the kinetic+potential energy splitting between the ground state and the quasi-degenerate odd first excited state of the GP equation. For a fixed $\Delta (\Delta > 2)$, there exists a critical $z_c = 2\sqrt{\Lambda - 1}/\Lambda$ such that for $0 < z << z_c$ there are Josephson-like os-
cillations of the condensate with period \( \tau = \tau_0 / \sqrt{1 + \Lambda} \), where \( \tau_0 = 2\pi h / \Delta E_0 \). But for \( z_c < z < 1 \) 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 \( (z \neq 0) \) 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 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 case, starting, for example, with the condensate in one well, it does not oscillate nor remains self-trapped but instead spreads over the two wells.

By solving the stationary GP equation in the MIT double-well trap with \( ^{23}\text{Na} \), we find that the parameter \( \Lambda \) 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 \( \sigma \) of the laser beam. In Table 4 it is shown that, as expected, the parameter \( \Lambda \) scales linearly with \( a_s \). This is an important point because recently it was confirmed experimentally the fact that it is now possible to control the two-body scattering length by placing atoms in an external field [25]. This fact opens the way to a direct observation of a macroscopic quantum tunneling of thousands of atoms through a potential barrier.

Note that also the geometry and the dimensions of the trap play an important role. In fact, if the condensate is less cigar-shaped (greater \( \lambda = \omega_z / \omega_x \)) 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 which have a different fate by increasing the strength of the barrier: an odd \( q = 0 \) mode that asymptotically goes to zero and a 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 \( ^{23}\text{Na} \) 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 damp the coherent oscillations.

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FIG. 1. Particle probability density in the ground state of $N = 5 \times 10^6$ $^{23}$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 $\hbar\omega_0 = 0.78$ peV. The laser power is given by the conversion formula $P = 0.09 \times U_0$ mW. Lengths are in units of $\alpha_z = 4.63 \mu m$.

![Density Plot](density_plot.png)

FIG. 2. Lowest elementary excitation $\hbar\omega^{(-)}$ with $q = 0$ vs barrier energy $U_0$ for $N = 5 \times 10^6$ $^{23}$Na atoms. Units as in Fig. 1.

| $U_0$ | $E/N$ | $\mu$ | $\sqrt{\langle \rho^2 \rangle}$ | $\sqrt{\langle z^2 \rangle}$ |
|------|-------|------|----------------|----------------|
| 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 1. Ground state of $N = 5 \times 10^6$ $^{23}$Na atoms. Energies are in units of $\hbar\omega_z = 0.78$ peV ($\omega_z = 2\pi \times 19$ Hz). Lengths are in units of $\alpha_z = 4.63 \mu m$. The laser power is given by the conversion formula $P = 0.09 \times U_0$ mW.

| $U_0$ | $\hbar\omega_1^{(-)}$ | $\hbar\omega_2^{(-)}$ | $\hbar\omega_3^{(-)}$ | $\hbar\omega_4^{(-)}$ | $\hbar\omega_5^{(-)}$ |
|------|----------------|----------------|----------------|----------------|----------------|
| 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 |

Table 2. Lowest elementary excitations of the $q = 0$ BdG spectrum for the ground state of $N = 5 \times 10^6$ $^{23}$Na atoms. $(-)$ and $(+)$ mean odd and even $z$-parity, respectively. Units as in Tab. 1.

| $U_0$ | $\hbar\omega_1^{(+)}/\hbar\omega_2^{(-)}/\hbar\omega_3^{(+)}/\hbar\omega_4^{(-)}/\hbar\omega_5^{(+)}/\hbar\omega_6^{(-)}$ |
|------|---------------------------------|
| 0    | 13.132 13.156 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 3. Lowest elementary excitations of the $q = 1$ BdG spectrum for the ground state of $N = 5 \times 10^6$ $^{23}$Na atoms. $(+)$ and $(-)$ mean even and odd $z$-parity, respectively. Units as in Tab. 1.

| $a_s/a_s^{Na}$ | $A$ | $\tau_0$ (sec) | $\omega_z$ |
|----------------|-----|----------------|-----------|
| $10^{-4}$      | 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 |

Table 4. Parameters of the MQT for different values of the scattering length $a_s$ with $a_s^{Na} = 3$ nm and $\tau_0 = 2\pi\hbar/\Delta E_0$. Condensate with $N = 5 \times 10^6$ atoms. Barrier with $U_0 = 20$ and $\sigma = 1.5 \mu m$. Unit of $U_0$ as in Tab. 1.