Bose-Einstein Condensation in Exotic Trapping Potentials

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Abstract

We discuss thermal and dynamical properties of Bose condensates confined by an external potential. First we analyze the Bose-Einstein transition temperature for an ideal Bose gas in a generic power-law potential and d-dimensional space. Then we investigate the effect of the shape of the trapping potential on the properties of a weakly-interacting Bose condensate. We show that using exotic trapping potentials the condensate can exhibit interesting coherent quantum phenomena, like superfluidity and tunneling. In particular, we consider toroidal and double-well potentials. The theoretical results are compared with recent experiments.

1 Introduction

In 1995 the Bose-Einstein condensation (BEC), i.e. the macroscopic occupation of the lowest single-particle state of a system of bosons, has been
experimentally achieved with clouds of confined alkali-metal atoms at ultra-low temperature (about 100 nK). In that year, three different groups (at JILA with $^{87}$Rb atoms [1], at MIT with $^{23}$Na atoms [2], and at Rice University with $^7$Li atoms [3]) have obtained the BEC by using the same technique: a laser cooling and confinement in a magnetic trap and an evaporative cooling. In 1997 the Nobel Prize in Physics has been given for the development of methods to cool and trap atoms with laser light [4]. Nowadays more than twenty experimental groups have achieved BEC by using different geometries of the confining trap and atomic species.

The BEC phase transition has been predicted for a homogeneous ideal gas of Bosons by Einstein [5] on the basis of a paper of Bose [6]. The idea of Bose condensate has been used by London to describe the superfluid behavior of $^4$He [7]. $^4$He is a strongly-interacting system and the condensed fraction does not exceeds 10%. Instead, in the dilute alkali-metal atoms of recent experiments, the condensed fraction can be more than 90%. Thus, dilute vapors are ideal systems to investigate thermal and dynamical properties of the Bose condensate and the role of the trapping potential.

In this review paper we discuss some recent theoretical results we have obtained for Bose gases confined in potentials with exotic shapes, like power-law, toroidal and double-well potentials. Exotic potentials can be used in future experiments to find signatures of new coherent matter-wave phenomena.
2 Confined Bose gas and BEC temperature

In this section we investigate a confined ideal quantum gas of Bosons. By using the semiclassical approximation, we derive analytical formulas for the BEC transition temperature.

In the grand canonical ensemble of equilibrium statistical mechanics \[8\], the average number \( N_\alpha \) of Bosons in the single-particle state \( |\alpha\rangle \) with energy \( \epsilon_\alpha \) is given by

\[
N_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - 1} ,
\]

where \( \mu \) is the chemical potential and \( \beta = 1/(kT) \) with \( k \) the Boltzmann constant and \( T \) the absolute temperature. In general, given the single-particle function \( N_\alpha \), the average total number \( N \) of particles of the system reads

\[
N = \sum_\alpha N_\alpha .
\]

This condition fixes the chemical potential \( \mu \). Thus, \( \mu \) is a function of \( \beta \) and \( N \). \( \mu \) cannot be higher than the lowest single-particle energy level \( \epsilon_0 \), i.e., it must be \( \mu < \epsilon_0 \). When \( \mu \) approaches \( \epsilon_0 \) the function \( N_0 \) becomes very large and consequently \( N_0 \) becomes of the same order of \( N \). The physical meaning is that the lowest single-particle state becomes macroscopically occupied and one has the so-called Bose-Einstein condensation (BEC). It is clear that if \( \mu = \epsilon \) then \( N_0 \) diverges. It is a standard procedure to calculate the condensed fraction \( N_0/N \) and also the BEC transition temperature \( T_B \) by studying the non divergent quantity \( N - N_0 \) at \( \mu = \epsilon_0 \) as a function of the temperature. This procedure is particularly effective by using the semiclassical approximation.
In the semiclassical approximation, the system is described by a continuum of states and, instead of $\epsilon_\alpha$, one uses the classical single-particle phase-space energy
\[
\epsilon(r, p) = \frac{p^2}{2m} + U(r),
\]
where $p^2/(2m)$ is the kinetic energy and $U(r)$ is the confining external potential. In this way one obtains the semiclassical single-particle phase-space distribution of Bosons
\[
n(r, p) = \frac{1}{e^{\beta(\epsilon(r, p) - \mu)} - 1}.
\]
Note that the accuracy of the semiclassical approximation is expected to be good if the number of particles is large and the energy level spacing is smaller than $kT$ [9].

For the sake of generality, let us consider a d-dimensional space. Then the quantum elementary volume of the single-particle 2d-dimensional phase-space is given by $(2\pi\hbar)^d$, where $\hbar$ is the Planck constant [9]. It follows that the average number $N$ of Bosons in the d-dimensional space can be written as
\[
N = \int \frac{d^d r}{(2\pi\hbar)^d} \int \frac{d^d p}{(2\pi\hbar)^d} n(r, p) = \int d^d r n(r),
\]
where
\[
n(r) = \frac{1}{\lambda^d} \frac{1}{\Gamma(n)} \int_{\infty} \frac{dy e^{-y}}{1 - ye^{-y}},
\]
is the spatial distribution, $\lambda = (2\pi\hbar^2 \beta/m)^{1/2}$ is the thermal length,
\[
g_n(z) = \frac{1}{\Gamma(n)} \int_{0}^{\infty} \frac{dy e^{-y}y^{n-1}}{1 - ye^{-y}},
\]
is the Bose function, and $\Gamma(n)$ is the factorial function.
It is important to observe that, while Eq. (4) is divergent at $\mu = \epsilon(r, p)$, Eq. (6) is not divergent at $\mu = U(r)$ because $g_{d/2}(1) = \zeta(d/2)$, where $\zeta(x)$ is the Riemann zeta-function. It means that the integration over momenta removes the divergent contribution coming from the ground-state. It follows that the Eq. (5) describes only the total number of non-condensed Bosons. Note that this number can also be written as

$$ N = \int_0^\infty d\epsilon \rho(\epsilon) \frac{1}{e^{\beta(\epsilon-\mu)} - 1}, \quad (7) $$

where $\rho(\epsilon)$ is the density of states. It can be obtained from the semiclassical formula

$$ \rho(\epsilon) = \int \frac{d^d r}{(2\pi \hbar d)} \frac{d^d p}{2\pi \hbar^2} \delta(\epsilon - \epsilon(p, r)) = \left(\frac{m}{2\pi \hbar^2}\right)^{\frac{d}{2}} \frac{1}{\Gamma(d/2)} \int d^d r \ (\epsilon - U(r))^{(d-2)/2}. \quad (8) $$

where $\delta(x)$ is the Dirac delta function and $\Gamma(n)$ is the factorial function. This result is the generalization of the formula for ideal homogeneous Bose gases in a box of volume $V$ [8]. It shows that, in the semiclassical limit, the non-homogeneous formula is obtained with the substitution $\mu \rightarrow \mu - U(r)$, also called local density approximation.

2.1 BEC temperature for power-law potentials

In many experiments with alkali-metal atoms, the external trap can be accurately described by a harmonic potential. More generally, one can consider power-law potentials, given by

$$ U(r) = A \ r^n = \frac{1}{2} \left(\frac{\hbar \omega_0}{r_0}\right)^n \ r^n, \quad (9) $$
where $n$ is the power-law exponent and $A$ is the trap constant. Clearly, with $n = 2$ one gets the harmonic potential. Here we have introduced an energy parameter $\hbar \omega_0$ and a length parameter $r_0$, which can be chosen as $r_0 = \sqrt{\hbar/(m \omega_0)}$. The power-law potential is interesting for studying the effects of adiabatic changes in the trap. The density of states of a quantum gas in the power-law potential can be calculated from Eq. (8) and reads

$$
\rho (\epsilon) = \frac{2^{\frac{d}{2}} \Gamma (\frac{d}{n} + 1)}{2^{\frac{d}{2}} \Gamma (\frac{d}{2} + 1) \Gamma (\frac{d}{2} + \frac{d}{n})} (\hbar \omega_0)^{\frac{2n}{d(n+2)}} \epsilon^{\frac{d(n+2)}{2n} - 1}.
$$

(10)

As previously stated, Eq. (5) and (7) give the total number of Bosons only above critical temperature $T_B$. Below $T_B$, Eq. (5) and (7) describe the non-condensed number of particles $N - N_0$, where $N_0$ is the number of condensed particles. At the Bose transition temperature $T_B$, the chemical potential is $\mu = 0$ and in this way one obtains the critical temperature. In the case of the power-law potential the critical temperature is

$$
kT_B = c(d, n) \hbar \omega_0 N^{\frac{2n}{d(n+2)}},
$$

(11)

where $c(d, n)$ is a numerical coefficient given by

$$
c(d, n) = \left[ \frac{2^{\frac{d}{2}} \Gamma (\frac{d}{n} + 1)}{2^{\frac{d}{2}} \Gamma (\frac{d}{n} + 1) \zeta (\frac{d}{n} + \frac{d}{2})} \right]^{\frac{2n}{d(n+2)}}
$$

(12)

Below the critical temperature $T_B$, one has $N_0 \neq 0$ and from Eq. (5) and (7) one gets the $T$ dependence of the condensed fraction

$$
\frac{N_0}{N} = 1 - \left( \frac{T}{T_B} \right)^{\frac{d(n+2)}{2n}},
$$

where $N$ is the number of Bosons in the gas.
It is important to observe that from the previous formulas one easily derives the thermodynamic properties of quantum gases in harmonic traps and in a rigid box. In fact, by setting \( n = 2 \) one gets the formulas for the Bose and Fermi gases in a harmonic trap (in the case of a anisotropic harmonic potential, \( \omega_0 \) is the geometric average of the frequencies of the trap). The results for a rigid box are instead obtained by letting \( \frac{d}{n} \to 0 \), where the density of particles per unit length is given by \( N/\Omega_d \) and \( \Omega_d = d\pi^{\frac{d}{2}}/\Gamma(\frac{d}{2} + 1) \) is the volume of the \( d \)-dimensional unit sphere.

Finally, one notes that in the formula of the BEC transition temperature \( T_B \) it appears the function \( \zeta(\frac{d}{2} + \frac{4}{n}) \). Because \( \zeta(x) < \infty \) for \( x > 1 \) but \( \zeta(1) = \infty \), one easily deduces the following theorem [9].

**Theorem.** Let us consider an ideal Bose gas in a power-law isotropic potential \( U(r) = A r^n \) with \( r = |r| = (\sum_{i=1}^{d} x_i^2)^{1/2} \). BEC is possible if and only if the following condition is satisfied

\[
\frac{d(n+2)}{2n} > 1 ,
\]

where \( d \) is the space dimension and \( n \) is the exponent of the confining power-law potential.

This is a remarkable inequality. For example, for \( d = 2 \) one finds the familiar result that there is no BEC in a homogeneous gas \( (\frac{d}{n} \to 0) \) but BEC is possible in a harmonic trap \( (n = 2) \). Moreover, one obtains that for \( d = 1 \) BEC is possible with \( 1 < n < 2 \).
3 Bose condensate in external potential

In this section we study in detail the static and dynamical properties of a trapped dilute Bose condensate at zero temperature. Note that, if the system of Bosons is dilute, at zero temperature the non-condensed fraction can be neglected [10].

Let us consider a \( N \)-body quantum system with Hamiltonian \( \hat{H} \). The exact time-dependent Schrödinger equation can be obtained by imposing the quantum least action principle to the action

\[
S = \int dt \ < \Phi(t)|i\hbar \frac{\partial}{\partial t} - \hat{H}|\Phi(t)> ,
\]

where \( \Phi \) is the many-body wave-function of the system and

\[
< \Phi(t)|\hat{A}|\Phi(t)> = \int d^3r_1...d^3r_N \ \Phi^*(r_1,...,r_N,t)\hat{A}\Phi(r_1,...,r_N,t) ,
\]

for any quantum operator \( \hat{A} \). Looking for stationary points of \( S \) with respect to variation of the conjugate wave-function \( \Phi^* \) gives

\[
i\hbar \frac{\partial}{\partial t} \Phi(r_1,...,r_N,t) = \hat{H} \Phi(r_1,...,r_N,t) ,
\]

which is the many-body time-dependent Schrödinger equation.

As is well known, except for integrable systems, it is impossible to obtain the exact solution of the many-body Schrödinger equation and some approximation must be used. Here we discuss the zero-temperature mean-field approximation for a system of trapped weakly-interacting bosons in the same quantum state, i.e. a Bose-Einstein condensate. In this case the Hartree-Fock equations reduce to only one equation, the Gross-Pitaevskii equation, which
describes the dynamics of the condensate. As previously discussed, this equation is intensively studied because of the recent experimental achievement of Bose-Einstein condensation for atomic gasses in magnetic traps at very low temperatures.

The Hamiltonian operator of a system of \( N \) identical bosons of mass \( m \) is given by

\[
\hat{H} = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + U(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{i,j=1}^{N} V(\mathbf{r}_i, \mathbf{r}_j),
\]

where \( U(\mathbf{r}) \) is an external potential and \( V(\mathbf{r}, \mathbf{r}') \) is the interaction potential. In the mean-field approximation the totally symmetric many-particle wave-function of the Bose-Einstein condensate reads

\[
\Phi(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \Psi(\mathbf{r}_1, t)\Psi(\mathbf{r}_2, t) ... \Psi(\mathbf{r}_{N-1}, t)\Psi(\mathbf{r}_N, t),
\]

where \( \Psi(\mathbf{r}, t) \) is the single-particle wave-function. Note that such factorization of the total wave-function is exact in the case of a non-interacting condensate. The quantum action of the system is then simply given by

\[
S_{GP} = N \int dt \left< \Psi(t) | i\hbar \frac{\partial}{\partial t} - \hat{h}_s | \Psi(t) \right>,
\]

where

\[
\hat{h}_s = -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) + \frac{1}{2} (N-1) \int d^3\mathbf{r}' |\Psi(\mathbf{r}', t)|^2 V(\mathbf{r}, \mathbf{r}') .
\]

We call \( S_{GP} \) the Gross-Pitaevskii (GP) action of the Bose condensate [10]. By using the quantum least action principle we get the Euler-Lagrange equation

\[
i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) + (N-1) \int d^3\mathbf{r}' V(\mathbf{r}, \mathbf{r}') |\Psi(\mathbf{r}', t)|^2 \right] \Psi(\mathbf{r}, t),
\]

(20)
which is an integro-differential nonlinear Schrödinger equation. Such equation and the effect of a finite-range interaction have been analyzed only by few authors [11,12]. In fact, at low energies, it is possible to substitute the true interaction with a pseudo-potential

\[ V(r, r') = g \delta^3(r - r') , \]

(21)

where \( g = 4\pi \hbar^2 a_s/m \) is the scattering amplitude and \( a_s \) the s-wave scattering length. The scattering length is positive (repulsive interaction) for \(^{87}\)Rb and \(^{23}\)Na atoms but negative (attractive interaction) for \(^{7}\)Li atoms. Moreover, for large \( N \), the factor \((N - 1)\) can be substituted with \( N \). In this way one obtains the so-called time-dependent GP equation

\[
i\hbar \frac{\partial}{\partial t} \Psi(r, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + gN|\Psi(r, t)|^2 \right] \Psi(r, t) ,
\]

(22)

that is the starting point of many calculations [13]. Note that the GP equation is accurate to describe the condensate of weakly-interacting bosons only near zero temperature, where thermal excitations can be neglected. The ground-state solution \( \psi(r) \) of the GP equation is found setting \( \Psi(r, t) = e^{-i\mu/\hbar} \psi(r) \) in the previous equation. In this way one gets the stationary GP equation

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + gN|\psi(r)|^2 \right] \psi(r) = \mu \psi(r),
\]

(23)

where \( \mu \) is the chemical potential. Note that this equation can be also found by minimizing the GP energy functional

\[
E = N \int d^3 r \frac{\hbar^2}{2m} |\nabla \psi(r)|^2 + U(r)|\psi(r)|^2 + \frac{1}{2} gN|\psi(r)|^4 ,
\]

(24)
with the normalization condition

$$\int d^3r \, |\psi(r)|^2 = 1 , \quad (25)$$

which fixes the chemical potential $\mu$, that is the Lagrange multiplier of the stationary minimization problem.

To calculate the energy and wavefunction of the zero-temperature elementary excitations, one must solve the so-called Bogoliubov–de Gennes (BdG) equations [14]. The BdG equations can be obtained from the linearized time-dependent GP equation. Namely, one can look for zero angular momentum solutions of the form

$$\Psi(r,t) = e^{-i\mu t} \left[ \psi(r) + u(r)e^{-i\omega t} + v^*(r)e^{i\omega t} \right] , \quad (26)$$

corresponding to small oscillations of the wavefunction around the ground state solution $\psi(r)$. By keeping terms linear in the complex functions $u(r)$ and $v(r)$, one finds the following BdG equations

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(\rho, z) - \mu + 2gN|\psi(r)|^2 \right] u(r) + gN|\psi(r)|^2 v(r) = \hbar \omega \, u(r) ,$$

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(\rho, z) - \mu + 2gN|\psi(r)|^2 \right] v(r) + gN|\psi(r)|^2 u(r) = -\hbar \omega \, v(r) . \quad (27)$$

The BdG equations allow one to calculate the eigenfrequencies $\omega$ 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.
3.1 Bose condensate in a toroidal potential

In this section we consider a 3-D toroidal trap given by a quartic Mexican hat potential along the cylindrical radius and a harmonic potential along the $z$ axis. As we have recently shown [15], the resulting toroidal 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. Moreover, the toroidal trap can be used to create a superfluid, namely persistent currents in absence of imposed rotation.

The toroidal trap we are discussing can be described by the following potential

$$U(r) = \frac{1}{4} \lambda (\rho^2 - \rho_0^2)^2 + \frac{1}{2} m \omega_z^2 z^2,$$

(28)

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

In the Thomas-Fermi approximation, i.e. neglecting the kinetic energy in the stationary GP equation, we find

$$\psi(r) = \left[ \frac{1}{gN} (\mu - U(r)) \right]^{1/2} \Theta(\mu - U(r)),$$

(29)

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 $\mu \sim N^{1/2}$.

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.
We have performed the numerical minimization of the GP functional by using the steepest descent method. This method consists of projecting onto the minimum of the energy functional an initial trial state by propagating it in imaginary time. We have discretize the space with a grid of points taking advantage of the cylindrical symmetry of the problem. We have used grids up to $200 \times 200$ 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. In calculations we have adopted $z$–harmonic oscillator units. We write $\rho_0$ in units $a_z = (\hbar/(m\omega_z))^{1/2} = 1 \mu m$, $\lambda$ 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 have used the following values for the scattering length: $a_s = 50 \ (-13)$ Å for $^{87}$Rb ($^7$Li).

In the case of positive scattering length ($^{87}$Rb) we can control the density profile of the BEC by modifying the parameters of the potential and also the number of particles. For small number of particles the condensate is essentially confined along the minimum of $U(r)$, 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 $\lambda$ and of $\rho_0$ and, within Thomas-Fermi approximation, scales like $\lambda^{3/2}\rho_0^8$.

In the case of negative scattering length ($^7$Li), 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 (see also [16]). We obtain
the same qualitative behavior for the $^7Li$ condensate in our Mexican hat 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 $z = 0$. We notice that, for a fixed $\rho_0$, the critical number of bosons $N_c$ is only weakly dependent on the height of the barrier of the Mexican potential. These results suggest that we can not use toroidal traps to significantly enhance the metastability of the BEC with negative scattering length.

It is useful to study states having a vortex line along the $z$ axis and all bosons flowing around it with quantized circulation. The observation of these vortex states is a signature of macroscopic phase coherence of trapped BEC. The axially symmetric condensate wave function can be written as

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

where $\theta$ is the angle around the $z$ axis and $k$ is the integer quantum number of circulation. The resulting GP energy functional can be written in terms of $\psi_k(r)$ by taking advantage of the cylindrical symmetry of the problem:

$$E = N \int \rho \, d\rho \, dz \, d\theta \, \frac{\hbar^2}{2m} \left[ \frac{\partial^2 \psi_k(\rho, z)}{\partial \rho^2} \right]^2 + \frac{\partial^2 \psi_k(\rho, z)}{\partial z^2} + \frac{\hbar^2 k^2}{2m\rho^2} \left| \psi_k(\rho, z) \right|^2 + U(\rho, z) \left| \psi_k(\rho, z) \right|^2 + \frac{1}{2} gN \left| \psi_k(\rho, z) \right|^4.$$  

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.

As previously stated, vortex states are important to characterize the macroscopic quantum phase coherence and also superfluid properties of Bose systems. It is not difficult to calculate the critical frequency $\Omega_c$ at which a
vortex can be produced. One has to compare the energy of a vortex state in a frame rotating with angular frequency $\Omega$, 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 1 we show some numerical 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.

| $N$  | $E_1/N$ | $\mu_1$ | $h\Omega_c$ |
|------|---------|---------|-------------|
| 5000 | 6.00    | 7.87    | 0.15        |
| 10000| 7.61    | 10.44   | 0.16        |
| 20000| 10.02   | 14.22   | 0.18        |
| 30000| 11.93   | 17.20   | 0.20        |
| 40000| 13.57   | 19.75   | 0.21        |
| 50000| 15.04   | 22.04   | 0.23        |

Table 1. Toroidal trap. Vortex states of $^{87}$Rb atoms with $k = 1$ in the toroidal trap with $\rho_0 = 2$ and $\lambda = 4$ within Hartree-Fock approximation. Chemical potential and energy are in units of $\hbar \omega_z = 0.477$ peV ($\omega_z = 0.729$ kHz). Lengths are in units of $a_z = 1 \mu m$.

Once a vortex has been produced, the Bose condensate is superfluid if the circulating flow persists, in a metastable state, in the absence of an externally imposed rotation. Vortex solutions centered in harmonic traps
have been found, but such states turn out to be unstable to single particle
excitations out of the condensate. The vortex state is superfluid if only
if its lowest elementary excitation is positive [17]. To have the complete
spectrum of elementary excitations, one must solve the BdG equations (see
Eq. (27)). We have solved the two BdG eigenvalue equations by finite-
difference discretization with a lattice of $40 \times 40$ points in the $(\rho, z)$ plane. In
this way, the eigenvalue problem reduces to the diagonalization of a $3200 \times
3200$ real matrix.

| $N$   | $5 \times 10^3$ | $10^4$ | $2 \times 10^4$ | $3 \times 10^4$ | $4 \times 10^4$ | $5 \times 10^4$ |
|-------|-----------------|-------|-----------------|-----------------|-----------------|-----------------|
| $\bar{\hbar \omega}$ | 1.22 | 1.48 | 1.73 | 1.88 | 1.99 | 2.08 |

Table 2. Toroidal trap. Bogoliubov elementary excitation for a vortex sta-
te of $^{87}$Rb atoms with $k = 1$ in the toroidal trap with $\rho_0 = 2$ and $\lambda = 4$. Units
as in Tab. 1.

We have tested our program in simple models by comparing numerical
results with the analytical solution and verified that a $40 \times 40$ mesh already
gives reliable results for the lowest part of the spectrum. The results are
shown in Table 2: The lowest Bogoliubov excitation is always positive. 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. Thus, we can conclude that a strongly-interacting Bose
condensate in a toroidal potential is superfluid.
3.2 Bose condensate in a double-well potential

In a recent experiment at MIT [18], the macroscopic interference of two Bose condensates released from the double minimum potential has been demonstrated. Here, we consider the same double-well potential. We analyze the ground state properties of the condensate and calculate the spectrum of the Bogoliubov elementary excitations as a function of the double-well barrier. 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 [19].

The double-well trap is 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:

\[
U(r) = \frac{1}{2} m \omega_{\rho}^2 \rho^2 + \frac{1}{2} m \omega_z^2 z^2 + U_0 \exp \left( \frac{-z^2}{2\sigma^2} \right),
\]

where \(\rho = \sqrt{x^2 + y^2}\), \(z\) and the angle \(\theta\) are the cylindrical coordinates. The parameter values appropriate for Ref. [18] 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 have performed the numerical minimization of the GP energy functional by using the steepest descent method. 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 have used 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 have used 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 [19].

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. The numerically calculated density profiles are in good agreement with the phase-contrast images of the MIT experiment [18] 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 $U_0$ can be written as $U_0/k_B = (37\mu K)P/\sigma^2 (\mu m^2/mW)$, where $P$ is the total power of the laser beam perpendicular to the long axis of the condensate and $\sigma = 6\mu m$ is the beam radius. 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 [18].

Another important property of the BEC is the spectrum of elementary excitations. To calculate the energy and wavefunction of elementary excitations, one must solve the BdG equations. 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 $40 \times 40$ points in the $(\rho, z)$ plane. In this way, the eigenvalue problem reduces to the diagonalization of a $3200 \times 3200$ real matrix. We have tested our program in simple models by comparing numerical results
Figure 1: Double-well trap. 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 $\hbar \omega_z = 0.78$ peV. The laser power is given by the conversion formula $P = 0.09 \times U_0$ mW. Lengths are in units of $a_z = 4.63 \, \mu$m.
Figure 2: Double-well trap. Lowest elementary excitation $\hbar \omega_1$ vs barrier energy $U_0$ for $N = 5 \times 10^6 \ ^{23}\text{Na}$ atoms. Energies 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.

with analytical solutions [19].

In Figure 2 we show the 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 $\omega_z$, 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.

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 elementary excitation 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. [20]. They have found that the time-dependent behavior of the condensate in the tunneling energy range can be described by the two-mode equations

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

(33)

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 $\Delta E^0$ 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 $\Lambda$ ($\Lambda > 2$), there exists a critical $z_c = 2\sqrt{\Lambda - 1}/\Lambda$ such that for $0 < z < z_c$ 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 $z_c < z \leq 1$ 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.

| $a_s/a_s^{Na}$ | $\Lambda$      | $\tau_0$ (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  |

Table 3. Double-well trap. 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 $N = 5 \times 10^3$ atoms. Barrier with $U_0 = 20$ and $\sigma = 1.5$ $\mu$m. Energy barrier $U_0$ in units of $\hbar\omega_z = 0.78$ peV.

By solving the stationary GP equation in the MIT double-well trap with $^{23}$Na, we have found that the parameter $\Lambda$ is larger than $10^4$ also when few particles are present. Nevertheless, one can control the dynamics of the condensate by reducing the scattering length $a_s$ and the thickness $\sigma$ of the laser beam. In particular, as shown in Table 3, 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. This fact opens the way to a direct observation of a macroscopic quantum tunneling of thousands of atoms.
through a potential barrier.

4 Conclusions

We have studied Bose gases in various trapping potentials above and below the BEC transition temperature. By using the semiclassical approximation, we have derived analytical formulas for the BEC transition temperature of an ideal Bose gas in a generic power-law potential and d-dimensional space. Then we have analyzed the effects of the shape of the external potential on a zero-temperature Bose condensate by using the Gross-Pitaevskii equation, which describes the macroscopic wave-function of the condensate, and the Bogoliubov-de Gennes equations, which describe the elementary excitations of the condensate. We have shown that, contrary to the case of a Bose condensate in a harmonic potential, a strongly-interacting condensate in a toroidal potential is superfluid. Finally, we have investigated the conditions under which it is possible to find macroscopic quantum tunneling with a Bose condensate in a double-well potential.

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