Self-Trapping, Quantum Tunneling and Decay Rates for a Bose Gas with Attractive Nonlocal Interaction

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We study the Bose-Einstein condensation for a cloud of $^7$Li atoms with attractive nonlocal (finite-range) interaction in a harmonic trap. In addition to the low-density metastable branch, that is present also in the case of local interaction, a new stable branch appears at higher densities. For a large number of atoms, the size of the cloud in the stable high-density branch is independent of the trap size and the atoms are in a macroscopic self-trapped configuration. We analyze the macroscopic quantum tunneling between the low-density metastable branch and the high-density one by using the instanton technique. Moreover we consider the decay rate of the Bose condensate due to inelastic two- and three-body collisions.

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The Bose-Einstein condensation (BEC) for atoms with effective attractive interaction, i.e. negative scattering length, is an interesting subject of study because of the instability of the system: Recent experiments with $^7$Li vapors in a harmonic trap have shown that the BEC is achieved only by a finite and small number of atoms [1].

In a uniform system, $^7$Li atoms do not form a stable BEC state because the $s$-wave scattering length $a_s$ is negative and the attractive interaction causes the condensate to collapse upon itself [2]. In a harmonic trap, atoms acquire zero-point energies which counterbalance the attractive interaction: a metastable condensate can be obtained for a number of atoms below a critical value $N_c$, which is about $10^3$ under the condition of present experiments [1,3].

Recently, we have shown that the inclusion of a non-local interaction implies the existence of a new stable branch intermediate in density between the known very dilute metastable state and the collapsed state [4]. In this paper, we discuss the properties of the stable state and calculate the tunneling rate of macroscopic quantum tunneling (MQT) from the metastable state to the stable one by using the instanton technique. Moreover, we determine the decay rate of the Bose condensate due to inelastic two- and three-body collisions.

The system of $^7$Li atoms is quite dilute and at zero temperature the atoms are practically all in the condensate [1,3]. The action of the system is given by

$$S = \int dt \; d^3r \; \phi^*(\mathbf{r}, t) \left[ \frac{i\hbar}{2m} \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - U(r) \right] \phi(\mathbf{r}, t)$$

$$- \frac{1}{2} \int dt \; d^3r \; d^3r' \; \phi^*(\mathbf{r}, t) \phi^*(\mathbf{r}', t) V(|\mathbf{r} - \mathbf{r}'|) \phi(\mathbf{r}', t) \phi(\mathbf{r}, t) ,$$

where $\phi(\mathbf{r}, t)$ is the macroscopic wavefunction of the condensed atoms, $U(\mathbf{r})$ is the external potential and $V(|\mathbf{r} - \mathbf{r}'|)$ is the interatomic potential [5].

For alkali atoms, the atom-atom interaction is usually replaced by an effective zero-range pseudo-potential, $V(r) = g \delta^3(r)$, where $g = 4\pi\hbar^2 a_s/m$ is the scattering amplitude and $a_s$ is the $s$-wave scattering length. By using such an effective potential, and imposing the least action principle to Eq. (1), one gets the so-called Gross-Pitaevskii (GP) equation [6].

In the case of $^7$Li, that has negative scattering length, the scattering cross section has a significant momentum dependence already at very low momenta [7,8]. This momentum dependence implies that the effective interaction is non local changing from attractive to repulsive at a characteristic range $r_c$. We assume [4] that the attractive potential has a finite range $r_c$ and in addition we allow for the presence of a repulsive contribution which is modeled as a local positive term defined by a "high energy" scattering length $a_r > 0$. The effective interaction can be written in the following form:

$$V(k) = \frac{4\pi\hbar^2}{m} [a_r + (a_s - a_r)f(kr_c)] .$$

We have considered two choices for the shape function $f(x)$: a Lorentzian $f(x) = (1 + x^2)^{-1}$ and a Gaussian $f(x) = \exp (-x^2)$. The results do not depend on the specific choice of $f(x)$ and so we will discuss only the Lorentzian case. We use interaction parameters appropriate for $^7$Li (see Parola, Salasnich and Reatto [4]): $a_s = -27a_B$, $r_c = 10^3a_B$ and $a_r = 6.6a_B$, where $a_B$ is the Bohr radius.

To study the properties of the Bose condensate we perform a variational calculation. Because of the external trap, that we model with an isotropic potential $U(\mathbf{r}) = (1/2)m\omega_0^2r^2$, we use a Gaussian trial wavefunction to describe the Bose condensate and minimize the quantum action. In the rest of the paper we write the lengths in units of the characteristic length of the trap $a_0 = \sqrt{\hbar/(m\omega_0)}$, the time in units $\omega_0^{-1}$, the action in units $\hbar$ and the energy in units $\hbar\omega_0$. A good choice for the wavefunction is the following:

$$\psi(\mathbf{r}, t) = \psi_0(\mathbf{r}) \exp \left[ \frac{i}{\hbar} \int dt' \; \mathbf{r}' \mathcal{A}^{*} \left( \mathbf{r}', t' \right) \mathcal{A} \left( \mathbf{r}', t' \right) \right] ,$$

where $\mathcal{A}(\mathbf{r}, t)$ is the amplitude to find a single particle in the trap, $\psi_0(\mathbf{r}) = \psi_0(\mathbf{r}, t)$ is the ground state wavefunction in the absence of the trap, and $\mathcal{A}(\mathbf{r}, t)$ is the amplitude to find a single particle in the trap. The amplitude $\mathcal{A}(\mathbf{r}, t)$ is determined by the wavefunction $\psi(\mathbf{r}, t)$ in the absence of the trap. The action of the system is given by

$$S = \int dt \; d^3r \; \phi^*(\mathbf{r}, t) \left[ \frac{i\hbar}{2m} \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - U(r) \right] \phi(\mathbf{r}, t)$$

$$- \frac{1}{2} \int dt \; d^3r \; d^3r' \; \phi^*(\mathbf{r}, t) \phi^*(\mathbf{r}', t) V(|\mathbf{r} - \mathbf{r}'|) \phi(\mathbf{r}', t) \phi(\mathbf{r}, t) ,$$

where $\phi(\mathbf{r}, t)$ is the macroscopic wavefunction of the condensed atoms, $U(\mathbf{r})$ is the external potential and $V(|\mathbf{r} - \mathbf{r}'|)$ is the interatomic potential [5].
\[ \phi(\mathbf{r}, t) = N^{1/2} \frac{1}{\pi^{3/4} \sigma^{3/2}(t)} \exp \left\{ -\frac{r^2}{2\sigma^2(t)} + i\beta(t)r^2 \right\} , \]

where \( N \) is the number of condensed atoms and \( \sigma \) and \( \beta \) are time-dependent variational parameters. \( \sigma \) is the width of the condensate. Note that, in order to describe the time evolution of the variational function, the phase factor \( i\beta(t)r^2 \) is needed \([9]\). The choice of a Gaussian shape for the condensate is well justified in the limit of weak interatomic coupling, because the exact ground-state of the linear Schrödinger equation with harmonic potential is a Gaussian. Moreover, for the description of the collective dynamics of Bose-Einstein condensates, it has already been shown that the variational technique based on Gaussian trial functions leads to reliable results even in the large condensate number limit \([9]\). By inserting the trial wavefunction in Eq. (1), after spatial integration, the action of the system reads

\[ S = \frac{N}{4} \int dt \ (3\dot{\sigma}^2 - W(\sigma)) , \]

where the effective potential energy is given by

\[ W(\sigma) = \frac{3}{\sigma^2} + 3\sigma^2 + 2N \left( \frac{\gamma_r}{\sigma^4} + \frac{\tau_1}{\sigma} - 2g(\chi^2 \sigma^2) \right) , \]

with \( \gamma_r = (2/\pi)^{1/2} a_r/a_0 \), \( \tau_1 = (2/\pi)^{1/2} a_0 (a_s - a_r)/\sigma^2 \), \( \chi = 2^{-1/2} a_0/r_e \), \( \tau_2 = a_0^2 (a_s - a_r)/r_e^3 \) and \( g(x) = \exp(x)(1 - \text{erf}(x)) \), where \( \text{erf}(x) \) is the error function. Note that the action does not depend explicitly on \( \beta \), which is fully determined by \( \sigma \) via the Euler-Lagrange equation \( \beta = -\dot{\sigma}/(2\sigma) \) (for further details see \([10]\)).

The extrema of \( W(\sigma) \) are obtained as solutions of an algebraic equation, which gives the number of bosons as a function of the size \( \sigma \) of the cloud

\[ N = (1 - \sigma^4) \left\{ -\gamma_r \sigma^{-1} - \frac{\tau_1 \sigma}{3} + \frac{2 \chi \tau_2 g(\chi^2 \sigma^2)}{3} - \frac{2 \chi^2 \tau_2 g(\chi^2 \sigma^2)}{3} \right\}^{-1} - 1 \]

(6)

This equation has either one or three positive roots depending on the parameters and on number \( N \) of atoms in the cloud. When three solutions are present, the intermediate one represents an unstable state (i.e. a local maximum of the energy), while the other two respectively describe a low-density metastable solution (local minimum) and a high-density stable solution (absolute minimum) within GP approximation. In the local case, Eq. (6) reduces to \( N = (\sigma^2 - \sigma)/\gamma_r \), where \( \gamma_r = (2/\pi)^{1/2} a_s/a_0 \).

The variational results for four trap sizes are shown in Fig. 1, where the size of the condensate is plotted as a function of \( N \) (see also Reatto, Parola and Salasnich \([4]\)). For comparison, we also show the radius of the cloud when a local interaction is assumed. In this case there is a critical number \( N_c \approx 0.67 a_0/a_s \) of bosons beyond which the cloud collapses \([3]\). Fig. 1 shows that the effects of non-locality are always important for very tight traps while for larger traps non-locality is important just when the radius of the cloud rapidly drops for increasing \( N \). This "transition" is discontinuous for large traps.

By reducing the trap size, however, this discontinuity is strongly reduced and, below about \( a_0 = 0.3 \mu \text{m} \), the unstable branch disappears and there is a smooth evolution from a very dilute cloud to a less dilute state with an increasing density as \( N \) grows. For large \( N \) the size of the cloud is independent of the trap size and the atoms are in a macroscopic quantum self-trapped (MQST) configuration. Note that we have also computed the exact solution of the GP equation, which is always very close to the exact solution \([4]\).

The condensate undergoes density oscillations around the minimum of the energy \( W(\sigma) \). By performing a quadratic Taylor expansion around the minimum one finds simple expressions for the monopole collective frequency. In the local case we have \( \omega = (5 - \sigma^{-4})^{1/2} \), such that \( \omega = 2 \) for \( \sigma = 1 \) (ideal gas), and \( \omega \to 0 \) for \( \sigma_0 \to 5^{-1/4} \) (i.e. for \( N \to N_c \)). Instead, in the nonlocal case we obtain

\[ \omega = \left[ 3\sigma^{-4} + 1 + N \left( \frac{4 \gamma_r}{\sigma^4} + \frac{2 \tau_1}{3 \sigma^2} - \frac{2 \chi^2 \tau_2 g(\chi^2 \sigma^2)}{3} \right) + \frac{4 \chi^2 \tau_2 g(\chi^2 \sigma^2)}{3 \sqrt{\pi}} \right]^{1/2} , \]

(7)

where \( \sigma \) is related to \( N \) by Eq. (6). For the larger traps, where the two branches are present, the frequency of the metastable branch is very close to the result given by the local approximation. In the stable branch \( \omega \) starts from zero and it rises rapidly as \( N^{1/2} \). For traps of intermediate size, \( \omega \) has a dip in the transition region between the low-density state and the self bound state. For very small traps, there is only one branch and the frequency increases smoothly with the number of bosons. Note that the variational monopole frequency and the numerical one (non local case), obtained by solving the nonlocal time-dependent GP equation, differ by less than 3% (see Reatto, Parola and Salasnich \([4]\)).

We have seen that the low-density and high-density branches represent local minima of the effective potential energy \( W(\sigma) \) of the condensate, given by Eq. (5). We know from quantum mechanics that a state that is concentrated in one minimum of the potential energy may tunnel into a lower one. Ueda and Leggett \([11]\) have shown that in the local case, very close to \( N_c \), there is macroscopic quantum tunneling (MQT) from the metastable branch to the collapsed state, which has zero radius and energy equal to minus infinity. In our more realistic picture, there is MQT from the low-density branch to the high-density one. The rate of MQT can be calculated by the semiclassical formula \( \Gamma_T = Ae^{-S/h} \), where
$S$ is the instantonic action, that is the action $S$ with imaginary-time (Euclidean action) evaluated along the trajectory that makes it extremal [12]. For a quadratic-plus-cubic potential the prefactor $A$ is given by $A = \omega (15S^2 / 2\pi \hbar)^{1/2}$ [11]. After some tedious but straightforward calculations, one finds

$$\Gamma_T = 36 \sqrt{3 \frac{\omega^2}{2\pi} \frac{N^{1/2}}{a \hbar \sigma}} \exp \left\{ - \frac{362}{5} \frac{N \omega^5}{(2\pi \hbar)^2} \right\}, \quad (8)$$

where $\omega$, $N$ and $\omega$ are given by Eq. (5), (6) and (7), respectively. In Fig. 2 we plot the rate of MQT for four different traps. As expected, this rate becomes large only near $N_c$, both in the local and nonlocal case. Moreover, $\Gamma_T$ increases strongly by reducing the trap size $a_0$. As previously discussed, in the nonlocal case, below about $a_0 = 0.3 \mu m$ the unstable branch disappears and there is no more MQT.

We observe that, also if the high density branch is mechanically stable, it has a very short life-time due to two-body dipolar collisions and three-body recombination. Atoms that inelastically collide acquire substantial energy and are ejected from the trap. The total loss rate due to two-body dipolar collision and three-body recombination collisions is given by $\Gamma_L = K \int d^3r |\phi(r)|^2 + L \int d^3r |\phi(r)|^6$, where $K = 1.2 \cdot 10^{-2} \mu m^3$ sec$^{-1}$ is the two-body coefficient and $L = 2.6 \cdot 10^{-4} \mu m^6$ sec$^{-1}$ the three-body coefficient [13]. By using the trial wavefunction of Eq. (3), we find

$$\Gamma_L = \frac{K}{(2\pi)^{3/2} a_0^3} \frac{N^2}{\sigma^3} + \frac{L}{(3\pi^2)^{3/2} a_0^6} \frac{N^3}{\sigma^6}. \quad (9)$$

In this formula the value of $N$ is related to that of $\sigma$ through Eq. (6). In Fig. 3 we plot the total loss rate $\Gamma_L$ as a function of the number of $^7$Li atoms. During MQT the condensate density grows rapidly, thereby increasing the decay rate from inelastic two- and three-body collisions. In the case of a unique stable branch, the loss rate increases very fast with the number of atoms due to the high-density of the system. For sake of completeness, in Fig. 4 we show the condensate size, the MQT rate and the loss rate for the trap of the Rice experiment ($a_0 = 3 \mu m$). Actually, the trap of the Rice group has a small anisotropy and we have used the geometric average of the frequencies [1,4]. It is interesting to observe that for this trap the high density branch exists also for a number of atoms much smaller than $N_c \simeq 1400$.

In conclusion, we have studied the effect of a nonlocal inter-atomic interaction for a Bose-Einstein condensate of $^7$Li atoms in an isotropic harmonic potential at zero temperature. We have shown that, in addition to the low-density metastable branch, which is present also in the case of local interaction, a new stable branch appears at higher densities. For a large number of atoms, the condensate is in a novel macroscopic quantum self-trapped (MQST) state. Very close to the low-density critical threshold, there is macroscopic quantum tunneling (MQT) between this low-density metastable tunneling and the high-density one. This prediction is more realistic than that of MQT from the metastable branch to a collapsed state, which has zero radius and energy equal to minus infinity. We have calculated the rate of MQT with the semiclassical technique of instantons. Finally, we have considered the decay rate of the Bose condensate due to inelastic two-body dipolar collisions and three-body recombination. The life-time of the condensate in the high-density branch is very short because of the small radius of the condensate in these configurations. Due to the very short life-time of $^7$Li, experimental studies of the high-density phase of the condensate are practically impossible. Nevertheless, this is only a technical difficulty, perhaps surmountable by using a different atom, and it is imaginable that in the future our predictions can be checked.

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REFERENCES

[1] C.C. Bradley, C.A. Sackett, J.J. Tollett, and R.G. Hulet, Phys. Rev. Lett. 75, 1687 (1995); C.C. Bradley, C.A. Sackett, and R.G. Hulet, Phys. Rev. Lett. 78, 885 (1997); C.A. Sackett, H.T.C. Stoof, and R.G. Hulet, Phys. Rev. Lett. 80, 2031 (1998).

[2] T.D. Lee, K. Huang, and C.N. Yang, Phys. Rev. 106, 1135 (1957).

[3] R.J. Dodd, M. Edwards, C.J. Williams, C.W. Clark, M.J. Holland, P.A. Ruprecht and K. Burnett, Phys. Rev. A 54, 661 (1996); G. Baym and C.J. Pethick, Phys. Rev. A 54, 6 (1996).

[4] A. Parola, L. Salasnich and L. Reatto, Phys. Rev. A 57, R3180 (1998); L. Reatto, A. Parola, and L. Salasnich, J. Low Temp. Phys. 113, 195 (1998); L. Salasnich, Mod. Phys. Lett. B 12, 649 (1998).

[5] A.L. Fetter and J.D. Walecka, Quantum Theory of Many-Particle Systems (McGraw-Hill, New York, 1971); K. Huang, Statistical Mechanics (Wiley, New York, 1963).

[6] E.P. Gross, Nuovo Cimento 20, 454 (1961); J. Math. Phys. 4, 195 (1963); L.P. Pitaevskii, Zh. Eksp. Teor. Fiz. 40, 646 (1961) [Sov. Phys. JETP 13, 451 (1961)].

[7] G.F. Gribakin and V.V. Flambaum, Phys. Rev. A 48, 546 (1993).
[8] R. Cotè, A. Dalgarno and M.J. Jamieson, Phys. Rev. A 50, 399 (1994).

[9] E. Cerboneschi, R. Mannella, E. Arimondo, L. Salasnich, Phys. Lett. A 249, 245 (1998).

[10] L. Salasnich, "Time-Dependent Variational Approach to Bose-Einstein Condensation", cond-mat/9908147, to be published in Int. J. Mod. Phys. B.

[11] M. Ueda and A.J. Leggett, Phys. Rev. Lett. 80, 1576 (1998).

[12] M. Kaku, Quantum Field Theory: a Modern Introduction (Oxford Univ. Press, Oxford, 1993).

[13] A.J. Moerdijk, H.M.J.M. Boesten, and B.J. Verhaar, Phys. Rev. A 53, 916 (1996); H. Shi and W.M. Zheng, Phys. Rev. A 55, 2930 (1997); C.A. Sackett, J.M. Gerton, M. Welling, and R.G. Hulet, Phys. Rev. Lett. 82, 876 (1999).

FIG. 1. Size of the condensate as a function of the number $N$ of $^7$Li atoms. Four different traps, from top to bottom and from left to right: $a_0 = 1.0 \, \mu m$, $0.6 \, \mu m$, $0.3 \, \mu m$, $0.1 \, \mu m$, respectively. The dashed lines represent the results with local interaction.

FIG. 2. Rate of MQT as a function of the number $N$ of $^7$Li atoms. Four different traps, from top to bottom and from left to right: $a_0 = 1.0 \, \mu m$, $0.6 \, \mu m$, $0.3 \, \mu m$, $0.1 \, \mu m$, respectively. The dashed lines represent the results with local interaction.

FIG. 3. Loss rate due to two- and three-body collisions as a function of the number $N$ of $^7$Li atoms. Four different traps, from top to bottom and from left to right: $a_0 = 1.0 \, \mu m$, $0.6 \, \mu m$, $0.3 \, \mu m$, $0.1 \, \mu m$, respectively. The dashed lines represent the results with local interaction.
FIG. 4. Condensate size $\sigma$, MQT rate $\Gamma_T$ and loss rate $\Gamma_L$ as a function of the number $N$ of $^7$Li atoms. Trap of Rice University with $a_0 = 3.0 \, \mu$m [1]. The dashed lines represent the results with local interaction.