Macroscopic Quantum Tunneling of a Bose-Einstein Condensate with Attractive Interaction

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(Received 19 May 1997)

A Bose-Einstein condensate with attractive interaction can be metastable if it is spatially confined and if the number of condensate bosons N_0 is below a certain critical value N_c. By applying a variational method and the instanton technique to the Gross-Pitaevskii energy functional, we find analytically the frequency of the collective excitation and the rate of macroscopic quantum tunneling. We show that near the critical point the tunneling exponent vanishes according to $(1 - N_0/N_c)^{5/4}$ and that macroscopic quantum tunneling can be a dominant decay mechanism of the condensate for N_0 very close to N_c. [S0031-9007(98)05384-8]

PACS numbers: 03.75.Fi, 05.30.Jp, 32.80.Pj, 73.40.Gk

An explosively increasing amount of research is being carried out on the phenomenon of Bose-Einstein condensation (BEC) in gases of ^{87}Rb [1], ^{7}Li [2], and ^{23}Na [3] atoms. Unlike the other two species, a uniform system of ^{7}Li atoms is usually believed not to form a stable BEC state [4] because the s-wave scattering length a is negative and the attractive interaction between the atoms causes the condensate to collapse upon itself. When atoms are spatially confined, however, they acquire zero-point energies which, under certain conditions, counterbalance the attractive interaction, thereby allowing a metastable condensate to form.

As the number of condensate bosons increases, the attractive interaction becomes strong and the energy barrier that prevents the condensate from collapsing becomes accordingly low. Given a confining potential which determines the zero-point energies, there exists a critical number N_c of condensate bosons at which the energy barrier vanishes. When the number of condensate bosons N_0 is slightly below N_c, the energy barrier will be so low that the condensate might undergo macroscopic quantum tunneling (MQT) to a dense state. Kagan *et al.* [5] estimated the overlap integral between the metastable condensate and the dense state to be proportional to $\exp(-\frac{3}{2}N_0 \ln \frac{l_0}{L^*})$, where l_0 is the amplitude of zero-point oscillations of the trap, and $L^* \sim 3|a|N_0$. Shuryak [6] estimated the MQT rate to be proportional to $\exp[-0.57(N_c - N_0)]$. Stoof [7] wrote down a WKB formula for the MQT rate but did not explicitly evaluate it near the critical point.

In this Letter we use a variational method and the instanton technique to show that the tunneling exponent vanishes faster than found in Refs. [5,6], namely, as $(1 - N_0/N_c)^{5/4}$, as N_0 approaches N_c. By comparing the MQT rate with other possible decay mechanisms, we argue that MQT can be a dominant decay mechanism of the condensate near the critical point at zero temperature, contrary to the conclusions of Refs. [5,6]. Since the formulas we obtain contain no fitting parameters, they can be used as stringent tests of the existence of BEC.

At sufficiently low temperatures, a condensate of weakly interacting bosons is described by a single wave function $\Psi(\mathbf{r})$, and the interaction between them is described by the s-wave scattering length a. The wave function is determined so as to minimize the Gross-Pitaevskii energy functional [8]

$$E[\Psi] = \int d\mathbf{r}\, \Psi^*(\mathbf{r}) \times \left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r}) + \frac{2\pi\hbar^2 a}{m} |\Psi(\mathbf{r})|^2 \right] \Psi(\mathbf{r}), \tag{1}$$

where m is the atomic mass, $V(\mathbf{r})$ is a confining potential, and $2\pi\hbar^2 a|\Psi(\mathbf{r})|^2/m$ is the local mean-field interaction energy per particle. The wave function Ψ is normalized so that $\int |\Psi|^2\, d\mathbf{r}$ is equal to the number of condensate bosons N_0. We assume an axially symmetric confining potential: $V(\mathbf{r}) = m(\omega_\perp^2 x^2 + \omega_\perp^2 y^2 + \omega_\parallel^2 z^2)/2$, where $\omega_\perp$ and $\omega_\parallel$ are, respectively, the frequency of the radial confining potential and that of the axial one.

To evaluate $E[\Psi]$, we assume a Gaussian trial wave function [9]

$$\Psi(\mathbf{r}) = \sqrt{\frac{N_0}{\pi^{3/2} d_\perp^2 d_\parallel}} \exp\left(-\frac{x^2 + y^2}{2d_\perp^2} - \frac{z^2}{2d_\parallel^2} \right), \tag{2}$$

where $d_\perp$ and $d_\parallel$ are variational parameters. Substituting Eq. (2) into Eq. (1), we obtain

$$\begin{aligned} f(r_\perp, r_\parallel) &\equiv \frac{4E}{N_0 \hbar (\omega_\perp^2 \omega_\parallel)^{1/3}} \\ &= 2\lambda^{-1/3}(r_\perp^2 + r_\perp^{-2}) + \lambda^{2/3}(r_\parallel^2 + r_\parallel^{-2}) \\ &\quad - \gamma r_\perp^{-2} r_\parallel^{-1}, \end{aligned} \tag{3}$$

where $r_\perp \equiv d_\perp \sqrt{m\omega_\perp/\hbar} \equiv d_\perp/d_{\perp 0}$ and $r_\parallel \equiv d_\parallel \sqrt{m\omega_\parallel/\hbar} \equiv d_\parallel/d_{\parallel 0}$ are the radial and axial widths of the condensate normalized by their noninteracting values;

$\lambda \equiv \omega_\parallel/\omega_\perp$ is the asymmetry parameter of the confining potential, and

$$\gamma \equiv \frac{4N_0}{\sqrt{2\pi}} \frac{|a|}{(d_{\perp 0}^2 d_{\parallel 0})^{1/3}} \tag{4}$$

is the dimensionless strength of interaction.

For a metastable condensate to exist, the function $f(r_\perp, r_\parallel)$ must have a local minimum which is determined from conditions

$$\frac{\partial f}{\partial r_\perp} = 0 \to r_\parallel = \frac{\lambda^{1/3}\gamma}{2(1 - r_\perp^4)}, \tag{5}$$

$$\frac{\partial f}{\partial r_\parallel} = 0 \to r_\perp^2 = \frac{\gamma r_\parallel}{2\lambda^{2/3}(1 - r_\parallel^4)}. \tag{6}$$

The metastability of the condensate is determined from the curvatures of $f(r_\perp, r_\parallel)$ which are calculated to be

$$\frac{\partial^2 f}{\partial r_\perp^2} = 16\lambda^{-1/3} > 0, \qquad \frac{\partial^2 f}{\partial r_\parallel^2} = 2\lambda^{2/3}(3 + r_\parallel^{-4}) > 0, \tag{7}$$

$$\frac{\partial^2 f}{\partial r_\perp \partial r_\parallel} = -2\gamma r_\parallel^{-2}\left[\frac{2\lambda^{2/3}(1 - r_\parallel^4)}{\gamma r_\parallel}\right]^{3/2} \leq 0. \tag{8}$$

The condition for a metastable condensate to exist is that the curvature of $f(r_\perp, r_\parallel)$ at the local minimum is positive in all directions, that is,

$$\frac{\partial^2 f}{\partial r_\perp^2}\frac{\partial^2 f}{\partial r_\parallel^2} - \left(\frac{\partial^2 f}{\partial r_\perp \partial r_\parallel}\right)^2 > 0. \tag{9}$$

It is clear from Eqs. (7) and (8) that the condition (9) is always satisfied at the limit of weak interaction $\gamma \to 0$, but that it is violated at the limit of strong interaction $\gamma \to \infty$. In between there must be a critical value of γ such that the left-hand side of (9) is zero. It is given by

$$\gamma_c = \frac{\lambda^{5/3}(1 - r_\parallel^4)^3}{r_\parallel^3(1 + 3r_\parallel^4)}. \tag{10}$$

For $\gamma > \gamma_c$ the local minimum becomes a saddle point and the condensate becomes unstable, collapsing into a dense state. Substituting Eq. (10) into Eq. (6) gives

$$r_{\perp c} = \frac{\lambda^{1/2}(1 - r_{\parallel c}^4)}{\sqrt{2r_{\parallel c}^2(1 + 3r_{\parallel c}^4)}}, \tag{11}$$

where $r_{\parallel c}$ denotes the value of $r_\parallel$ at the critical point. Substituting Eqs. (10) and (11) into Eq. (5) gives

$$\lambda^2 = \frac{4r_{\parallel c}^4(1 + 3r_{\parallel c}^4)^2}{(1 - r_{\parallel c}^4)^3(3 + 5r_{\parallel c}^4)}. \tag{12}$$

We may use Eq. (12) to simplify Eq. (10) somewhat,

$$\gamma_c = \frac{4r_{\parallel c}(1 + 3r_{\parallel c}^4)}{\lambda^{1/3}(3 + 5r_{\parallel c}^4)}. \tag{13}$$

For a given asymmetry parameter $\lambda \equiv \omega_\parallel/\omega_\perp$, a real positive root of Eq. (12) gives $r_{\parallel c}$. Substituting this into Eqs. (11) and (13) gives $r_{\perp c}$ and γ_c, respectively.

For an isotropic case ($\lambda = 1$), we obtain $r_{\perp c} = r_{\parallel c} = 5^{-1/4} \simeq 0.669$ and $\gamma_c \simeq 1.07$ in agreement with the results of Refs. [7,10]. Taking experimental data from the second reference in [2], where $a = -14.5$ Å, $d_{\perp 0} \simeq 3.08\ \mu$m, and $\lambda \simeq 0.867$, we obtain from Eq. (4) that $N_c \simeq 1460$. This is 17% greater than the more precise value of 1250 which is obtained by numerically solving the nonlinear Schrödinger equation [11]. In evaluating the MQT rate, we will use the latter value for the critical number of condensate bosons.

Figure 1 shows $r_{\perp c}$, $r_{\parallel c}$, and γ_c as a function of the asymmetry parameter λ. We see that the maximum value of γ_c can be attained for the case of an isotropic potential [12]. Also plotted is the ratio $d_{\perp c}/d_{\parallel c}$ of the width of the condensate along the radial direction to that along the axial one. We note that the ratio remains relatively constant for $\lambda < 1$, but it grows rapidly for $\lambda > 1$. In what follows we will focus on the case of an isotropic confining potential, and drop the subscripts $\perp$ and $\parallel$. The function f can then be written as $f(r) = 3r^{-2} + 3r^2 - \gamma r^{-3}$.

Collective excitation of the condensate.—The condensate undergoes density oscillations around the local minimum. Associated with this collective motion is a kinetic energy T which we may write as

$$T = 3\zeta N_0 m\dot{d}^2 = 3\zeta N_0 m d_0^2 \dot{r}^2 = 3\frac{\zeta N_0 \hbar}{\omega}\dot{r}^2, \tag{14}$$

where ζ is a constant to be determined below.

The dynamics of the collective excitation is determined by the kinetic-energy term (14) and the quadratic part of the potential energy which is obtained by expanding

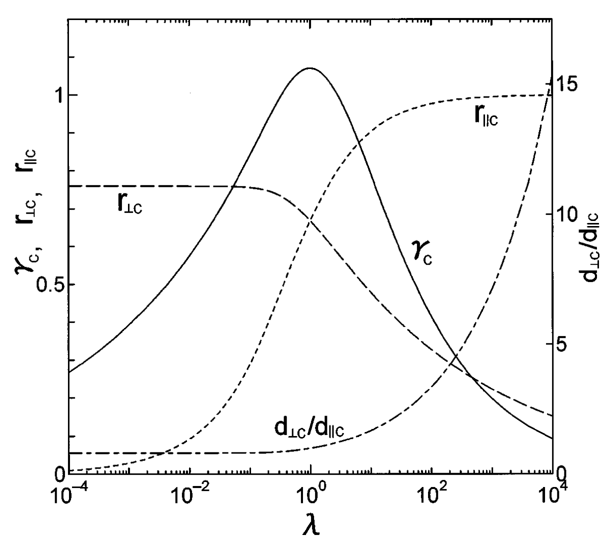

FIG. 1. Critical values of the normalized radii $r_{\perp c} \equiv d_{\perp c}/d_{\perp 0}$, $r_{\parallel c} \equiv d_{\parallel c}/d_{\parallel 0}$, and the dimensionless strength of interaction γ_c as a function of the asymmetry parameter $\lambda \equiv \omega_\parallel/\omega_\perp$, where $d_{\perp 0} \equiv (\hbar/m\omega_\perp)^{1/2}$ and $d_{\parallel 0} \equiv (\hbar/m\omega_\parallel)^{1/2}$. Also plotted is the ratio $d_{\perp c}/d_{\parallel c}$ of the width of the condensate along the radial direction to that along the axial one. Note that $r_{\perp c}$, $r_{\parallel c}$, and γ_c refer to the left scale, while $d_{\perp c}/d_{\parallel c}$ refers to the right one.

$f(r) - f(r^{\min})$ in powers of $r - r^{\min}$,

$$\frac{N_0 \hbar \omega}{4} \frac{f''(r^{\min})}{2} (r - r^{\min})^2, \tag{15}$$

where $r^{\min}$ is determined from $f'(r^{\min}) = 0$. For γ slightly below γ_c, $r^{\min}$ is close to $r_c = 5^{-1/4}$; that is, $r^{\min} = r_c + \delta r$, where δr is given to leading order in $\gamma_c - \gamma$ by

$$\delta r \simeq \frac{r_c^{1/2}}{2} (\gamma_c - \gamma)^{1/2}. \tag{16}$$

From Eqs. (3) and (16), $f''(r_\perp^{\min})$ is calculated to be

$$f''(r_\perp^{\min}) \simeq 120 \frac{\delta r}{r_{\perp c}}. \tag{17}$$

From Eqs. (14)–(17) we obtain the frequency ω_c of the collective mode near the critical point as

$$\frac{\omega_c}{\omega} = \sqrt{\frac{5}{\zeta} \frac{\delta r}{r_c}}. \tag{18}$$

The constant ζ can be determined by a variational method. According to Ref. [13], an upper bound of the frequency of a collective mode is given by $\omega_c^{\text{upper}} = \sqrt{m_3/m_1}/\hbar$, where $m_1 = \langle 0 | [F, [H, F]] | 0 \rangle / 2$ and $m_3 = \langle 0 | [[F, H], [H, [H, F]]] | 0 \rangle / 2$ are the energy-weighted moment and the cubic-energy-weighted moment of the dynamic structure factor, with F being an excitation operator. For the monopole mode the excitation operator is given by $F = \sum_{i=1}^{i=N_0} (x_i^2 + y_i^2 + z_i^2)$. Applying this formula to our Hamiltonian which is given in the square brackets of Eq. (1), we obtain Eq. (18) with $\zeta = 1/4$ and ω_c replaced by ω_c^{upper}. Stringari [14] has pointed out that for the case of repulsive interaction this method gives results in excellent agreement with numerically obtained exact frequencies. We expect that the same is true for the case of attractive interaction and identify ω_c^{upper} with ω_c. Substituting Eq. (16) into Eq. (18) and using Eq. (4), we obtain

$$\frac{\omega_c}{\omega} = 160^{1/4} \left(1 - \frac{N_0}{N_c}\right)^{1/4}. \tag{19}$$

We thus find that as the number of condensate bosons N_0 approaches its critical value N_c, the collective frequency ω_c vanishes as the one-fourth power of $1 - N_0/N_c$.

Rate of macroscopic quantum tunneling.—At sufficiently low temperature, the thermally activated decay of the condensate over the barrier is negligible, and we can expect MQT to provide a dominant decay mechanism. When the barrier is low enough for MQT to occur but still so high that the instanton approximation is valid, the MQT rate Γ is given by $\Gamma = A e^{-S^B/\hbar}$, where S^B is the bounce exponent, that is, the value of the imaginary-time action S evaluated along the bounce trajectory $r^B(\tau)$. Using Eq. (14) with $\zeta = 1/4$ we obtain

$$\frac{S}{\hbar} = \frac{N_0}{4} \int d\tau [3\dot{r}^2 + f(r) - f(r^{\min})], \tag{20}$$

where the imaginary time has been rescaled as $\omega\tau \to \tau$. The bounce trajectory $r^B(\tau)$ is the one that makes S extremal. From $\delta S/\delta r^B = 0$, we obtain an equation of motion for the bounce trajectory which can be integrated to give $(\dot{r}^B)^2 = \frac{1}{3}[f(r^B) - f(r^{\min})]$. Near the critical point, it is sufficient to expand the right-hand side of this equation in powers of $r^B - r^{\min}$ and keep terms up to the third power,

$$f(r^B) - f(r^{\min}) \simeq \frac{f''(r^{\min})}{2} \left[(r^B - r^{\min})^2 + \frac{(r^B - r^{\min})^3}{r^{\min} - r^L} \right], \tag{21}$$

where r^L is the left turning point of $f(r)$ such that $f(r^L) = f(r^{\min})$. The bounce trajectory is then obtained as

$$r^B(\tau) = r^{\min} - \frac{r^{\min} - r^L}{\cosh^2[\sqrt{f''(r^{\min})/24}\,\tau]}. \tag{22}$$

Substituting Eqs. (21) and (22) into Eq. (20), we obtain

$$\frac{S^B}{\hbar} = \frac{2}{15} N_0 \sqrt{6 f''(r^{\min})} (r^{\min} - r^L)^2. \tag{23}$$

Since $r^{\min} - r^L = 3 f''(r^{\min})/f'''(r^{\min})$, we find from Eq. (17) and $f'''(r^{\min}) \simeq 120/r_c$ that $r^{\min} - r^L = 3\delta r$. Hence

$$r^{\min} - r^L \simeq \frac{3}{2} \sqrt{r_c(\gamma_c - \gamma)}. \tag{24}$$

Substituting Eqs. (17) and (24) into Eq. (23), we obtain

$$\frac{S^B}{\hbar} \simeq 4.58 N_0 \left(1 - \frac{N_0}{N_c}\right)^{5/4}. \tag{25}$$

Thus if the condensate is formed and its decay is governed by MQT, the bounce exponent should be proportional to the five-fourths power of $1 - N_0/N_c$.

For a quadratic-plus-cubic potential, the prefactor A is given by $A = \omega_c (15 S^B / 2\pi\hbar)^{1/2}$ [15]. Substituting Eqs. (19) and (25) into this, we obtain

$$\frac{A}{\omega} \simeq 11.8 N_0^{1/2} \left(1 - \frac{N_0}{N_c}\right)^{7/8}. \tag{26}$$

Thus as N_0 approaches N_c, the prefactor vanishes as the seven-eighths power of $1 - N_0/N_c$. The crucial observation here is that the decrease in the prefactor as $N_0 \to N_c$ is outweighed by the much faster increase in the exponential factor. Because of this rapid growth in the MQT rate, MQT can be a dominant decay mechanism of the condensate near the critical point for experiments by the Rice group [2] as we now show.

Taking the experimental data of the second paper of Ref. [2], we have $\omega = (\omega_x \omega_y \omega_z)^{1/3} \simeq 908.4/\text{s}$, $\omega_c \simeq 3231(1 - N_0/N_c)^{1/4}$, $S^B/\hbar \simeq 4.58 N_0 (1 - N_0/N_c)^{5/4}$, and $A \simeq 10\,720 N_0^{1/2} (1 - N_0/N_c)^{7/8}$ with $N_c = 1250$. For $1 - N_0/N_c = 10^{-2}$, we obtain $\omega_c \simeq 1022/\text{s}$, $A \simeq 6707/\text{s}$, $S^B/\hbar \simeq 17.9$, and $\Gamma \simeq 1.12 \times 10^{-4}/\text{s}$. For this N_0 MQT is negligible, but if N_0 is a little bit closer to N_c, e.g., for $1 - N_0/N_c = 5 \times 10^{-3}$, we obtain $\omega_c \simeq 859/\text{s}$, $A \simeq 3666/\text{s}$, $S^B/\hbar \simeq 7.58$, and $\Gamma = 1.88/\text{s}$, and the MQT rate is therefore significant.

It has sometimes been argued that the decay rate of the condensate due to MQT is much slower than that due to two-body dipolar and three-body collisions, and is therefore unlikely [16]. The above numerical evaluation, however, shows that near the critical point the MQT rate is at least comparable to the decay rate due to those inelastic collisions evaluated in Refs. [17,18] because near the critical point the MQT rate grows at an enormous rate as numerically illustrated above. Kagan *et al.* pointed out yet another interesting decay mechanism due to exchange interaction [5]. This mechanism becomes important when the mean-field interaction energy per particle is larger than the single-particle energy-level spacing. For the experiments of Ref. [2], these energies are estimated to be 1 and 7 nK, respectively, so the condensate is not likely to decay via this mechanism.

In conclusion, we have used a variational method and the instanton technique to find analytically the frequency of the collective mode and the MQT rate of a Bose condensate with attractive interaction near the critical point of collapse. The maximum number of condensate bosons is found to be attained for the case of isotropic confining potential. By comparing MQT with other decay mechanisms, we have argued that MQT can be a dominant decay mechanism of the condensate for N_0 very close to N_c. The obtained formulas contain no fitting parameters and can therefore be used as rather stringent tests for the existence of BEC. The fact that we have demonstrated the tunneling of the condensate to indefinitely low energy to occur does not necessarily imply that the physical system actually collapses, because we have not taken into account any effect of higher-order interactions.

We would like to thank R. Hulet and C. Sackett for valuable discussions and for sending us Ref. [12] prior to publication. M. U. gratefully acknowledges helpful discussions with G. Baym and I. Kosztin. This work was supported by the Core Research for Evolutional Science and Technology (CREST) of the Japan Science and Technology Corporation (JST) and by the National Science Foundation under Grant No. DMR96-14133.

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