Periodic Instanton Method and Macroscopic Quantum Tunneling between two weakly-linked Bose-Einstein Condensates

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A new method is used to investigate the tunneling between two weakly–linked Bose–Einstein condensates confined in double–well potential traps. The nonlinear interaction between the atoms in each well contributes to a finite chemical potential, which, with consideration of periodic instantons, leads to a remarkably high tunneling frequency. This result can be used to interpret the newly found Macroscopic Quantum Self Trapping (MQST) effect. Also a new kind of first–order crossover between different regions is predicted.
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Following the first observation of Bose–Einstein condensation (BEC) in dilute gases of trapped alkali atoms, remarkable progress has been made both theoretically and experimentally [1]. In particular, interference between two freely expanding condensates has been observed after switching off the double–well potential that confines them [2]. By using a thinner barrier between the two condensates it should be possible to establish reliably a weak link and study quantum tunneling, or the Josephson effect, for atoms. Aspects of these questions have already been studied theoretically in the limit of noninteracting atoms [3] and for small–amplitude Josephson oscillations [4,5].

Here we develop another theoretical method for a sensitive and precise investigation of the tunneling between two condensates. The almost trivially looking problem of the tunneling behavior in a double–well potential has attracted much attention from theorists for decades. For a single particle, the solution can be found even in quantum mechanics textbooks [6]. The advantage of a nonperturbative method, as presented here, is that it gives not only a more accurate description of the tunneling phenomena but also a comprehensive physical understanding in the context of quantum field theory. The periodic instanton configurations, which have been shown to be a useful tool in several areas of research such as spin tunneling [7], bubble nucleation [8] and gauge field theory [9], enable also the investigation of the finite temperature behavior of these systems. In the case of the Bose–Einstein system, however, we need to evaluate the tunneling frequency for a finite chemical potential even at zero temperature, due to the nonlinear interaction between the confined atoms. Therefore the chemical potential here replaces the position of the excited energy and gives rise to an expected higher tunneling frequency.

A novel nonlinear effect has been predicted to occur in the Bose–Josephson Junction (BJJ) [10]: The self–trapping of a BEC population imbalance arises because of the interatomic nonlinear interaction in the Bose gas. This was considered to be a novel "macroscopic quantum self–trapping" (MQST) and was predicted to be observable under certain experimental conditions. The three parameters, i.e. the ground state energy E^0, the interaction energy U, and more importantly, the tunneling amplitude K, are still undetermined for a specific geometry of the potential well and have been taken as constants in refs. [10,11]. Here we present a rigorous derivation of these quantities and find that they actually depend on the number of atoms N. This N–dependence refines the conclusions and makes the self–trapping easier to observe.

The macroscopic wave function Φ associated with the ground state of a dilute Bose gas confined in the potential $V_{ext}(r)$ obeys the well–known Gross–Pitaevskii Equation (GPE), which can be obtained using a variational procedure, i.e. $i\hbar\partial\Phi/\partial t = \delta E/\delta\Phi^*$. The energy functional E is defined by

$$E[\Phi] = \int d^3r \left[\frac{\hbar^2}{2m}\left|\nabla\Phi\right|^2 + V_{ext}(r)\left|\Phi\right|^2 + \frac{g}{2}\left|\Phi\right|^4\right] \quad (1)$$

where $g = 4\pi\hbar^2 a/m$ is the interatomic coupling constant with a the $s-$wave scattering length. The three terms in the integral are the kinetic energy of the condensate E_{kin}, the (an)harmonic potential energy E_{ho}, and the mean–field interaction energy E_{int}, respectively. In the simplest case of an isotropic harmonic trap $V_{ext}(r) = m\omega_0^2 r^2/2$, these energies can be calculated beyond the Thomas–Fermi (TF) approximation [1,4,12] as

$$\frac{E_{kin}}{N} = \frac{5}{2}C_{TF}, \qquad \frac{E_{ho}}{N} = \frac{3}{7}\mu_{TF} + C_{TF},$$
$$\frac{E_{int}}{N} = \frac{2}{7}\mu_{TF} - C_{TF}, \qquad C_{TF} = \frac{\hbar^2}{mR^2}\ln\left(\frac{R}{1.3a_{ho}}\right)$$

by using nontrivial relationships among the various energy components, i.e. the virial theorem $2E_{kin} - 2E_{ho} + 3E_{int} = 0$, the expression for the chemical potential $\mu = (E_{kin} + E_{ho} + 2E_{int})/N$ and the thermodynamic definition $\mu = \partial E/\partial N$. Here N is the number of atoms and the harmonic oscillator length $a_{ho} = (\hbar/m\omega_0)^{1/2}$ is introduced for simplicity. The chemical potential in the TF approximation is evaluated as $\mu_{TF} = \frac{\hbar\omega_0}{2}(15Na/a_{ho})^{2/5}$ and is related to the radius of the condensate R through $\mu_{TF} = m\omega_0^2 R^2/2$. We note that in the derivation, the

TF wave function is normalized to N. If one uses instead a wave function normalized to unity, the following correspondence should be realized

$$U_{1,2}N_{1,2} \to 2\frac{E_{int}}{N}, \qquad E^0_{1,2} \to \frac{E_{kin}}{N} + \frac{E_{ho}}{N}$$

and we obtain the ground state energy $E^0_{1,2}$ and the interaction self energy $U_{1,2}N_{1,2}$ for the isolated traps with $N_1 = N_2 = N$ as in ref. [10]

$$E^0_{1,2} = \frac{3}{7}\mu_{TF} + \frac{7}{2}C_{TF}, \qquad U_{1,2}N_{1,2} = \frac{4}{7}\mu_{TF} - 2C_{TF}$$

Considering a condensate of $N = 5000$ sodium atoms confined in a symmetric spherical trap with frequency $\omega_0 = 100Hz$, we have $E^0 = 1.18n\mathrm{K}, UN = 1.03n\mathrm{K}$, quite close to the values estimated in [10].

Calculation of the tunneling frequency by means of the periodic instanton method: We study the amplitude for tunneling between the two condensates confined in the wells of an external double–well potential

$$V_{ext}(x) = \frac{m\omega_0^2}{8x_0^2}(x^2 - x_0^2)^2 \tag{2}$$

The two minima are located at $\pm x_0$ on the x–axis, and the harmonic oscillation frequency near these minima is ω_0. The barrier height between the two wells $V_0 = \frac{1}{8}m\omega_0^2 x_0^2$ is assumed to be high enough so that the overlap between the wave functions relative to the two traps occurs only in the classically forbidden region where interaction can be ignored and one can safely use the WKB wave function approximately [4]. The tunneling amplitude K in ref. [10] can be calculated by different methods, and we demonstrate in this work the use of the nonperturbative instanton approach. It is easily shown that this tunneling amplitude is just the quantity $\mathcal{R}$ of [11] (up to a minus sign), if one observes the orthogonality property of the eigenfunctions $\int dx \Phi_i^*(x)\Phi_j(x) = \delta_{ij}, i, j = 1, 2$, with $\Phi_{1,2}(x)$ the local modes in each well, which are taken as the harmonic oscillator single particle ground state wave function in ref. [11]. The nonlinear interaction between the atoms in the same well will be included, which modifies only the chemical potential μ to or beyond the TF approximation.

Now we turn to the field theory description of the GPE. To this end we consider a scalar field in a 1–dimensional time plus 1–dimensional space. After a Wick's rotation $t = -i\tau$ the Euclidean–Lagrangian equation of motion for a finite chemical potential takes the form

$$\frac{1}{2}m\left(\frac{dx}{d\tau}\right)^2 - V_{ext}(x) = -\mu \tag{3}$$

The reason why we can handle a nonlinear problem by means of a linear equation of motion is that we discuss the tunneling behavior in the barrier region where the nonlinear interaction is negligible. However, there are obvious differences between the BEC tunneling system and the usual one-body problem, i.e. the nonlinear interaction contributes a finite chemical potential, which is just the integration constant on the right hand side of eq.(3). The classical turning points on both sides of the barrier can be determined by the relation $V(x_{1,2}) = \mu$ as suggested in ref. [4]. For a noninteracting system the chemical potential approaches the ground state energy corresponding to the vacuum instanton case in [13].

Solving this Euclidean time classical equation in the usual way [13] one obtains the periodic instanton solution in terms of the Jacobian elliptic function $x_c = 2x_0 kb(k)/\omega_0 \,\mathrm{sn}\,(b(k)\tau)$ with the parameters defined as

$$b(k) = \frac{\omega_0}{2}\sqrt{\frac{2}{1+k^2}}, \qquad k^2 = \frac{1-u}{1+u}, \qquad u = \sqrt{\frac{\mu}{V_0}}$$

The Euclidean action for this solution in half of the imaginary period $T = 2\mathcal{K}(k)/b(k)$ can be obtained through $S = \int_{-T/2}^{T/2} d\tau \left(\frac{1}{2}m(dx/d\tau)^2 + V_{ext}(x)\right) = W + \mu T/2$ with

$$W = \frac{2}{3}\frac{8V_0}{\omega_0}(1+u)^{1/2}\left(\mathcal{E}(k) - u\mathcal{K}(k)\right) \tag{4}$$

where $\mathcal{K}(k)$ and $\mathcal{E}(k)$ are complete elliptic integrals of the first and second kinds with modulus k, respectively. The frequency of tunneling between the two condensates is then given by the energy level splitting of the two lowest states, i.e. $\Omega = \Delta E/\hbar = 2K/\hbar = 2\mathcal{R}/\hbar$ and can be calculated by means of the path integral method as [13]

$$\Omega = \frac{1}{\hbar}Ae^{-W/\hbar} = \frac{\sqrt{1+u}}{2\mathcal{K}(k')}\omega_0 \exp\left[-W/\hbar\right] \tag{5}$$

We emphasize here that this formula has been proven to be valid for the whole region when the chemical potential is below the barrier height. The condition $V_0 = \mu$ determines the sphaleron configuration, where a type of phase transition may occur. In the TF approximation this means

$$x_0 = 2R = 2a_{ho}\left(\frac{15N_T a}{2a_{ho}}\right)^{1/5}$$

where $N_T = N_1 + N_2$ is the total number of atoms in both wells together. Therefore for a specific type of trapped atoms and a given double–well potential with separation x_0 (atom number N_T) there exists a critical number of atoms N_{c1} (critical separation x_{c1}) determined by the above equation, below (above) which the tunneling process will give the main contribution to the tunneling amplitude. However, above this critical number of atoms or below this critical separation value another process, i.e. the over–barrier activation will dominate (which is definitely not "thermal activation" as in spin tunneling since the temperature is zero) (cf. Fig. 1). Between these

two processes there exists a crossover. A more explicit condition for this critical number of atoms (separation between the two minima) can be derived beyond the TF approximation, i.e.

$$x_0 = 2R\sqrt{1+\frac{3}{5}\left(\frac{15N_T a}{2a_{ho}}\right)^{-4/5}\ln\left(\frac{15N_T a}{2a_{ho}1.3^5}\right)}$$

As an example, we consider two weakly–linked condensates of $N_T = 10^4$ sodium atoms, confined in two symmetric spherical traps with frequency $\omega_0 = 100Hz$ as in ref. [10]. The critical value for x_{c1} is $x_{c1} = 24.58\mu m$ or more accurately $x_{c1} = 25.29\mu m$. We note that here the height of the potential barrier is $V_0 = 2.21n$K and the ground state is located at $\hbar\omega_0/2 = 0.38n$K so that there are several energy levels beneath the barrier height. This means the interaction between the atoms contributes to the chemical potential, which effectively raises the classical turning points to a remarkably high level. Although the atoms remain in the ground state, the interaction energy is so strong that the vacuum instanton method can no longer be applied. We have to resort to the periodic instanton method, as will be shown below.

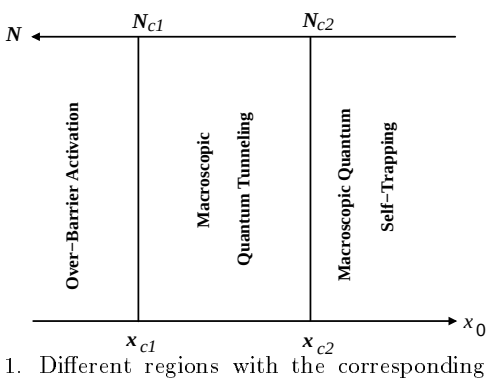

FIG. 1. Different regions with the corresponding critical parameter

Low–energy limit: We now consider the "low-energy" limit, $\mu \to 0$. As in the case of a uniform Bose gas, the number of atoms in the ground state can be macroscopic, i.e., of the order of the total number in one potential well, when the chemical potential becomes equal to the energy of the lowest state, which, in our 1–dimensional case here, is $\mu \to \mu_c = \frac{1}{2}\hbar\omega_0$. The lower boundary for the chemical potential in fact implies that $R_c = a_{ho}$, i.e. the radius of the condensate should never be less than the harmonic oscillator length a_{ho}. We thus have a result similar to that in the vacuum instanton case [13] and the "low energy" limit here is only meaningful in this sense. Expanding eq. (5) far below the barrier height, i.e., around the modulus $k \to 1$, or equivalently evaluating the tunneling amplitude in the vacuum instanton method [13], we obtain for the tunneling frequency

$$\Omega = 2\sqrt{\frac{6S_c}{\pi\hbar}}\omega_0 \exp\left(-S_c/\hbar\right) \tag{6}$$

with the Euclidean action

$$\frac{S_c}{\hbar} = \frac{2}{3}\frac{8V_0}{\hbar\omega_0} = \frac{2}{3}\frac{x_0^2}{a_{ho}^2}$$

This result can be compared with that of ref. [11] where the problem of tunneling in the BEC system is considered. We reexpress the tunneling frequency of ref. [11] in the notation of the harmonic oscillator length a_{ho} as

$$\Omega = \frac{x_0^2}{a_{ho}^2}\omega_0 e^{-x_0^2/a_{ho}^2} \tag{7}$$

which, however, gives not only a smaller exponential contribution $8V_0/\hbar\omega_0$ (there is a 2/3 factor) but also an inaccurate prefactor $x_0^2\omega_0/2\triangle = \omega_0 S_c/\hbar$. The source of this inaccuracy is the adoption of the too simple harmonic oscillator wave function of a single particle, which obviously oversimplifies the Bose–Einstein condensation tunneling problem. At least one should use the WKB wave function in the tunneling region, and it can be shown that this corresponds to the vacuum instanton result we present here. For the agreement between WKB and vacuum instanton methods we refer to ref. [14].

Observation of Macroscopic Quantum Self Trapping: The periodic instanton result will lead to an exponentially growing behavior for the tunneling frequency when the chemical potential, i.e. the number of atoms, is increased. According to ref. [10], for a fixed value of the initial population imbalance (for simplicity we consider here only the zero–phase case $\phi(0) = 0$ which describes the interwell atomic tunneling dynamics with a zero time–average value of the phase across the junction), if the parameter $\Lambda = UN_T/2K$ exceeds a critical value Λ_c, the population becomes macroscopically self–trapped with a nonzero average population difference $N_1 - N_2$. There are different ways in which this state can be achieved, and all of them correspond to the so-termed MQST condition that

$$\Lambda = \frac{UN_T}{2K} > \Lambda_c = 2\left(\frac{\sqrt{1-z(0)^2}+1}{z(0)^2}\right) \tag{8}$$

This requirement is actually that the modulus of the elliptic function, which appears in the population oscillation solution, should be larger than 1 so that the elliptic function cn will be replaced by dn and the oscillation period is shortened from $8k\mathcal{K}(k)/C\Lambda$ to $4k\mathcal{K}(k)/C\Lambda$. The parameters UN_T and K are taken as constants in ref. [10]. Considering the fact that they are actually N–dependent as in our calculation above, we can refine the conclusions of refs. [10,11]. To access the region of self–trapping, that is, $\Lambda > \Lambda_c$, it is better to lower the value of K by making a higher barrier height V_0 through increasing the separation x_0 or the oscillation frequency ω_0, than to increase the number of atoms as suggested in ref. [10]. In fact, the quantity UN_T here is proportional to $\mu_{TF} \sim N^{2/5}$ which means that increasing the

number of atoms will not increase the interaction energy significantly, and at the same time the tunneling amplitude will be increased more drastically. Thus, contrary to the result of ref. [10,11], we find that the MQST will occur when the number of atoms is smaller (instead of larger) than a critical value N_{c2}, i.e. we should decrease the number of atoms instead of increasing it (Fig. 1). Inserting the values of the interaction energy and the tunneling amplitude into eq.(8) we can obtain this critical number of atoms for a given potential geometry. The parameters which can be adjusted are the number of atoms N_T, the oscillation frequency ω_0, and the separation distance between the two condensates x_0. Fig 1. shows the three different regions for different numbers of atoms and distances between the potential wells. When x_0 (N_T) is smaller (larger) than the critical value $x_{2c}(N_{c2})$, the atoms will oscillate between these two potential wells. Once we increase the separation above (or decrease the number of atoms below) this critical value, the MQST will occur, i.e., most of the atoms will tend to remain in their appropriate wells, leading to only a small oscillation around a fixed population difference.

We take the initial condition for the population difference to be $z(0) = 0.4$ as an example. For sodium atoms confined in the double–well potential with $\omega_0 = 100$, we show numerically in Fig. 2 the critical line between the three different regions. The upper region marks the self–trapping region, the lower the over–barrier activation. Quantum tunneling occurs only for a small range of the parameter. The solid line is the result beyond the TF approximation and the dashed line corresponds to TF results. We also find that the tunneling will be suppressed when the separation or the number of atoms satisfies $x_0 > 24\mu m$ or $N > 7000$. The crossover will occur directly between the self–trapping and the over–barrier regions, quite similar to the first–order transition in spin tunneling [7]. The TF result pushes this critical point out to $x_0 \sim 25\mu m$, $N_T \sim 12000$.

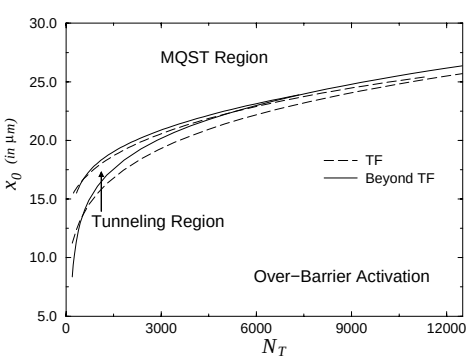

FIG. 2. Critical line for MQST effect

In conclusion we can say, we have shown that the periodic instanton method can be used to investigate the tunneling problem in BEC systems at zero temperature. The tunneling amplitude and the nonlinear interaction energy between the atoms can be calculated analytically beyond the TF approximation. The MQST effect is more easily observed if one takes into account the N–dependence of the tunneling amplitude K and the self interaction energy UN_T. The crossover between the different regions may be of the first–order type when the two minima of the potential wells are separated sufficiently far or the number of confined atoms in the potential well is large enough.

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[1] F. Dalfovo, S. Giorgini, L. P. Pitaevskii and S. Stringari, Rev. Mod. Phys **71**, 463 (1999).

[2] M. R. Andrews, C. G. Townsend, H.–J. Miesner, D. S. Durfee, D. M. Hurn and W. Ketterle, Science **275**, 637 (1997).

[3] J. Javanainen, Phys. Rev. Lett. **57**, 3164 (1986).

[4] F. Dalfovo, L. P. Pitaevskii and S. Stringari, Phys. Rev. **A54**, 4213 (1996).

[5] I. Zapata, F. Sols and A. Leggett, Phys. Rev. **A57**, R28 (1998);J. Williams, R. Wasler, I. Cooper, E. Cornell and M. Holland, Phys. Rev. **A69**, R31 (1999).

[6] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics, 3rd ed.* (Pergamon Press, Oxford, 1977); E. Merzbacher, *Quantum Mechanics, 3rd ed.*(John Wiley Sons Inc, 1998).

[7] J.-Q. Liang, H. J. W. Müller–Kirsten, D. K. Park and F. Zimmerschied, Phys. Rev. Lett. **81**, 216 (1998); J.-Q. Liang, Y.-B. Zhang, H. J. W. Müller–Kirsten, J. G. Zhou, F. Zimmerchied and F.-C. Pu, Phys. Rev. **B57**, 529(1998).

[8] J.–Q. Liang, H. J. W. Müller–Kirsten, Y.-B. Zhang, A. V. Shurgaia, S. P. Kou and D. K. Park, Phys. Rev. **D62**, 025017 (2000).

[9] D. K. Park, H. J. W. Müller–Kirsten and J.–Q. Liang, Nucl. Phys. **B579**,728 (2000).

[10] A. Smerzi, S. Fantoni, S. Giovanazzi and S. R. Shenoy, Phys. Rev. Lett. **79**, 4950 (1997); S. Raghavan, A. Smerzi, S. Fantoni and S. R. Shenoy, Phys. Rev. **A59**, 620 (1999).

[11] G. J. Milburn, J. Corney, E. M. Wright and D. F. Walls, Phys. Rev. **A55**, 4318 (1997).

[12] A. L. Fetter and D. L. Feder, Phys. Rev. **A58**, 3185 (1998); E. Lundh, C. J. Pethick and H. Smith, Phys. Rev **A55**, 2126 (1997).

[13] E. Gildener and A. Patrascioiu, Phys. Rev. **16**, 423 (1977);J.-Q. Liang, H. J. W. Müller–Kirsten, Phys. Rev. **D46**, 4685(1992).

[14] P. Achuthan, H. J. W. Müller–Kirsten and A. Wiedemann, Fortschr. Phys. **38**, 77 (1990).