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Numerical simulation on tunnel splitting of Bose-Einstein condensate in multi-well potentials

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Abstract. The low-energy-level macroscopic wave functions of the Bose-Einstein condensate (BEC) trapped in a symmetric double-well and a periodic potential are obtained by solving the Gross-Pitaevskii equation numerically. The ground state tunnel splitting is evaluated in terms of the even and odd wave functions corresponding to the global ground and excited states respectively. We show that the numerical result is in good agreement with the analytic level splitting obtained by means of the periodic instanton method.

PACS. 03.75.Lm Tunneling, Josephson effect, Bose-Einstein condensates in periodic potentials, solitons, vortices and topological excitations – 02.60.Cb Numerical simulation; solution of equations

1 Introduction

The experimental realization of Bose-Einstein condensation (BEC) in double-well trap [1–5] and optical lattice [6–10] has stimulated active research into various aspects of quantum tunneling phenomena such as the Josephson junction [11–14], atomic interferometry [4], the two-wire waveguide [2], etc. Dalfovo [11] suggested a Josephson like effect by considering a confining potential with two wells separated by a barrier. A difference between the chemical potentials of the atoms in the two traps can be achieved, for example, by loading a different number of atoms in the traps. The first experimental evidence [7] of the oscillating atom current was observed instead in an one-dimensional Josephson Junction array realized with condensates in a laser standing wave, i.e., an optical lattice [15]. The latest techniques of coherently splitting the condensate by deforming the single optical trap into two wells serve as a model system for tunneling in the condensate and provide a perfect demonstration of a trapped-atom interferometer [4,5].

The coherent tunneling of BEC between double-well traps results in the level splitting of the macroscopic ground state and hence the macroscopic coherence, which has been observed in interference experiments [1,4]. Recently, the energy-band structure and level splitting due to quantum tunneling in two weakly linked condensates in the "phase" representation have been evaluated in terms of the periodic instanton method [16], which manifests itself as a powerful tool for the calculation of the tunneling rate and a good approximation for the dilute boson gas [17]. It, nevertheless, is not able to explicitly take into account the nonlinear interaction term in the Gross-Pitaevskii equation (GPE) describing the atom-atom collisions in BEC [18]. It is naturally expected that as the number density of atoms in the condensates increases, the effect of the nonlinear interaction between atoms would become important. In the present paper we solve the GPE numerically in order to have a quantitative evaluation of the energy level splitting of the ground state for BEC confined in a symmetric double-well trap and an optical lattice and explore the dependence of the energy level splitting on the chemical potential and the s-wave scattering length between atoms.

Although the numerical solution of GPE has been developed into a standard procedure, this never prevents us from seeking efficient analytical methods. The advantage of a nonperturbative method is that it gives not only an good 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, bubble nucleation and string theory, enable also the investigation of the finite temperature behavior of these systems. In the case of the Bose-Einstein system, it turns out that the periodic instanton method is reliable in evaluating the tunnel splitting for BEC trapped in both the double-well and optical lattice in the regime of experimental values of the chemical potential and scattering length. The intention of this

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paper is to quantitatively compare the deviation of the instanton result from the exact numerical solution and to address the applicability of the instanton method to actual experimental situations.

We restricted our discussion to a quasi-one-dimensional (Q1D) BEC since it is mathematically simple, in which the BEC is prepared in optical and magnetic traps by putting atoms in cylindrical traps long enough that the one-particle energy-level spacing in the radial direction exceeds the interatomic-interaction energy, and the atoms can move effectively in the axial direction [19].

The paper is organized as follows. In Section 2 we give a brief review of the mean-field analysis for BEC trapped in external potentials. In Section 3 the energy level splitting is derived in terms of the instanton method based on the GPE with, however, the nonlinear interaction term included implicitly in the chemical potential. In Section 4 we present the numerical procedure for solving the GPE and evaluation of the ground state level splitting. The numerical level splitting is compared with the instanton result in Section 5 and a brief summary is given in Section 6.

2 GPE for one-dimensional Bose gas

We are interested in the macroscopic quantum tunneling between the condensates separated by potential barriers and the main concern here is how the nonlinear interaction between the atoms would affect the level splitting. We begin with the energy functional for the condensed bosons of mass m confined in the external potential $V(x)$ given by

$$E=\int dx\left[\frac{\hbar^2}{2m}\left|\frac{d\psi\left(x\right)}{dx}\right|^2+V(x)\left|\psi\left(x\right)\right|^2+\frac{U_0}{2}\left|\psi\left(x\right)\right|^4\right] \tag{1}$$

where the order parameter of the condensate $\psi\left(x\right)$ are normalized to the number of atoms in the condensate $\int dx\left|\psi\left(x\right)\right|^2=N$ and the 1D effective interaction constant $U_0=2\hbar^2a/ma_\perp^2$ [20,21] characterizes the nonlinear interaction in the condensate through s-wave scattering length a. Here the radial extension of the ground state wavefunction $a_\perp=\sqrt{\hbar/m\omega_\perp}$ is a typical length scale in the transverse trap with a confinement frequency $\omega_\perp$. The first-order variation of the energy functional leads to the Gross-Pitaevskii equation (GPE), $H\psi\left(x\right)=\mu\psi\left(x\right)$, with the chemical potential $\mu=\left\langle\psi\left|H\right|\psi\right\rangle/N$ calculated as the expectation value of the Hamiltonian

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)+U_0\left|\psi\left(x\right)\right|^2. \tag{2}$$

The transverse confinement frequency $\omega_\perp$ should be large compared with $\mu/\hbar$ so that the condensate is prepared in one dimension. On the other hand, for a less strong transverse confinement, atoms will oscillate in all directions which makes the model not exactly solvable. As can be seen in the last part of the paper, tunneling would be greatly enhanced in 3D.

Consider two models of the external potential where atoms can tunnel through the barriers. The double-well trapping potential of the form

$$V_{dw}(x)=V_0\left(1-x^2/x_0^2\right)^2 \tag{3}$$

allows us to investigate the interwell coupling which results in the splitting of the energy level. The potential barrier of depth V_0 between the two minima $\pm x_0$ is assumed to be large enough so that the overlap between the wave functions relative to the two traps occurs only in the classically forbidden region where the interaction can be ignored. The optical lattice trapping potential

$$V_{ol}(x)=V_0\cos^2\left(k_0x\right), \tag{4}$$

on the other hand, formed by the standing wave laser beams with wavevector k_0 [8], simulates the sine-Gordon potential which is widely used in quantum field theory as a periodic field model [22]. Quantum tunneling between many wells leads to the formation of energy bands due to the spatially periodic potential (4). A path integral calculation [22] was done for these quantum tunneling models both for vacuum and excited states neglecting, however, the nonlinear interaction. In our previous work [18], the nonlinear interaction between the atoms was included in the finite chemical potential and we realized that tunneling occurs at the level of chemical potential. Here we will solve the GPE numerically and compare the numerical results with the analytical ones.

For convenience we rescale the energies and distances in units of $\hbar\omega_0$ and oscillator lengths $a_0=\sqrt{\hbar/m\omega_0}$, with $\omega_0=\sqrt{V''(x_b)/m}$ being the frequency of small oscillations at the bottom of each well x_b in double-well or optical lattice traps. The wave function is correspondingly rescaled in units of $\sqrt{1/a_0}$ so that it remains normalized to N. The GPE thus takes the following dimensionless form

$$\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)+U_0\left|\psi\left(x\right)\right|^2\right]\psi\left(x\right)=\mu\psi\left(x\right) \tag{5}$$

with the potential barrier V_0 and chemical potential μ measured in units of $\hbar\omega_0$ and the nonlinear interaction parameter becomes $U_0=2aa_0/a_\perp^2$. Furthermore, we fix the potential parameters as $x_0=\sqrt{8V_0}$ and $k_0=1/2\sqrt{V_0}$ in order to leave us with only one adjustable parameter, i.e., the potential depth V_0. The tunnel splitting depends on these parameters x_0 and k_0, which are effectively the separations between the well bottoms, in a similar way as on V_0. In the case of an optical lattice, the depth of the barrier is usually measured in units of the recoil energy $E_r=\hbar^2k_0^2/2m$ of the atoms. It is, however, not difficult to transfer the energy units between this convention and ours.

3 The tunnel splitting evaluated with instanton method

Quantum tunneling between noninteracting particles localized in two adjacent wells with macroscopic wave

functions ψ_+, ψ_- leads to an effective energy level splitting $\Delta\mu$, which removes the asymptotic degeneracy. The wave functions of the ground state ψ_e with even parity and the first excited state ψ_o with odd parity are superpositions of the localized wave functions ψ_+ and ψ_-

$$\psi_e = (\psi_+ + \psi_-)/\sqrt{2} \tag{6}$$

$$\psi_o = (\psi_+ - \psi_-)/\sqrt{2} \tag{7}$$

with energy eigenvalues $\mu \pm \Delta\mu/2$, respectively. When the interatomic coupling constant U_0 vanishes, the problem reduces to the solution of a linear Schröndinger equation with the Hamiltonian $H = -(1/2)d^2/dx^2 + V(x)$. The nonlinear interaction increases the chemical potential and even for the system at zero temperature, tunneling occurs at a higher level μ than the ground state. The tunnel splitting can be found with the instanton method [18,22] and is generally expressed as

$$\Delta\mu = \frac{\omega(\mu)}{\pi}\exp[-S(\mu)] \tag{8}$$

where the imaginary time action $S(\mu)$ is calculated through the barrier region ($\mu < V(x)$) once from turning point $-b$ to turning point b:

$$S(\mu) = \int_{-b}^{b}\sqrt{2(V(x)-\mu)}dx \tag{9}$$

and the frequency $\omega(\mu)$ appearing in the prefactor is the frequency of the classical periodic oscillations at energy $\mu > V(x)$ in the classically accessible region with the boundary determined by the turning points b and a

$$\omega(\mu) = \frac{\pi}{\int_b^a \frac{dx}{\sqrt{2(\mu - V(x))}}}. \tag{10}$$

The path integral method [23] has been used in the evaluation of the tunneling rate prefactor and the barrier V_0 between two wells is assumed to be high enough to safely use the WKB wave functions [11] in the calculation of the transition amplitude. For the potential in the form of (3) the level splitting reduces to

$$\Delta\mu = \frac{\sqrt{1+u}}{2\mathcal{K}(k')}\exp(-W) \tag{11}$$

$$W = \frac{16V_0}{3}(1+u)^{1/2}\left(\mathcal{E}(k) - u\mathcal{K}(k)\right), \tag{12}$$

where $\mathcal{K}(k)$ and $\mathcal{E}(k)$ denote the complete Jacobian elliptic integral of the first and second kinds respectively. The corresponding parameters are defined as $u = \sqrt{\mu/V_0}$, $k^2 = (1-u)/(1+u)$, and $k'^2 = 1 - k^2$. When the nonlinear interaction vanishes, the dimensionless chemical potential reduces to $\mu = 1/2$ and the above result turns out to be

$$\Delta\mu = \sqrt{\frac{2}{\pi}}8V_0^{1/2}\exp\left(-\frac{16V_0}{3}\right). \tag{13}$$

which resembles the case of the vacuum instanton.

Tunneling between many potential wells splits the level further into as many sublevels as the number of wells. The Bloch theorem tells us that the eigenvalues of the periodic potential exhibits an energy band structure in the tight-binding approximation

$$E(\theta) = \mu + \frac{\Delta\mu}{2}\cos(\theta a) \tag{14}$$

with $\Delta\mu$ the band width of the quantum state with energy μ. Here the Bloch wave vector θ is confined to the first Brillouin zone $[-\pi/a, \pi/a]$ of the optical lattice with a lattice constant $a = \lambda/2$. For the periodic potential of the optical lattice (4), the energy band width reads

$$\Delta\mu = \frac{1}{2\sqrt{2}\mathcal{K}(k')}\exp(-W) \tag{15}$$

$$W = 4\sqrt{2}V_0\left(\mathcal{E}(k) - k'^2\mathcal{K}(k)\right) \tag{16}$$

with $k^2 = 1 - \mu/V_0$.

4 Numerical procedure

There exist various numerical approaches for studying the energy spectrum and dynamics of BEC trapped in the external potentials [24]. In the present paper, we solve the GPE numerically and find the ground- and first excited-state wave functions $\psi_e(x)$, $\psi_o(x)$ where the corresponding energy expectation values μ_e and μ_o are obtained by direct calculation. The level splitting $\Delta\mu = \mu_e - \mu_o$ is described as a function of parameters N and U_0.

We adopt the Gauss-Seidel method to solve equation (5) numerically and hence start from the diffusion equation

$$\partial_t\psi = -H\psi =: \frac{1}{2}\frac{d^2\psi}{dx^2} - \frac{1}{2}\rho, \tag{17}$$

with a diffusion constant of 1/2 and a source term ρ. As $t \to +\infty$, the wave function relaxes to an equilibrium solution which means that all time derivatives vanish. As a matter of fact the diffusion equation (17) is obtained from the NLSE equation (5) with the time being replaced by a negative imaginary time.

We use the following Crank-Nicholson scheme to discretize equation (17) by using the space step h and time step Δ

$$\begin{aligned}\frac{\psi_i^{n+1} - \psi_i^n}{\Delta} = \frac{1}{2h^2}[&\left(\psi_{i+1}^{n+1} - 2\psi_i^{n+1} + \psi_{i-1}^{n+1}\right) \\ &+ \left(\psi_{i+1}^{n} - 2\psi_i^{n} + \psi_{i-1}^{n}\right)] \\ &- \frac{1}{2}\left[V_i(x_i) + U_0|\psi_i^n|^2\right]\left(\psi_i^{n+1} + \psi_i^n\right)\end{aligned} \tag{18}$$

where $\psi_i^n = \psi(x_i, t_n)$ denotes the exact solution at $x_i = ih$ and $t_n = n\Delta$. The method is stable, unitary, and second-order accurate in space and time [25–27]. In a lattice of s points equation (18) represents a tridiagonal set with open boundary conditions or a cyclic tridiagonal set

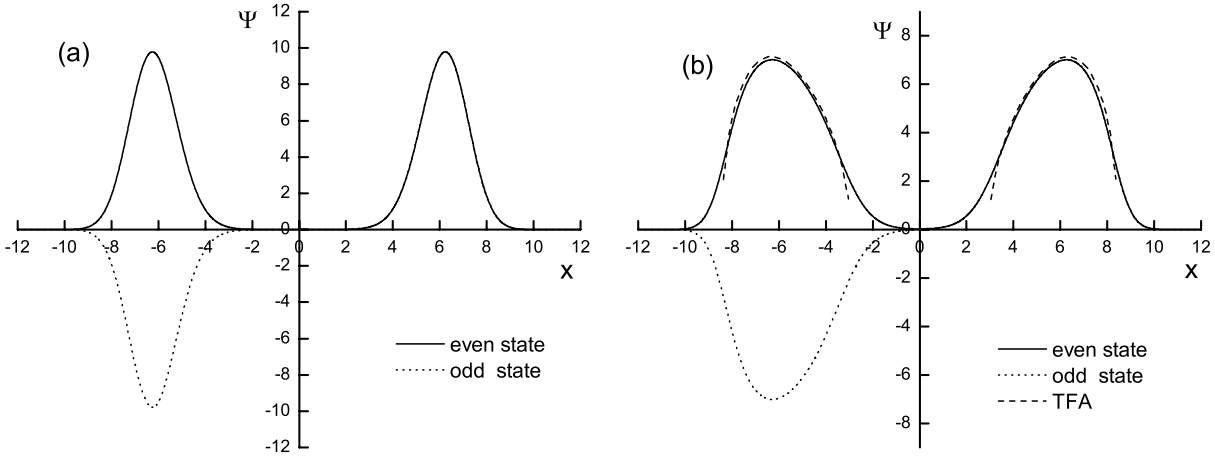

Fig. 1. Level splitting and wavefunctions of condensates confined in a double well potential for $V_0 = 5$. (a) The symmetric (full line) and antisymmetric (dotted lines) wave functions of the ground state with $U_0 = 0$ (noninteracting case). (b) The same as (a) but for $U_0 = 0.06$. The Thomas–Fermi solution $\psi_{TF} = [(\mu - V(x))/U_0]^{1/2}$ is shown by the dashed lines.

with periodic boundary conditions for $i = 2, 3, ..., s-1$. For tridiagonal sets, the whole solution can be encoded very concisely using the procedures of LU decomposition, forward- and back- substitution while for cyclic tridiagonal sets, the procedure of Sherman-Morrison Formula is used [25]. For the double-well case we choose the space step $h = 0.01$, time step $\Delta = 0.001$ and, $s = 2400$. For the optical lattice, $\Delta = 0.02$ and $s = 2500$. The values of these parameters are chosen to satisfy the stability criterion of the Crank-Nicholson code.

We start from the initial, trial wave functions ($t = 0$) given in equations (6) and (7) and choose the eigenstates in the non-interacting limit as our trial wave functions such that ψ^+, ψ^- are the degenerate eigenstates in the left- and right-well with the same energy eigenvalue. In our procedure, all of the wavefunctions with even parity finally evolve into the lowest eigenstate with even parity, i.e., the lower level state for the double well or the bottom of energy band for the optical lattice. Similarly those states with odd parity evolve into the lowest state with odd parity, i.e., the upper level state for the double well or the top of the energy band for the optical lattice. The boundary and normalization conditions are implemented at each time step. To test the validity of our code, the numerical wave functions for a stationary GPE in a spherical trap is compared with the corresponding results given in [28] and the agreement is perfect.

5 Numerical result with the nonlinear interaction

As an example we consider weak-linked condensates of ^{87}Rb atoms confined in multi-traps with frequency $\omega_0 = 100$ Hz as in reference [12] and the corresponding oscillator length is $a_0 = 2.70 \times 10^{-4}$ cm. The s-wave scattering length is in the range $85a_{bohr} < a_{sc} < 140a_{bohr}$, where a_{bohr} is the Bohr radius [29]. In our analysis we use $a_{sc} = 100a_{bohr}$. The transverse confinement frequency $\omega_\perp$ is taken to be $2\pi \times 250$ Hz. The corresponding radial extension $a_\perp = 6.81 \times 10^{-4}$ cm and the interatomic-interaction constant $U_0 = 0.06$ (in units of $\hbar\omega_0$), which corresponds to a weak [30] nonlinear interaction such that we could examine its effect on the level splitting. We always measured energies in units of $\hbar\omega_0$ and lengths in units of the oscillator length a_0, so V_0 is all we need.

As a comparison we first of all deal with the "noninteracting" case. When $V_0 = 5$, the analytical tunnel splitting of the instanton approach given in equation (11) is $\Delta\mu = 3.74 \times 10^{-11}$ and our numerical result is $\Delta\mu = 3.60 \times 10^{-11}$. This again proves the validity of our numerical simulation. The corresponding wave function is shown in Figure 1a. In this paper we are mainly interested in the ground state, and for this purpose the choice of $s = 2400$ is seen to be adequate for most of the calculations. In Figure 1b we show the profiles of the even (solid line) and odd (dotted line) wave functions $\psi_{e,o}(x)$ for 344 atoms confined in the trap with height $V_0 = 5$, which are the even- and odd-eigenstates of the Hamiltonian with the nonlinear interaction term $U_0 |\psi(x)|^2$. Also the Thomas-Fermi approximation $\psi_{TF} = [(\mu - V(x))/U_0]^{1/2}$ for $V(x) < \mu$ is given by the dashed lines.

Now we turn to examine the difference of level splitting obtained from the instanton method and the numerical simulation for the double-well trap. In Figure 2, $\Delta\mu$ on a logarithmic scale to base 10 as a function of the chemical potential is depicted for barrier heights, $V_0 = 4$ and $V_0 = 5$. Results from both the numerical simulation (solid line) and instanton approach (dotted line) exhibit an enhancement of the tunneling with increasing chemical potential. To show how large the difference is, in the insets, we plot the splitting divided by the exponential factor of the analytical result. The results of the two approaches always have the same order of magnitude and are close to each other. The periodic instanton method evaluates fairly well the tunneling splitting even if the nonlinear interaction is included. Quantitatively, however, it always overestimates the splitting for the whole range of the chemical

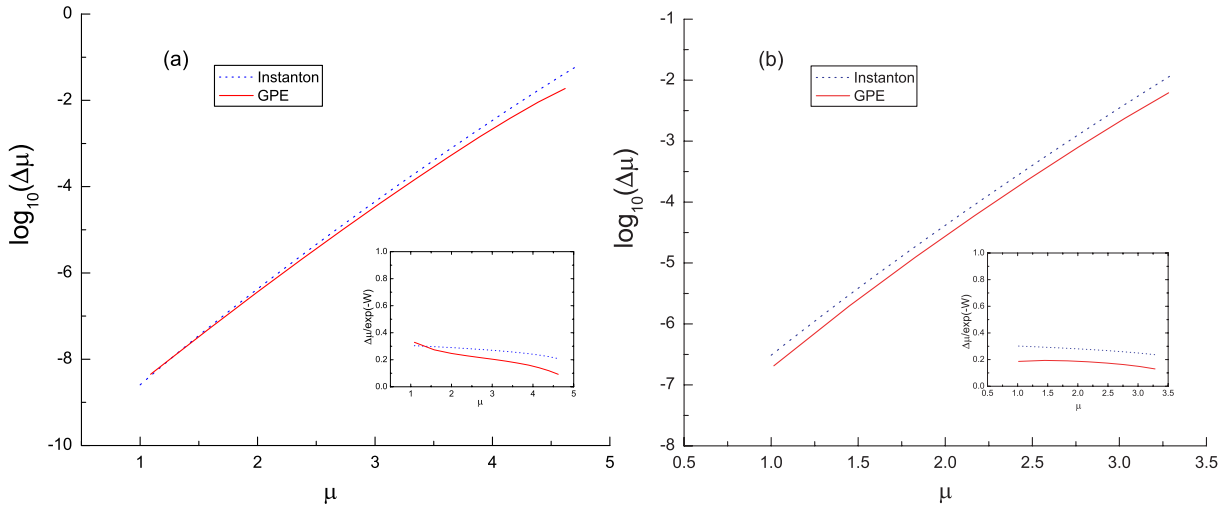

Fig. 2. Level splitting as a function of chemical potential μ for two values of the barrier height $V_0 = 5$ (a) and $V_0 = 4$ (b). Insets: the splitting divided by the exponential factor of the analytical result in the insets. Solid lines: GPE results $\Delta\mu_{\rm GPE}/\exp(-W)$, dotted lines: periodic instanton results $\Delta\mu_{\rm Instanton}/\exp(-W)$.

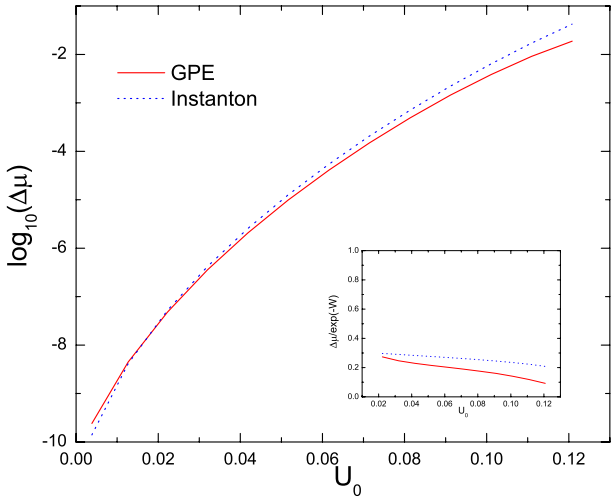

Fig. 3. The interaction constant U_0 dependence of level splitting for condensates in a double-well for $V_0 = 5$. The inset shows the splitting divided by the exponential factor of analytical result. Solid lines: GPE results, $\Delta\mu_{\rm GPE}/\exp(-W)$, dotted lines: periodic instanton results $\Delta\mu_{\rm Instanton}/\exp(-W)$.

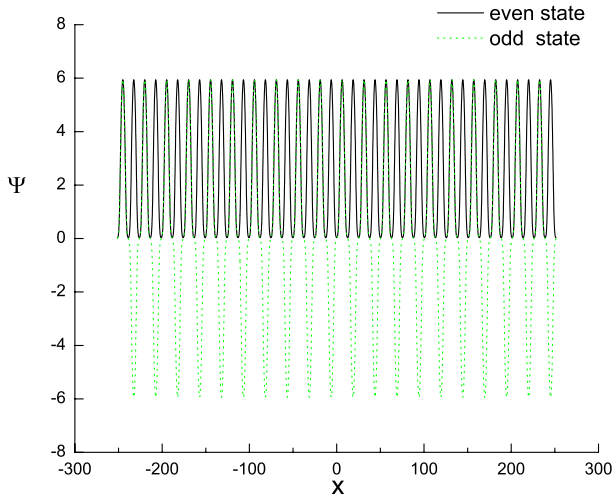

Fig. 4. The symmetric (full line) and antisymmetric (dotted lines) wave functions in an optical lattice for $V_0 = 5$.

potential. These can be seen more clearly from the interacting constant U_0 dependence of the level splitting displayed in Figure 3 and its inset for $V_0 = 5$. We emphasize here that a peculiar feature of this periodic instanton result for the level splitting is that the prefactor depends on the chemical potential as displayed in the insets of Figure 2. This result is important, as has been shown in [18].

For the case of the optical lattice potential we still choose the same parameters as in the case of the double-well. The nonlinear interaction constant between atoms in the same well, $U_0 = 0.06$ for the repulsive interaction. The typical profile of the condensate wave function $\psi_e(x)$, shown by the solid line, and $\psi_o(x)$, shown by the dotted lines, are plotted in Figure 4 for $V_0 = 5$ and 150 atoms in each well. The even wave function is symmetric, and the odd wave function is maximally antisymmetric, i.e., the wavefunction segment in each well is antisymmetric with respect to those of its neighbors. Figures 5a and 5b display the chemical potential dependence of the level splitting for $V_0 = 5$ and $V_0 = 4$, as determined by the method outlined above. Again, we find the results from the periodic instanton method and GPE have the same order of magnitude.

By comparing Figures 2 and 5, it is shown that when the nonlinear interaction between atoms is included, the level splitting is smaller than the instanton result in the double-well case, but the splitting is larger in the optical lattice case. This distinction depends on the structure of the trapping potentials, for example, atoms in the optical lattice can tunnel through the barrier in two directions,

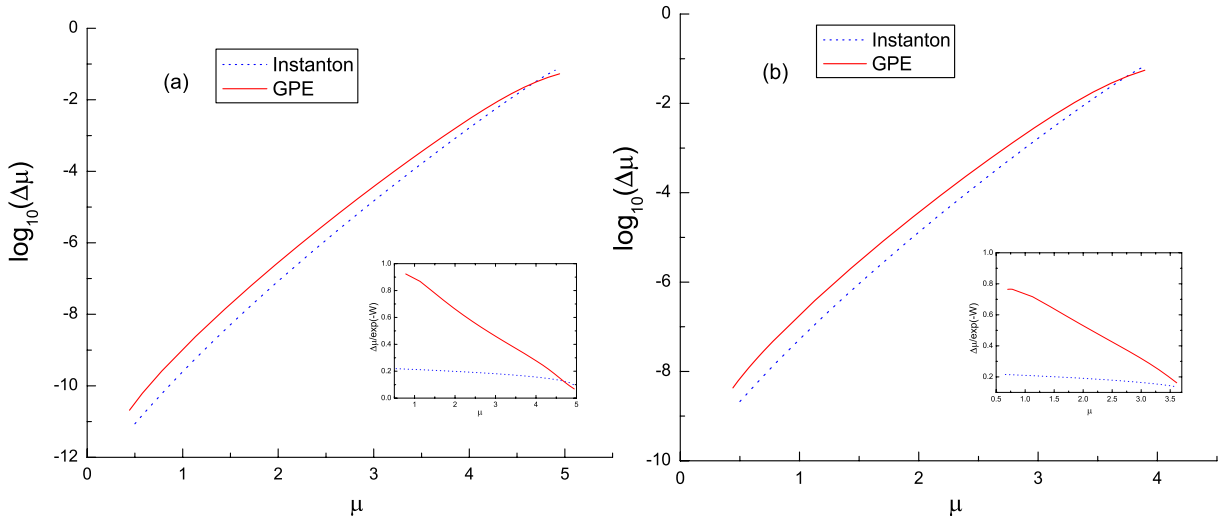

Fig. 5. Level splitting as a function of chemical potential μ in an optical lattice for $V_0 = 5$ (a) and $V_0 = 4$ (b). The insets show the splitting divided by the exponential factor of the analytical result. Solid lines: GPE results $\Delta\mu_{\mathrm{GPE}}/\exp(-W)$, dotted lines: periodic instanton results $\Delta\mu_{\mathrm{Instanton}}/\exp(-W)$.

while the tunnel path for those in the double-well is one-way only. This makes the periodic instanton result different from the double well case. In spite of this, the periodic instanton method remains good enough to describe the level splitting for the BEC.

Recently a single bosonic Josephson junction [31] has been implemented by two weakly linked BEC in a double-well potential. In previously reported realizations of condensates in double-well potentials [5] the time scale of tunneling dynamics was in the range of thousands of seconds. In contrast, their set-up allows the realization of nonlinear tunneling times on the order of 50 ms, which makes the direct observation of the nonlinear dynamics in a single bosonic Josephson junction possible for the first time. We emphasize here the distinction between tunneling in 3D and that in quasi-1D systems. The important parameter, the "tunneling matrix element" K [12] between two condensates is related to the energy level splitting through $K = \Delta\mu/2$. The period of oscillation T can be obtained by numerically integrating equation (1) in reference [31] for each given parameter $\Lambda = NU_0/2K$. In the 3D case, K is often assumed to be of the order 0.1 nK or 25 Hz, which gives a relative small value for $\Lambda \sim 10$. In contrast, in the 1D case, the tight confinement in the other 2 directions would suppress drastically the tunneling and make the link between the condensates even weaker. According to our calculation the parameter K obviously takes typical values of $10^{-3} \sim 1$ Hz and Λ may be as large as $10^3 \sim 10^6$. As a consequence, the atoms tend to be trapped in the potential wells and the observation of Josephson oscillation becomes almost impossible, e.g., the initial population imbalance must be less than 0.06 for $\Lambda \sim 10^3$. A simple calculation shows that for $N = 600$, $U_0 = 0.06$, $V_0 = 5$, the Josephson oscillation may be observed with a period 2 ms, which is less than that in the 3D experiments.

According to our calculation, the energy splitting is very small compared with the chemical potential of the system and increases exponentially with the chemical potential. The tunneling effect gives rise to the macroscopic phase coherence of BEC across the barriers, which results in the significant observable interference phenomena between different BEC segments.

6 Summary

In this paper we have investigated the tunnel splitting of the ground state for a weakly-linked BEC trapped in double-well potential and in optical lattice by solving the Gross-Pitaevskii equations numerically. It turns out that the periodic instanton method is a reliable tool in the evaluation of the tunnel splitting for the BEC. The reason for this is that for the quantum tunneling through the potential barrier, the nonlinear interaction is negligibly small and contributes overall to a finite chemical potential. Our numerical scheme could easily be improved for the investigation of the dynamical behavior of the condensates in multi-well potentials.

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