Macroscopic quantum tunneling of Bose-Einstein condensate with $\phi^6$ interaction

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Abstract. Macroscopic quantum tunneling of Bose-Einstein Condensate in a double-well potential is discussed in the frame of an experimentally realizable Hamiltonian with $\phi^6$ interaction under the two-mode approximation. Concentrating on a special case $\Delta E = \Lambda = 0$, we analyze the stationary states and dynamics of the system to find that such system possesses very small phase spaces for Josephson oscillation and usually lies in the macroscopic quantum self-trapping state (MQST). Importantly we obtain three kinds of MQSTs and in terms of them show the phase diagrams of the system.

1. Introduction
The coherent oscillation of Bose-Einstein condensate (BEC) in a double-well potential, generally denoted by the boson Josephson junction (BJJ) and widely studied theoretically [1-5] and observed experimentally [6, 7], has provided an atomic analogy of the superconductor Josephson junction (SJJ) [8]. Depending on the nonlinear interaction and its isolation [2], the BJJ allows investigations of dynamical regimes for the phase difference and population imbalance across the junction and shows much more interesting phenomena, such as $\pi$-phase oscillation and macroscopic quantum self-trapping state (MQST) [2], which are not accessible with the SJJ. The appearance of the MQST is characterized by a population imbalance between two wells of the trapping potential and is linked to a nonlinearity-induced phase locking between the nonlinear eigenstates of the system [9, 10]. Especially, the MQST in a symmetric double-well potential represents a classical paradigm of spontaneous symmetry breaking.

Basically the researches on the BJJ are based on the Gross-Pitaevskii equation (GPE) [11, 12] with $\phi^4$ interaction using the two-mode approximation [2]. However the inclusion of $\phi^6$ interaction in the GPE is possible and can be realized at least in two different ways. A direct introduction of $\phi^6$ term is to consider the three-body interaction among bosons. In fact, researches on the three-body interaction originated from accurate calculations of the ground state energy of bosonic systems in 1959 [13]. Following the achievements of BEC in 1995, the determinations on detailed properties of the three-body interaction were revived [14-16]. Furthermore Buchler et al. [17] have suggested that polar molecules driven by microwave fields give naturally rise to the strong three-body interaction. Ensuing from these fundamental works, the phase diagrams of Bose-Hubbard model with the three-body interaction without [18] or with [19] the magnetic field are also derived. Another origin of the term $\phi^6$ can be realized by the induction of fermions. Considering the mixture of a BEC and a single
component Fermi gas with the interspecies interaction strength controlled by Feshbach resonances [20, 21], the Fermi degrees of freedom can be completely integrated out owing to Pauli exclusion principle
and an effective GPE with $\phi^6$ interaction can be produced [22, 23]. By contrast, this method permits more controllabilities by adjusting the concentration of fermions and interspecies interaction. Recently Benítez et al. [24] have discussed coherent macroscopic quantum tunnelings in boson-fermion mixtures on the basis of the quasi-static approximation for the fermionic density, where fermions are considered to form large impurities spatially localized around the minima of the double-well potential. Under this quasi-static approximation, which is essentially equivalent to the mean field method for the boson-fermion interaction, fermions play the similar role with an exterior field coupling with boson density operator, thus the $\phi^6$ term does not appear.

In the light of the availabilities of $\phi^6$ term, the dynamics of the BJJ including $\phi^6$ interaction has also been investigated in the frame of the two-mode approximation [25, 26]. Considering the fact that the effects of three-body recombination on the BEC can be regarded as $\phi^6$ interaction with the imaginary coefficient, Ref. [25] studied an attractive BEC with the atomic feeding and found that the stability region of the system could be enlarged by increasing the three-body losses. By contrast Ref. [26] supposed a real $\phi^6$ interaction and discussed the stable stationary solutions of the system for some special cases. Importantly when a periodically time-varying scattering length is applied, the existence of chaotic behaviours and the dependence of chaos on $\phi^6$ interaction are demonstrated.

In this paper we extend the contents in [26] to another special case ($\Delta E = \Lambda = 0$, see below), which is realizable in an experiment, and analyze stationary and dynamical properties of the system. The plan of this paper is as follows. In section 2, we obtain dynamical equations of the BJJ with $\phi^6$ interaction, called the extended BJJ (EBJJ), then analyze fixed points of equations and their stabilities. In section 3, from a mechanical analogy we classify MQSTs and investigate phase diagrams of the EBJJ. A brief conclusion is given in section 4.

2. EBJJ and fixed points

The EBJJ can be described in terms of the Hamiltonian

$$\begin{align*}
H &= -K(b_i^* b_i + b_i^0 b_i) + \sum_{i=1}^2 \left[ \frac{U_i}{2}(b_i^*)^2(b_i)^2 + \frac{W_i}{6}(b_i^*)^3(b_i)^3 + E_i b_i^* b_i \right],
\end{align*}$$

(1)

where $b_i^*$ ($b_i$) is the bosonic creation (annihilation) operator with $n_i = b_i^* b_i$ being the particle number operator for bosons in the well $i$ ($i=1,2$). The parameters $K, U_i, W_i$ are the amplitude of tunneling between two wells, effective two- and three-body repulsive interaction strengths, respectively. $E_i$ is the zero-point energy in the well $i$, reflecting the symmetry of the double-well potential.

At the mean field level the equations of motion for $b_i$ are

$$\begin{align*}
\frac{i\hbar}{\Delta t} b_i &= -K b_i + E_i b_i + U_i n_i b_i + \frac{W_i}{2} n_i^2 b_i, \\
\frac{i\hbar}{\Delta t} b_i^2 &= -K b_i + E_i b_i^2 + U_i n_i b_i^2 + \frac{W_i}{2} n_i^2 b_i^2.
\end{align*}$$

(2)

Substituting $b_i = \sqrt{n_i} e^{i\theta}$ and introducing two variables $z = \frac{n_1 - n_2}{n_1 + n_2}$, $\theta = \frac{\theta_2 - \theta_1}{2}$, we obtain dynamical equations of the EBJJ

2
\[
\frac{dz}{d\tau} = -\sqrt{1-z^2}\sin\theta, \\
\frac{d\theta}{d\tau} = \Delta E + \Lambda z + \beta z^2 + \frac{z}{\sqrt{1-z^2}}\cos\theta,
\]

with

\[
\Delta E = \frac{E_1 - E_2 + n(U_1 - U_2) / 2 + n^2(W_1 - W_2) / 8}{2K}, \\
\Lambda = \frac{n(U_1 + U_2) / 2 + n^2(W_1 + W_2) / 4}{2K}, \\
\beta = \frac{n^2(W_1 - W_2) / 8}{2K},
\]

where we have rescaled \( t \) to a dimensionless time \( \tau = \frac{2K}{h} t \) and \( n = n_1 + n_2 \) is the total particle number in the double-well potential. So the equations of two complex variables (3) have been reduced to those of two real variables (3) due to the conservation of particle number and the uncertainty of the global phase. These two equations (3) have also been derived in [26] from the viewpoint of the continuum limit. By contrast in [25], there is another equation describing the dynamical behaviours of the total particle number \( n \) owing to imaginary \( \phi^z \) interaction and atomic feeding.

It is known that above description has a canonical structure of classical dynamics with \( z \) and \( \theta \) representing a pair of canonically conjugate variables [27]. The total classical energy is

\[
H_c = \Delta E z + \frac{\Lambda}{2} z^2 + \frac{\beta}{3} z^3 - \sqrt{1-z^2}\cos\theta
\]

and the equations of motion can be written in the Hamiltonian form

\[
\frac{dz}{d\tau} = -\frac{\partial H_c}{\partial \theta}, \quad \frac{d\theta}{d\tau} = \frac{\partial H_c}{\partial z}.
\]

Until now all formulae adapt to symmetrical and asymmetrical double-well potentials. For a symmetric double-well potential \( E_1 = E_2 \), \( U_1 = U_2 \), \( W_1 = W_2 \), \( \Delta E = \beta = 0 \), the dynamics of the EBJ is the same as that of the BJJ [2] except that the nonlinear parameter \( \Lambda \) has been renormalized by \( W_1 \) and \( W_2 \). In order to study pure effects in relation to the \( \beta \) term and as a supplementary to [26], we assume an asymmetric double-well potential and \( \Delta E = \Lambda = 0 \). The latter is possible in light of highly controllabilities of cold atom gases. The offset \( \Delta E \) between two wells can be compensated by an accelerated double-well potential or a direct current electric field, while \( \Lambda \) can be tuned by Feshbach resonances on \( U_1 \) and \( U_2 \). So below we will concentrate on the situation \( \Delta E = \Lambda = 0 \) and \( \beta > 0 \).

The fixed points of the classical Hamiltonian system (5) have one-to-one correspondences to the eigenstates of quantum system [28]. Easily proved, the number of the fixed points strongly depends on the value of \( \beta \). For \( \beta < 2 \), there are two symmetrical fixed points \( (\theta_{z1, z_2}^0) = (0, 0) \) and \( (\theta_{z1, z_2}^\pi) = (\pi, 0) \). For \( \beta > 2 \), the system develops four more asymmetrical fixed points

\[
(\theta_{z1, z_2}^0, z_{z1}^0) = (0, -\sqrt{1 - 4/\beta^2}) \quad \text{and} \quad (\theta_{z1, z_2}^\pi, z_{z1}^\pi) = (\pi, \sqrt{1 - 4/\beta^2}).
\]

While at the critical point \( \beta = 2 \), \( (\theta_{z1, z_2}^0, z_{z1}^0) = (0, -1/\sqrt{2}) \) and \( (\theta_{z1, z_2}^\pi, z_{z1}^\pi) = (0, 1/\sqrt{2}) \), two more fixed points exist. In figure 1 we show the relations between energies of these fixed points and the parameter \( \beta \). Easily
found that the energies of fixed points \( (\theta_{a-}, z_{a-}) \) and \( (\theta_{c-}, z_{c-}) \) tend to those of \( (\theta_{s1}, z_{s1}) \) and \( (\theta_{s2}, z_{s2}) \) respectively in the limit of \( \beta \rightarrow \infty \). Besides, the crossings of energy levels also happen between \( (\theta_{s1}, z_{s1}) \) and \( (\theta_{a+}, z_{a+}^0) \), \( (\theta_{s2}, z_{s2}) \) and \( (\theta_{a+}, z_{a+}^\pi) \), which signifies that the adiabatic approximation is not valid if \( \beta \) changes very slowly with the time.

\[ J = \begin{pmatrix}
\frac{\partial^2 H_c}{\partial \theta^2} & -\frac{\partial^2 H_c}{\partial \theta \partial z} \\
-\frac{\partial^2 H_c}{\partial \theta \partial z} & \frac{\partial^2 H_c}{\partial z^2}
\end{pmatrix} \]  

Figure 1. The relation between energies of fixed points and parameter \( \beta \). The circle line, square line and triangle line correspond to the fixed points in (a) \( (\theta_{s1}, z_{s1}) \), \( (\theta_{a+}, z_{a+}^0) \), \( (\theta_{c-}, z_{c-}) \) and in (b) \( (\theta_{s2}, z_{s2}) \), \( (\theta_{a+}, z_{a+}^\pi) \), \( (\theta_{c+}, z_{c+}) \) respectively.

The criterion of the stability of fixed points is that the eigenvalues of Jacobian of the classical energy \( H_c \)

\[ J = \begin{pmatrix}
\frac{\partial^2 H_c}{\partial \theta^2} & -\frac{\partial^2 H_c}{\partial \theta \partial z} \\
-\frac{\partial^2 H_c}{\partial \theta \partial z} & \frac{\partial^2 H_c}{\partial z^2}
\end{pmatrix} \]  

3. Dynamics of EBJJ

The dynamics of the EBJJ is the same as that of a classical particle with the energy \( w_0 \) moving in a potential \( w(z) \). The effective equation of motion is
\[
\left( \frac{dz}{d\tau} \right)^2 + w(z) = w_0, \tag{8}
\]

where

\[
H_{eo} = H(z(0), \theta(0)), \quad w_0 = 1 - H_{eo}^2,
\]

\[
w(z) = z^2 \left( \frac{\beta^2}{9} z^3 - \frac{2}{3} \beta H_{eo} z + 1 \right). \tag{9}
\]

In order to find the differences between the dynamics of the EBJJ and BJJ, we briefly comment on the BJJ. In the BJJ the potential \( w(z) \) has the parabolic or double-well structure and is symmetrical about \( z = 0 \) [2]. The motions in a parabolic or double well potential with energy \( w_0 \) larger than the barrier between two wells are Josephson oscillations with a zero time-average value of \( z \). While \( w_0 \) is less than the barrier between two wells the system enters into the MQSTs. By contrast the potential \( w(z) \) in the EBJJ is generally asymmetrical about \( z = 0 \) except \( H_{eo} = 0 \), thus the phase space of the Josephson oscillation in the EBJJ is very small and the system is usually in the MQSTs. Essentially this conclusion also pointed out in [26] is very general and does not depend on special assumption \( \Delta E = \Lambda = 0 \). Below we analyze the structure of the potential \( w(z) \) and classify the MQSTs in the EBJJ.

![Figure 2](image-url)

**Figure 2.** Phase diagrams for \( \theta(0) = 0 \) in (a) and \( \theta(0) = \pi \) in (b). Gray, black and blue regimes correspond to MQST-I, MQST-II and MQST-III respectively. Note that Josephson oscillation is not included owing to its small phase space.

In addition to a stationary point \( z^{**} = 0 \), which is a minimum of \( w(z) \), other possible stationary points are the real roots of the equation

\[
z^4 - \frac{3H_{eo}}{\beta} z^2 + \frac{3}{\beta^2} = 0. \tag{10}
\]

Easily found that if \( \beta H_{eo}^2 < 16/9 \), (10) has no real root so that the potential \( w(z) \) has only one stationary point \( z^{**} \) and the system oscillates around \( z^{**} \), which we call MQST-I. If \( \beta H_{eo}^2 > 16/9 \), there are two real roots for (10). Numerically we have proved that both real roots are in the area (-1, 1),
so the potential $w(z)$ becomes a double well and has two more stationary points, one of which corresponds to the minimum called $z^{s2}$ and the other the maximum called $z^{s3}$. Furthermore if $H_{e0} < 0$ the relation among three stationary points is $z^{s2} < z^{s3} < z^{s1}$, conversely $z^{s1} < z^{s3} < z^{s2}$. At this time the dynamics of the EBJJ becomes complicated. On the one hand if $w(z^{s3}) < w_0$, in other words the effective energy of the particle is larger than the height of potential barrier, the particle will move between the two wells and it is called MQST-II. On the other hand if $w(z^{s3}) > w_0$ the particle will be constrained into one well. Depending on the initial condition $z(0)$, there are two cases. For $H_{e0} < 0, z(0) > z^{s3}$ or $H_{e0} > 0, z(0) < z^{s3}$ the system is localized around $z^{s1}$ and is also in the MQST-I. If $H_{e0} < 0, z(0) < z^{s3}$ or $H_{e0} > 0, z(0) > z^{s3}$, the system localizes around $z^{s2}$ and enters into the MQST-III. From the above argument, figure 2 shows phase diagrams of the EBJJ in the plane of $z(0)$ and $\beta$ for $\theta(0) = 0$ and $\theta(0) = \pi$. In the light of the fact that the classical energy satisfies the relation $H_c(z,0) = -H_c(-z,\pi)$, the phase diagram (b) can also be obtained by reflecting the phase diagram (a) about the $z(0) = 0$, and vice versa. Note that in figure 2 we do not include the Josephson oscillation due to its small phase spaces, which lies in the region of MQST-I.

![Figure 3](image-url)

**Figure 3.** Dynamical evolution of the EBJJ for $\theta(0) = 0$ and $\beta = 6$. (a) $z(0) = -0.1, w_0 = 0.006, z^{s3} = -0.169, w(z^{s3}) = 0.009$, (b) $z(0) = 0.3, w_0 = 0.19, z^{s3} = -0.188, w(z^{s3}) = 0.012$, (c) $z(0) = -0.8, w_0 = -1.637, z^{s3} = -0.103, w(z^{s3}) = 0.004$ correspond to respectively the MQST-I, MQST-II, MQST-III, which are consistent with the figure 2. In (d) $z(0) = 0.707$ and $H_{e0} = 0$, the system is in the Josephson oscillation.
In figure 3, we numerically solve the equations of motion (3) to observe dynamical behaviours of the EBJJ for $\theta(0) = 0$. The case for $\theta(0) = \pi$ is available by the relation $H_c(z,0) = -H_c(-z, \pi)$. These results validate the correctness of phase diagrams in figure 2.

4. Conclusions
In conclusion we have discussed the macroscopic quantum tunneling of BEC in a double-well potential in the frame of an experimentally realizable Hamiltonian with $\phi^6$ interaction. Using the two-mode approximation we have derived two coupled equations of phase difference and population imbalance between two wells. Focusing on a special case $\Delta E = \Lambda = 0$, we analyze the stationary states and dynamics of the system. Importantly we obtain three kinds of MQSTs and in terms of them show the phase diagrams of the system.

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