Finite-size effects in a bosonic Josephson junction

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We investigate finite-size quantum effects in the dynamics of $N$ bosonic particles which are tunneling between two sites adopting the two-site Bose-Hubbard model. By using time-dependent atomic coherent states (ACS) we extend the standard mean-field equations of this bosonic Josephson junction, which are based on time-dependent Glauber coherent states. In this way we find $1/N$ corrections to familiar mean-field (MF) results: the frequency of macroscopic oscillation between the two sites, the critical parameter for the dynamical macroscopic quantum self trapping (MQST), and the attractive critical interaction strength for the spontaneous symmetry breaking (SSB) of the ground state. To validate our analytical results we perform exact numerical simulations of the quantum dynamics. In the case of Josephson oscillations around a balanced configuration we find that also for a few atoms the numerical results are in good agreement with the predictions of time-dependent ACS variational approach, provided that the time evolution is not too long. Also the exact numerical results of SSB are better reproduced by the ACS approach with respect to the MF one. Instead the onset of MQST is correctly reproduced by ACS theory only in the large $N$ regime and, for this phenomenon, the $1/N$ correction to the MF formula is not reliable.

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I. INTRODUCTION

The Josephson junction is a quantum mechanical device made of two superconductors, or two superfluids, separated by a tunneling barrier [1]. The Josephson junction can give rise to the direct-current (DC) Josephson effect, where a supercurrent flows indefinitely long across the barrier, but also to the alternate-current (AC) Josephson effect, where due to an energy difference the supercurrent oscillates periodically across the barrier [2]. The superconducting quantum interference devices (SQUIDs), which are very sensitive magnetometers based on superconducting Josephson junctions, are widely used in science and engineering [3]. Moreover, DC SQUIDs sandwiched between two metal islands are now used as qubits of quantum computers (see, for instance, [4]).

The achievement of Bose-Einstein condensation with ultracold and dilute alkali-metal atoms [5] has renewed and increased the interest on macroscopic quantum phenomena and, in particular, on the Josephson effect [6]. Indeed, contrary to the case of superconducting Josephson junctions, with atomic Josephson junctions it is possible to have a large population imbalance with the appearance of the self-trapping phenomenon [7]. A direct experimental observation of macroscopic quantum tunneling and nonlinear self-trapping in a single bosonic Josephson junction was made in 2005 with $^{87}$Rb atoms [8]. More recently, in 2015, Josephson effect has been detected in fermionic superfluids across the BEC-BCS crossover with $^6$Li atoms [9].

The fully quantum behavior of Josephson junctions is usually described by using the phase model [10], which is based on the quantum commutation rule [11] between the number operator $\hat{N}$ and the phase angle operator $\hat{\phi}$. Within this model it has been found that quantum fluctuations renormalize the mean-field Josephson oscillation [12, 13]. However, the phase angle operator $\hat{\phi}$ is not Hermitian, the exponential phase operator $\exp(i\hat{\phi})$ is not unitary, and their naive application can give rise to wrong results. Despite such problems, the phase model is considered a good starting point in many theoretical studies of Josephson junctions, because the phase-number commutation rule is approximately correct for systems with a large number of condensed electronic Cooper-pairs or bosonic atoms [14].

In this paper we study finite-size quantum effects in a Josephson junction avoiding the use of the phase operator. The standard mean-field theory is based on the Glauber coherent state $|CS\rangle$ which however is not eigenstate of the total number operator $\hat{N}$. Here we adopt the atomic coherent state $|ACS\rangle$, which is instead eigenstate of the total number operator, and it reduces to the Glauber coherent state only in the limit of a large num-
Quite remarkably, this time-evolution equation can be derived by extremizing the following action

$$S = \int dt \langle \psi(t) \rangle \left( i\hbar \frac{\partial}{\partial t} - \hat{H} \right) |\psi(t)\rangle ,$$

characterized by the Lagrangian

$$L = i\hbar \langle \psi(t) | \frac{\partial}{\partial t} |\psi(t)\rangle - \langle \psi(t) | \hat{H} |\psi(t)\rangle .$$

### III. STANDARD MEAN-FIELD DYNAMICS

The familiar mean-field dynamics of the bosonic Josephson junction can be obtained with a specific choice for the quantum state $|\psi(t)\rangle$, namely

$$|\psi(t)\rangle = |CS(t)\rangle ,$$

where

$$|CS(t)\rangle = |\alpha_1(t)\rangle \otimes |\alpha_2(t)\rangle$$

is the tensor product of Glauber coherent states $|\alpha_j(t)\rangle$, defined as

$$|\alpha_j(t)\rangle = e^{-\frac{1}{2}|\alpha_j(t)|^2} e^{\alpha_j(t)\hat{a}_j^\dagger}|0\rangle$$

with $|0\rangle$ the vacuum state, and such that

$$\hat{a}_j|\alpha_j(t)\rangle = \alpha_j(t)|\alpha_j(t)\rangle .$$

Thus, $|\alpha_j(t)\rangle$ is the eigenstate of the annihilation operator $\hat{a}_j$ with eigenvalue $\alpha_j(t)$ [15]. The complex eigenvalue $\alpha_j(t)$ can be written as

$$\alpha_j(t) = \sqrt{N_j(t)} e^{i\phi_j(t)} ,$$

with $N_j(t) = \langle \alpha_j(t) | \hat{N}_j |\alpha_j(t)\rangle$ the average number of bosons in the site $j$ at time $t$ and $\phi_j(t)$ the corresponding phase angle at the same time $t$.

Adopting the coherent state [17] with Eq. 8, the Lagrangian [15] becomes

$$L_{CS} = i\hbar \langle CS(t) | \frac{\partial}{\partial t} |CS(t)\rangle - \langle CS(t) | \hat{H} |CS(t)\rangle$$

$$= N\hbar z \dot{\hat{\phi}} - \frac{U N^2}{2} z^2 + JN \sqrt{1 - z^2} \cos(\hat{\phi}) ,$$

where the dot means the derivative with respect to time $t$,

$$N = N_1(t) + N_2(t)$$

is the average total number of bosons (that is a constant of motion),

$$\phi(t) = \phi_2(t) - \phi_1(t)$$

is the relative phase, and

$$z(t) = \frac{N_1(t) - N_2(t)}{N}$$
is the population imbalance. The last term in the Lagrangian (11) is the one which makes possible the periodic oscillation of a macroscopic number of particles between the two sites.

In the Lagrangian $L_{CS}(\phi, z)$ of Eq. (11) the dynamical variables $\phi(t)$ and $z(t)$ are the generalized Lagrangian coordinates (see, for instance, [25]). The extremization of the action (11) with the Lagrangian (11) gives rise to the Euler-Lagrange equations

$$\frac{\partial L_{CS}}{\partial \phi} - \frac{d}{dt} \frac{\partial L_{CS}}{\partial \dot{\phi}} = 0, \quad \frac{\partial L_{CS}}{\partial z} - \frac{d}{dt} \frac{\partial L_{CS}}{\partial \dot{z}} = 0,$$

which, explicitly, become

$$\dot{\phi} = J \frac{z}{\sqrt{1 - z^2}} \cos(\phi) + UNz, \quad \dot{z} = -J \sqrt{1 - z^2} \sin(\phi).$$

These equations describe the mean-field dynamics of the macroscopic quantum tunneling in a Josephson junction, where $\phi(t)$ is the relative phase angle of the complex field of the superfluid (or superconductor) between the two junctions at time $t$ and $z(t)$ is the corresponding relative population imbalance of the Bose condensed particles (or Cooper pairs).

Assuming that both $\phi(t)$ and $z(t)$ are small, i.e. $|\phi(t)| \ll 1$ and $|z(t)| \ll 1$, the Lagrangian (11) can be approximated as

$$L^{(2)}_{CS} = \hbar z \dot{\phi} - \frac{JN}{2} \phi^2 - \frac{(JN + UN^2)}{2} z^2,$$

removing a constant term. The Euler-Lagrange equations of this quadratic Lagrangian are the linearized Josephson-junction equations

$$\hbar \ddot{\phi} = (J + UN)z, \quad \hbar \ddot{z} = -J \phi,$$

which can be rewritten as a single equation for the harmonic oscillation of $\phi(t)$ and the harmonic oscillation of $z(t)$, given by

$$\ddot{\phi} + \Omega^2 \phi = 0, \quad \ddot{z} + \Omega^2 z = 0,$$

both with frequency

$$\Omega = \frac{1}{\hbar} \sqrt{J^2 + UNJ},$$

that is the familiar mean-field frequency of macroscopic quantum oscillation in terms of tunneling energy $J$, interaction strength $U$, and number $N$ of particles [26].

It is straightforward to find that the conserved energy of the mean-field system described by Eqs. (17) and (18) is given by

$$E_{CS}(z(0), \phi(0)) > H_{CS}(0, \pi),$$

if the condition

$$E_{CS}(z(0), \phi(0)) > H_{CS}(0, \pi)$$

is satisfied then $\langle z \rangle \neq 0$ since $z(t)$ cannot become zero during an oscillation cycle. This situation is known as macroscopic quantum self trapping (MQST) [27]. Introducing the dimensionless strength

$$\Lambda = \frac{NU}{J},$$

the expression (25) and the trapping condition (26) give

$$\Lambda_{MQST} = \frac{1 + \sqrt{1 - z^2(0) \cos(\phi(0))}}{z(0)^2/2}$$

for the critical value of $\Lambda$ above which the self trapping occurs. Indeed,

$$\Lambda > \Lambda_{MQST}$$

is the familiar mean field condition to achieve MQST in BECs [27].

Let us study the stationary solutions of (11). From the system of Eqs. (17) and (18) we obtain the symmetric solutions

$$\langle \tilde{z}, \tilde{\phi} \rangle = (0, 2n\pi) \quad \text{(30)}$$

$$\langle \tilde{z}_+, \tilde{\phi} \rangle = (0, (2n + 1)\pi) \quad \text{(31)}$$

with $n \in \mathbb{Z}$, respectively with energies $\tilde{E}_- = -JN$ and $\tilde{E}_+ = JN$. Due to the nonlinear interaction there are degenerate solutions that break the $z$-symmetry

$$z_\pm = \pm \sqrt{\frac{1}{\Lambda^2} - 1} \quad \text{(32)}$$

$$\phi_n = n\pi \quad \text{(33)}$$

where $n \in \mathbb{Z}$. These solutions give a minimum of the energy with $\phi = 0$ only for $\Lambda = UN/J < 0$. Thus, the spontaneous symmetry breaking (SSB) of the balanced ground state ($z = 0, \phi = 0$) appears at the critical dimensionless strength

$$\Lambda_{SSB} = -1.$$ 

In other words, for $\Lambda = UN/J < \Lambda_{SSB} = -1$ the population imbalance $z$ of the ground state of our bosonic system becomes different from zero.

### IV. FINITE-SIZE EFFECTS

Different results are obtained by choosing another quantum state $|\psi(t)\rangle$ in Eqs. (14) and (15). In this section, our choice for the quantum state $|\psi(t)\rangle$ is

$$|\psi(t)\rangle = |ACS(t)\rangle,$$

(35)
where

$$|ACS(t)\rangle = \left(\frac{\sqrt{1+z(t)} a_1^+ + \sqrt{1-z(t)} e^{-i\phi(t)} a_2^+}{\sqrt{N!}}\right) |0\rangle$$

(36)

is the atomic coherent state [16], also called SU(2) coherent state or Bloch state or angular momentum coherent state [17], with |0⟩ the vacuum state. This atomic coherent state depends on two dynamical variables φ(t) and z(t) which, as we shall show, can be again interpreted as relative phase and population imbalance of the Josephson junction [18–21, 26, 27].

Contrary to the Glauber coherent state |CS(t)⟩ of Eq. (7), the atomic coherent state of Eq. (36) is an eigenstate of the total number operator [2], i.e.

$$\hat{N}|ACS(t)\rangle = N|ACS(t)\rangle .$$

(37)

Moreover, the atomic coherent state ACS(t) becomes the Glauber coherent state CS(t) only in the regime N ≫ 1 [14, 21, 24, 27].

Adopting the atomic coherent state ACS the Lagrangian [5] becomes

$$L_{ACS} = i\hbar \langle ACS(t)| \frac{\partial}{\partial t}|ACS(t)\rangle - \langle ACS(t)|\hat{H}|ACS(t)\rangle$$

$$= N\hbar \: z \dot{\phi} - \frac{U N^2}{2} \left(1 - \frac{1}{N}\right) z^2 + J N \sqrt{1-z^2} \cos(\phi).$$

(38)

both with frequency

$$\Omega_A = \frac{1}{\hbar} \sqrt{J^2 + NUJ \left(1 - \frac{1}{N}\right)},$$

(46)

that is the atomic-coherent-state frequency of macroscopic quantum oscillation in terms of tunneling energy J, interaction strength U, and number N of particles. Quite remarkably, this frequency is different and smaller with respect to the standard mean-field one, given by Eq. (24). However, the familiar mean-field result is recovered in the limit of a large number N of bosonic particles. In addition, for N = 1, Eq. (46) gives ΩA = J/ℏ that is the exact Rabi frequency of the one-particle tunneling dynamics in a double-well potential.

In the same fashion as in the previous section, the conserved energy associated to Eqs. (39) and (40) reads

$$E_{ACS} = \frac{UN^2}{2} \left(1 - \frac{1}{N}\right) z^2 - JN \sqrt{1-z^2} \cos(\phi).$$

(47)

and using the condition (20) we get the inequality

$$\Lambda > \Lambda_{MQST,A} = 1 + \sqrt{1-z^2(0)\cos(\phi(0))} - \frac{1}{z(0)^2/2} \left(1 - \frac{1}{N}\right),$$

(48)

where ΛMQST,A is the atomic-coherent-state MQST critical parameter in terms of tunneling energy J, interaction strength U, and number N of particles. Remarkably this value is bigger than the standard mean field one, given by Eq. (28), which is recovered in the semiclassical approximation of a large number N of bosonic particles.

In addition to the usual symmetric stationary solutions [50] and [51] we obtain from the system of Eq. (39) and
a correction to the symmetry breaking ones
\[ z_{ACS} = \pm \sqrt{1 - \frac{1}{\Lambda^2} \left(1 - \frac{1}{N}\right)^2} \] (49)
\[ \phi_n = n\pi \] (50)
with \( n \in \mathbb{Z} \) and \( \Lambda = NU/J \). It follows that, within the approach based on the atomic coherent state, the critical strength for the SSB of the balanced ground state \((z = 0, \phi = 0)\) reads
\[ \Lambda_{SSB,A} = -\frac{1}{(1 - \frac{1}{N})} \] (51)
This means that for \( \Lambda = UN/J < \Lambda_{SSB,A} = 1/(1 - 1/N) \) the ground state is not balanced. Clearly, for \( N \gg 1 \) from Eq. (51) one gets Eq. (44), while for \( N = 1 \) one finds \( \Lambda_{SSB,A} = -\infty \): with only one boson the spontaneous symmetry breaking cannot be obtained.

V. EXACT NUMERICAL RESULTS

To test our analytical results we compare them with exact numerical simulations. The initial many-body state \(|\Psi(0)\rangle\) for the time-dependent numerical simulations is the coherent state \(|ACS(0)\rangle\) from Eq. (46), with a given choice of \( z(0) \) and \( \phi(0) \). The time evolved many-body state is then formally obtained as
\[ |\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi(0)\rangle \] (52)
with \( \hat{H} \) given by Eq. (1).

Knowing \(|\Psi(t)\rangle\) the exact population imbalance at time \( t \) is given by
\[ z_{ex}(t) = \langle \Psi(t)|\hat{N}_1 - \hat{N}_2|\Psi(t)\rangle/N \] (53)

In Fig. 1 we plot the Josephson frequency \( \Omega \) as a function of the number \( N \) of bosons, but with a fixed value of \( UN/J = 1 \). As shown in the figure, the standard mean-field prediction (dashed curve), Eq. (24), predicts an horizontal line. The exact numerical results (filled circles), which are very far from the standard mean-field predictions, are instead reproduced extremely well by Eq. (46), based on atomic coherent states. Indeed, as previously stressed, for \( N = 1 \) Eq. (46) gives the correct Rabi frequency.

We investigate numerically also the onset of macroscopic quantum self trapping (MQST). In Fig. 2 we report the exact time evolution of the population imbalance \( z_{ex}(t) \) for different values of the number \( N \) of bosons and of the interaction strength \( NU/J \). In the figure the numerical results are obtained with an initial ACS state \(|ACS(0)\rangle\) where \( z(0) = 0.5 \) and \( \phi(0) = 0 \). In general, during the time evolution the many-body quantum state \(|\Psi(t)\rangle\) does not remains close to an atomic coherent state. This is especially true in the so-called Fock regime, where \( U/J \gg N \) [22]. Unfortunately, this is the regime where the MQST can be achieved. Fig. 2 illustrates the problems in determining a critical value for MQST: for \( N \lesssim 10 \) interwell oscillations possibly occur with a very long period even for very large values of \( \Lambda \). For larger \( N = 10, \ldots, 100 \), MQST is found, yet the loss of it occurs smoothly diminishing the interaction parameter (not shown in the figure), making it hard to define a critical value. We opted for the definition that just no crossing of zero imbalance should happen. This defini-
The amplitude probabilities \( c_j \) are obtained numerically by diagonalizing the Hamiltonian matrix obtained from (54). Clearly these amplitude probabilities \( c_j \) strongly depend on the values of the hopping parameter \( J \), on-site interaction strength \( U \), and total number \( N \) of bosons. For \( U > 0 \) the distribution \( P(|c_j|^2) \) of the probabilities \( |c_j|^2 \) is unimodal with its maximum at \( |c_{N/2}|^2 \) (if \( N \) is even) [28]. However, for \( U < 0 \) the distribution \( P(|c_j|^2) \) becomes bimodal with a local maximum at \( |c_{N/2}|^2 \) (if \( N \) is even) when \( |U| \) exceeds a critical threshold [28].

The semiclassical SSB, described by Eqs. (34) and (51), corresponds to a full quantum mechanical treatment to the onset of the bimodal structure in the distribution \( P(|c_j|) \). In Fig. 4, we report the dimensionless interaction strength \( (|U|/J)_{SSB} \) for the spontaneous symmetry breaking (SSB) as a function of the number \( N \) of bosons. In the figure we compare the exact numerical results (filled circles) with the semiclassical predictions based on Glauber coherent states (dashed curve) and atomic coherent states (solid curve). The figure shows that the exact numerical results of SSB are quite well approximated by the ACS variational approach, which is more accurate with respect to the standard mean-field one. For large \( N \) the exact numerical results end up in the analytical curves, which become practically indistinguishable.

VI. CONCLUSIONS

In this paper we have adopted a second-quantization formalism and time-dependent atomic coherent states to study finite-size effects in a Josephson junction of \( N \) bosons, obtaining experimentally detectable theoretical predictions. The experiments with cold atoms in lattices and double wells reported in [29-32], for instance, showed that atom numbers well below \( N = 100 \) can be reached and successfully detected with an uncertainty of...
the order one atom. In particular we have obtained an analytical formula with $1/N$ corrections to the standard mean-field treatment for the frequency of Josephson oscillations. We have shown that this formula, based on atomic coherent states, is in very good agreement with exact numerical simulations and it reduces to the familiar mean-field one in the large $N$ limit. We have also investigated the spontaneous symmetry breaking the population-balanced configuration is no more the one with maximal probability. Also in this case the agreement between the analytical predictions of the atomic coherent states and exact numerical results is good. Finally, we have studied the critical interaction strength for the macroscopic quantum spontaneous symmetry breaking the population-balanced configuration is no more the one with maximal probability. In particular we have obtained an analytical formula with $1/N$ corrections to the standard mean-field theory predicted by the atomic coherent states do not work. Summarizing, the time-dependent variational ansatz with atomic coherent states is quite reliable in the description of the short-time dynamics of the bosonic Josephson junction both in the Rabi regime, where $0 \leq U/J \ll 1/N$, and in the Josephson regime, where $1/N \ll U/J \ll N$ [22]. Instead, in the Fock regime, where $U/J \gg N$, a full many-body quantum treatment is needed.

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