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Quantum dynamics of bosons in a double-well potential: Josephson oscillations, self-trapping and ultralong tunneling times

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Abstract. The dynamics of the population imbalance of bosons in a double-well potential is investigated from the point of view of many-body quantum mechanics in the framework of the two-mode model. For small initial population imbalances, coherent superpositions of almost equally spaced energy eigenstates lead to Josephson oscillations. The suppression of tunneling at population imbalances beyond a critical value is related to a high concentration of initial state population in the region of the energy spectrum with quasi-degenerate doublets. Negligible coherences among adjacent doublets result in imbalance oscillations with a very small amplitude. For unaccessible long times, however, the system recovers the regime of Josephson oscillations.

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The understanding of many-body quantum systems from the theoretical and experimental points of view has undergone a considerable development during the past decade. Unifying concepts of several branches of physics are under development, creating an interdisciplinary scenario for the understanding of quantum mechanical paradigms. One of the simplest many-body systems to be realized experimentally and studied theoretically are ultra-cold bosons in a double-well potential. This system is very rich exhibiting a great variety of quantum phenomena such as interference [1], tunneling/self-trapping [2–11], and the entanglement of macroscopic superpositions [12]. Lately this system has been extensively studied, especially after the realization of several experiments in the area. The usual theoretical approach to weakly interacting Bose-Einstein condensates (BECs) is a mean-field approximation, namely the nonlinear Gross-Pitaevski equation [3, 9, 13–16], which has proven to adequately explain a wide variety of experimental observations. Corrections to the mean-field [17] and quantum solutions [3,5,10,11] have also been explored.

Recently, the dynamics of a bosonic gas confined in two or more wells of an optical lattice has been experimentally investigated. In particular, Josephson oscillations in a one-dimensional optical lattice [18,19] and macroscopic tunneling of bosons in a double-well [2] were observed. In the latter experiment, the population in the two wells exhibits Josephson oscillations if the initial difference in population is below a critical value, which depends on the tunneling rate, the strength of the interparticle interaction and the total number of bosons. Above this critical population imbalance, tunneling appears to be suppressed and the populations are locked in each potential well. Based on a mean field treatment, this macroscopic "self-trapping" is attributed to the non-linearity of the Gross-Pitaevski equation [4,8].

In this article, we discuss the experimental non-observation of tunneling for initial population imbalances larger than a critical value in the framework of the quantum many-body theory. The dynamics of bosons in a double-well potential is based on a largely explored soluble two-mode approximation to the many-body Hamiltonian (the two-site Bose-Hubbard Hamiltonian). We review and use the well-known structure of the energy spectrum of the model and its correspondent eigenstates for the symmetric and asymmetric double-well potentials to investigate the time evolution of the imbalance population, in particular the self-trapping phenomena. The time evolution of the population imbalance and the spectral properties of the two-site Bose-Hubbard Hamiltonian have been studied before in several papers (see for example [3,5,10,11]). As a new feature, we find that the change of behavior of the dynamics of the population imbalance is related to the structure of the energy spectrum and the role of

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populations and coherences contained in the initial many-body wave function.

The two-site Bose-Hubbard Hamiltonian is written as

$$\begin{aligned} H = &-\frac{J}{2}(a_1^\dagger a_2 + a_2^\dagger a_1) \\ &+ \frac{U}{2}(n_1(n_1-1) + n_2(n_2-1)) + \frac{\delta}{2}(n_1 - n_2), \end{aligned} \quad (1)$$

where $a_i^\dagger$ and a_i are creation and annihilation operators for a boson in the ith site ($i = 1, 2$), $n_i = a_i^\dagger a_i$, U is the on-site two-body interaction parameter, J is the hopping parameter and δ is an asymmetry parameter corresponding the difference of the one-boson energies in the two sites, so that the perfectly symmetric two site trap corresponds to $\delta = 0$. This Hamiltonian has been shown to adequately describe the dynamics of bosons in a two-well potential under the assumption that the interaction energy U is much smaller than the level spacing of the external trap, allowing for a two-mode approximation [3]. Extensions of this model including two-body hopping terms related to the two-boson interaction have been considered [16,20], but will be ignored here as they do not affect the main argument. The total number of bosons is clearly a conserved quantity, and consequently the exact energy spectrum can be obtained numerically by diagonalizing finite matrices. A convenient base for N bosons consists of the states $|n_1, n_2\rangle = |n, N-n\rangle$, $n_0, \ldots, N$, the labels n_i being the eigenvalues of the corresponding number operators. Note that in the no-hopping, symmetric limit, $J = 0$, $\delta = 0$, H is diagonal in this basis and the states $|n, N-n\rangle$ and $|N-n, n\rangle$ are degenerate (whenever different). The distance between successive doublets *increases* with population imbalance, while hopping matrix elements decrease due to intervening bosonic factors. When the effects of hopping are perturbatively small, also small admixtures of components $|n', N-n'\rangle$ (with $n' \neq n$) will occur, and doublet degeneracy will be slightly removed. The upper graph in Figure 1 shows a numerical calculation of the energy spectrum for $N = 100$ bosons in a symmetric double well ($\delta = 0$) with $J/U = 3.33$. This choice of parameters corresponds to $\Lambda \equiv NU/(2J) = 15$ corresponding to the experimental situation of reference [2]. The resulting spectrum is seen to consist of two qualitatively different regions: a lower region of nearly equidistant energy levels dominated by smaller population imbalances with stronger hopping effects and a region still consisting of nearly degenerate doublets in which the effects of hopping are perturbative (cf. Ref. [3]). A semi-classical analysis of this spectrum can be found in references [15,21]. In the classical phase space the low-lying excited states are related to librations in a pendulum-like energy landscape, while the higher-lying states correspond to trapping around population asymmetric energy maxima in the energy landscape. As the relative tunneling parameter J/U is increased, this separation shifts towards larger energies and, correspondingly, quantum numbers. As a consequence, the doublet region becomes smaller.

The tunneling dynamics of the initial state $|\psi(0)\rangle$ is characterized by the temporal evolution of the population

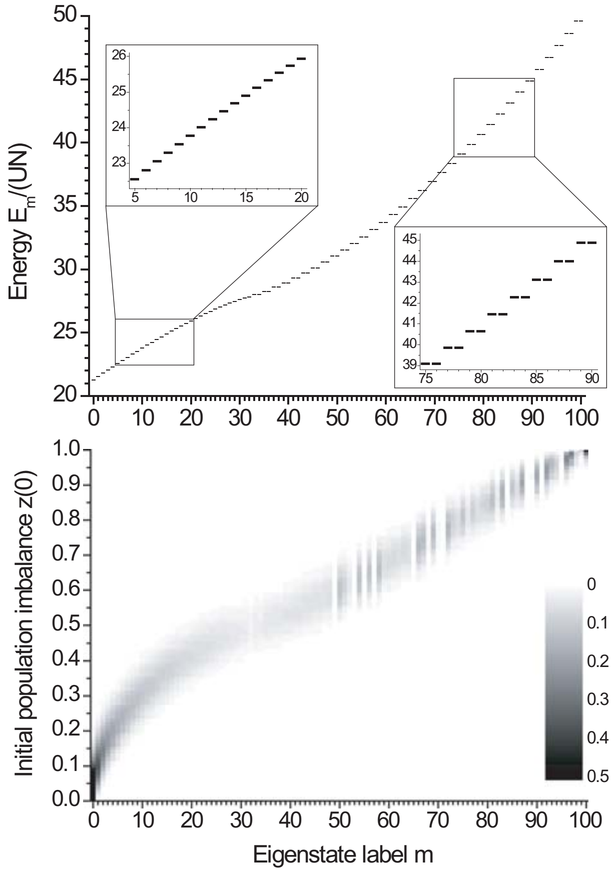

Fig. 1. Upper graph: Hamiltonian energy spectrum for 100 bosons in a symmetric double-well potential for $J/U = 3.333$ corresponding to $\Lambda = 15$. Lower graph: density plot of the occupation probability of symmetric Hamiltonian eigenstates $|m\rangle$ as a function of the initial population imbalances $z(t=0)$ for the same parameters as the upper graph. The gray scale gives the population of the corresponding eigenstate. Below a critical value $z_c \approx 0.5$, only states with almost equal energy spacing are populated, while above z_c the quasi-degenerate doublet states are occupied.

imbalance

$$z(t) \equiv \frac{1}{N}\langle\psi(t)|(n_1 - n_2)|\psi(t)\rangle,$$

the time evolution of the initial state being given as

$$|\psi(t)\rangle = \sum_m c_m e^{-iE_m t}|E_m\rangle$$

with $c_m = \langle E_m|\psi(0)\rangle$, E_m and $|E_m\rangle$ being, respectively, the eigenvalues and eigenstates of the symmetric Hamiltonian ($\delta = 0$ in Eq. (1)). In this way one obtains

$$z(t) = \sum_m z_{mm} + 2\sum_{m<n} z_{mn} \cos\left[\frac{(E_m - E_n)t}{\hbar}\right] \quad (2)$$

where

$$z_{mn} = \frac{1}{N} c_m^* c_n \langle E_m|(n_1 - n_2)|E_n\rangle. \quad (3)$$

Following the experimental procedure adopted in reference [2] the system is initially prepared in the ground state of an asymmetric double-well potential ($\delta \neq 0$) which is then suddenly changed to the symmetric regime ($\delta = 0$), under which it is left to evolve. The relevant features of the initial state for this subsequent dynamics are contained in its spectral decomposition in the symmetric well eigenstates.

The relative importance of two regions of the energy spectrum can be varied through the value of δ chosen for the preparation of the initial state. In the lower graph of Figure 1 the occupation probability $|c_m|^2$ of the eigenstates $|m\rangle$ as a function of the initial population imbalance $z(0)$ is depicted. For small $z(0)$ only the lowest few energy eigenstates are populated. The spread of the distribution of populated states increases as $z(0)$ increases, but for $z(0)$ below a critical value $z_c \approx 0.5$ only energy eigenstates with nearly equal energy splitting are occupied (see upper graph in Fig. 1). As follows from equation (2), coherences between these states will lead to a macroscopic oscillation of the population imbalance at a frequency given by this energy splitting. For larger values $z(0) > z_c$ the scenario changes and only doublet states are occupied. As these two states are almost degenerate, coherences among them do not contribute to the oscillatory term in equation (2).

The dynamical behavior of the system $z(t)$ crucially depends on the competition of two ingredients of z_{mn}, namely the correlation matrix of the initial state in the basis of the eigenstates of the symmetric Hamiltonian $c_m^* c_n$, and the correlation matrix of the observable, the population imbalance in the basis of the eigenstates of the symmetric Hamiltonian $\langle E_m|(n_1 - n_2)|E_n\rangle$. Actually, the correlation matrix of the population imbalance is responsible for the suppression of oscillations allowed by the first term. This suppression can be easily understood in terms of the perturbative character of the hopping effects in the upper region of the spectrum. In fact, the population imbalance operator $n_1 - n_2$ will only connect states $|n, N-n\rangle$ to themselves. Thus, for perturbatively weak hopping, large components of one doublet will connect only to small components of a different doublet, leading to small matrix elements of this operator between different doublets.

As the occupied eigenstates are almost equally spaced for $z(0) < z_c$, the population imbalance $z(t)$ oscillates around zero at a fundamental oscillation frequency given by the mean energy spacing of the occupied states, which is given by the plasma frequency $\omega_p = 2J\sqrt{1+\Lambda}$, with $\Lambda = (UN/2J)$ [4]. This behavior constitutes the regime of Josephson oscillations as shown by the left graph of the upper curves in Figure 2. Small deviations from equal energy spacing lead to a dephasing of the oscillations on a time scale inversely proportional to the number of occupied states and the corresponding differences in energy splitting. The oscillations undergo revivals on time scales given by the inverse of the frequency difference of adjacent eigenstates. The revivals can be seen in the right graph of the upper curves in Figure 2.

For values of $z(0) > z_c$, where doublet states are occupied with negligible coherences between adjacent doublets, one has ideally two widely different time scales. For short times, the population imbalance is locked to its initial value with small residual oscillations as shown by the left graph of the lower curves in Figure 2. The frequency of these small oscillations is determined by the inverse of the energy separation of two quasi-degenerate doublets, i.e. $\Delta E \simeq NU$. This regime is commonly referred to as the "self-trapping" regime observed in reference [2]. The presence of small oscillations is related to the weak mixture of adjacent doublet pairs, since in the doublet region of the energy spectrum the on-site interaction is dominant and the hopping term can be treated as a perturbation. It should however be noted, that on the much larger time scale $T \simeq \hbar/\Delta E_{doublet}$ associated with the small splitting of energy doublets, which can be estimated as $\Delta E_{doublet}/U = [2N(J/U)^N]/(N-1)!$ through a non-perturbative method [23] or via perturbation theory [24], the atoms still undergo collective tunneling resulting in oscillatory behavior of the population imbalance around zero. This oscillatory behavior is guaranteed by the high occupation of the quasi-degenerate doublets due to the the initial condition (see the lower graph of Fig. 1) and the population imbalance correlation matrix guarantees a high coherence among pairs of quasi-degenerate doublets. However, this Josephson regime is far beyond experimental observation, since those doublets are almost degenerate. For instance, for $N = 100$ particles and $J/U = 0.333$ the energy splitting of the topmost doublet can be estimated to $\Delta E_{doublet}/U \sim 10^{-202}$ which is indistinguishable from zero and thus nor resulting in observable oscillatory behavior. Note furthermore that this ultralong tunneling phenomenon requires tuning the symmetry of the two wells, which is here modeled by the $\delta = 0$ condition, to a precision better than the scale set by the splitting of the relevant quasi-degenerate doublets, and is therefore easily destroyed in practice, especially for the most narrowly spaced upper doublets. Such slight breaking of the two well

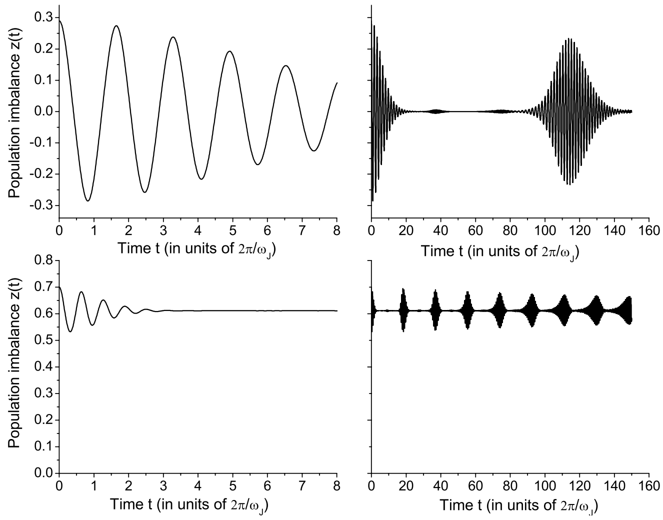

Fig. 2. Time evolution of the population imbalance for 100 particles with $J/U = 3.333$ and initial conditions $z(0) = 0.3$ (upper graph) and $z(0) = 0.7$ (lower graph).

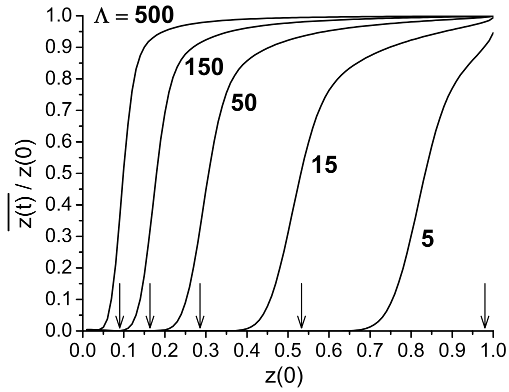

Fig. 3. Time average of $\bar{z(t)}/z(0)$ over 50 plasma periods as a function of the initial population imbalance $(z(0))$ for 100 particles. Josephson oscillations result in $\bar{z(t)} = 0$ while $\overline{z(t)} \neq 0$ indicates the regime of suppressed tunneling. The parameter $\Lambda = NU/2J$ determines the critical population imbalance separating these two regimes. The arrows indicate the semi-classical value of the critical imbalance population $z_c \simeq 2\sqrt{1+\Lambda}/\Lambda$ [4].

symmetry, while having a dramatic effect on the pair of energy eigenstates corresponding to each of the doublets, has otherwise essentially no effect, so that it does not, in particular, affect the preceding analysis of the suppression of tunneling.

In order to distinguish between oscillatory and non-oscillatory behavior, we take the time average of the population imbalance $\bar{z(t)}$ over 50 plasma periods $(2\pi/\omega_p)$, which is shown in Figure 3 as a function of the initial population imbalance $z(0)$ for different values of the parameter Λ. The transition between the two regimes is marked by the change of this average from zero to one, which provides a quantitative measure of the critical value z_c. From Figure 3 one finds that as the parameter Λ decreases, the critical value z_c increases for a fixed number of particles N. This behavior can be traced back to the structure of the energy spectrum: the number of quasi-degenerate doublets decreases as the tunneling parameter J/U increases. As a consequence, the quasi-degenerate doublets states are situated at higher energies which can only be accessed by larger values of $z(0)$. The critical values z_c follows very well the semi-classical prediction $z_c \simeq 2\sqrt{1+\Lambda}/\Lambda$ [4] as indicated by the arrows in Figure 3.

In conclusion, we have investigated the dynamics of bosons in a double-well potential in the framework of a two-mode Bose-Hubbard model. The evolution of the population imbalance in the two wells, prepared by suddenly switching from an asymmetric to a symmetric double-well potential, is explained solely in terms of the initial many-body wave function and the spectral properties of the Hamiltonian. The appearance of oscillatory and self-trapping behavior is related to the occurrence of two distinct regions of the energy spectrum, one of them consisting of quasi-equidistant energy levels, the other of quasi-degenerate doublets. Populations and coherences of the initial wave function determine which parts of the spectrum contribute to the dynamics. For initial population imbalance smaller than a critical value the occupation probability are larger in the lower part of the energy spectrum with quasi-equidistant levels, contributing with large oscillation amplitude with a plasma frequency ω_p. For initial population imbalances larger than a critical value the system oscillates with very small amplitude, with oscillation period of $t \simeq \hbar/(U(N-1))$. The small oscillations are related to hindered coherences among pairs of quasi-degenerate doublets, since they are weak mixtures of adjacent pairs of doublets. However, for longer times beyond possible experimental observation $t \simeq \Delta E_{doublet}/U = (\frac{2N(J/U)^N\hbar}{(N-1)!})$, the system is apt to recover the Josephson oscillation behavior due to high occupation of both members of quasi-degenerate doublets and to coherences between them. We explored the dependence of the critical population imbalance, which separates the two dynamical regimes, on the relative tunneling parameter J/U and find good agreement with semi-classical predictions.

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