Comparative study of quantum dynamics of a few bosons in a one-dimensional split hard-wall trap: exact results versus Bose–Hubbard-model approximations

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Abstract
We study the dynamical properties of a few bosons confined in a one-dimensional split hard-wall trap with the interaction strength varying from the weakly to strongly repulsive regime. The system is initially prepared on one side of the double well by setting the barrier strength of the split trap to be infinity, and then the barrier strength is suddenly changed to a finite value. Both the exact diagonalization method and Bose–Hubbard-model (BHM) approximation are used to study the dynamical evolution of the initial system. The exact results based on exact diagonalization verify the enhancement of correlated tunnelling in the strongly interacting regime. Comparing results obtained by two different methods, we conclude that one-band BHM approximation can well describe the dynamics in the weakly interacting regime, but is not efficient to give quantitatively consistent results in the strongly interacting regime. Despite the quantitative discrepancy, we validate that the form of correlated tunnelling gives an important contribution to tunnelling in the large interaction regime. To get a quantitative description for the dynamics of bosons in the strongly interacting regime, we find that a multi-band BHM approximation is necessary.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Bose–Einstein condensates in double-well potentials have attracted much attention in the past decades. As a paradigm model for studying the competition effect of quantum tunnelling and interaction, the double-well systems have been widely studied from many aspects. Due to the experimental progress in manipulating ultracold atomic gases, both the trap potential and interaction between atoms can be implemented with unprecedented tunability, and thus the dynamics of many-body quantum states of interacting bosons can be experimentally explored by loading the ultracold atoms in double wells. For the atomic double-well system, the atom–atom interactions in Bose–Einstein condensates have been found to play important roles in the dynamics of the system. The competition between tunnelling and interaction leads to many rich and interesting effects, such as the Josephson oscillation and self-trapping phenomena. Moreover, novel correlated tunnelling dynamics in interacting atomic systems characterized by a small number of particles has recently been observed experimentally, which attracted particular attention in the study of the dynamics of few-atom systems. Particularly, few-boson tunnelling in a one-dimensional (1D) double well from a weakly to strongly interacting regime has been systematically studied, where the authors found that a fermionized atom pair can tunnel coherently.

So far most of the theoretical works for double-well systems are based on the two-mode approximation. For atoms confined in a double-well potential, if all of them are prepared in one well initially, they will oscillate in the form of Josephson oscillation for interactions that are weak to moderate. However, when the interatomic interaction becomes strong, this simple concept no longer holds. The fractions of particles in the two wells are determined by the interplay of tunnelling and interactions, which results in a systematic change of the tunnelling probability with respect to the strength of the interaction.
enough, or they will stay in one well (self-trapping) when
the interaction is above a critical value. Both Josephson
oscillation and self-trapping phenomena can be understood
within the two-mode approximation and have been observed
experimentally in cold atomic systems [16]. However, if
interactions are strong enough, the mean-field theory and
the two-mode approximation are not expected to be valid
as higher orbits are occupied. In the strongly interacting
regime, strong interactions between atoms may fundamentally
alter the tunnel dynamics and result in a correlated tunnelling,
which was explored most recently in ultracold atoms [13, 14].
Theoretically, the correlated paring tunnelling was studied
by the multi-configuration time-dependent Hartree method
[13, 15], and also in the scheme of the extended Bose–Hubbard
model (BHM) with an additional term of correlated pair
tunnelling [14]. In order to understand the dynamics of double-
well systems from a weakly to strongly interacting regime in an
unified scheme, in this work we study the dynamical properties
of a few bosons confined in a 1D split hard-wall trap with the
repulsive interaction strength varying from zero to infinity.
Experimentally, the effective interaction strength can be tuned
by using the Feshbach resonance or the confinement-induced
resonance to the strongly interacting Tonks–Girardeau (TG)
limit [17, 18], which makes it possible to explore the novel
dynamics even in the TG limit.

In the TG limit, the bosonic systems exhibit the feature of
fermionization [19–24]. In the strongly interacting regime, the
mean-field theory generally fails to describe the properties
of fermionization. In order to characterize the crossover from
weakly interacting condensation to strongly interacting TG
gas, some sophistical theoretical methods, such as the exact
diagonalization method [10, 21, 22] and the multi-orbital self-
consistent Hartree method [23, 24], have been applied to study
the static few-boson systems. In this work, we shall apply the
exact diagonalization method to study the dynamical problem
in the 1D double-well system. The exact diagonalization
method can produce numerically exact results and allows us
to give a unified description for both the weakly and strongly
interacting regimes. For comparison, we also investigate the
dynamics based on the two-site BHM by considering both
the two-mode and multi-mode approximations. Comparing
the results obtained from different methods, we conclude that
the one-band (two-mode) BHM approximation is efficient
at describing dynamics in a small interaction regime, but
the multi-band BHM approximation is needed if we want
to describe the dynamics of bosons with large interaction
quantitatively. We also validate that the form of pair tunnelling
gives an important contribution to tunnelling in the large
interaction regime.

2. Model and method

We consider a few bosons with mass \( m \) confined in a 1D
split hard-wall trap, which is described by the Hamiltonian
\( \hat{H} = m a^2 \frac{\partial^2}{\partial x^2} + V(x) + \kappa \delta(x) \)
\( + c \int \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') \delta(x - x') \hat{\psi}(x) \hat{\psi}(x') \ dx \ dx' \). (1)

Here, \( V(x) \) is a hard-wall trap which is zero in the region
\( (-a, a) \) and infinite outside, \( \kappa \) is a tunable parameter
which describes the strength of a zero-ranged barrier at the centre
of the trap, and \( c \) is the interaction strength between particles
determined by the effective 1D s-wave scattering length. Here,
the double well is modelled by the 1D split hard-wall trap
with a \( \delta \)-type barrier located at the origin, and the tunnelling
amplitude between the left and right wells can be tuned by the
barrier strength \( \kappa \) [9, 10]. To study the tunnelling dynamics,
the barrier strength \( \kappa \) is initially set to be infinity and the system
is prepared in the ground state of the left well. At time \( t = 0 \),
we suddenly change \( \kappa \) to a finite value and study the dynamical
evolution of the initially prepared system.

For \( c = 0 \), the single-particle stationary Schrödinger equation
associated with the Hamiltonian (1) can be written as
\[
-\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) + \kappa \delta(x) \psi_n(x) = \epsilon_n \psi_n(x),
\] (2)
where \( \psi_n(x) \) are the complete set of orthonormal
eigenfunctions and \( \epsilon_n \) are the corresponding eigenenergies.
Here, \( n = 1, 2, 3, \ldots \) gives the ordering number of the single-
particle energies. According to the parity symmetry of the
eigenfunctions, the state \( \psi_n(x) \) is symmetric for odd \( n \) (\( n = 2i - 1 \)) and antisymmetric for even \( n \) (\( n = 2i \)). The
single-particle energies are ordered alternatively corresponding
to symmetric and antisymmetric states. For convenience, we also represent \( \psi_{2i-1}(x) = \psi_i(x) \) and \( \psi_{2i}(x) = \psi_i(x) \)
with the subscript \( S \) (A) indicating the symmetric (antisymmetric)
function. The single-particle antisymmetric eigenfunctions
are \( \psi_i(A) = \frac{1}{\sqrt{a}} \sin \left( \frac{\pi x}{a} \right), i = 1, 2, 3, \ldots \) with their
corresponding eigenenergies \( \epsilon_{i,A} = \epsilon_{2i} = (\pi/a)^2/2 \), and
the single-particle symmetric eigenfunctions are \( \psi_i(S) = C[\cos(px) - \frac{1}{p} \sin(px)] \theta(-x) + C[\cos(px) + \frac{1}{p} \sin(px)] \theta(x) \)
with their corresponding eigenenergies \( \epsilon_{i,S} = \epsilon_{2i-1} = p^2/2 \), where the wave vector \( p \) is determined by the
transcend equation \( p/\kappa + \tan(pa) = 0 \) and \( C \) is the
normalization constant. It is true that the barrier only influences
symmetric eigenfunctions, but does not influence antisymmetric
eigenfunctions for any barrier strength \( \kappa \). Furthermore, the \( (2i - 1) \)th eigenenergy is close to the \( 2i \)th
eigenenergy (\( i = 1, 2, 3, \ldots \)) gradually with the increase of
barrier strength, and they become degenerate in the limit
\( \kappa \rightarrow \infty \). For simplicity, we set \( a = 1 \) and discuss
a large barrier strength \( \kappa = 50 \) in this paper. In this case,
single-particle eigenenergies in a split hard-wall trap are
\( \epsilon_1 = 4.74341, \epsilon_2 = \pi^2/2, \epsilon_3 = 18.9764, \epsilon_4 = 2\pi^2, \epsilon_5 = 42.7073, \ldots \) respectively, see figure 1(a). In
contrast to the small energy gap between the \( (2i - 1) \)th state and the \( 2i \)th state, there is a relatively very large
energy gap between the \( 2i \)th state and \( (2i + 1) \)th state, i.e. \( \epsilon_{i,A} \ll \epsilon_{i+1,S} \approx \epsilon_{i,A} \).

Expanding field operators as \( \hat{\psi}(x) = \sum_{n=1}^{\infty} \psi_n(x) a_n \),
the many-body Hamiltonian (1) takes the form
\[
\hat{H} = \sum_n \epsilon_n a_n^\dagger a_n + c \sum_{n,m,p,q} I_{npq} a_n^\dagger a_m^\dagger a_p a_q,
\] (3)
where \( a_n^\dagger(a_n) \) is a bosonic creation (annihilation) operator for
a particle in the single-particle energy eigenstate \( \psi_n \). The
interaction integral parameters \( I_{\alpha\beta\gamma\delta} \) are calculated through
\[
I_{\alpha\beta\gamma\delta} = \int D\psi \psi_{\alpha}(x) \psi_{\beta}(x) \psi_{\gamma}(x) \psi_{\delta}(x) \, dx.
\]
The eigenstate of this Hamiltonian can be obtained by numerically exact diagonalization in the subspace of the energetically lowest eigenstates of a non-interacting many-particle system [10, 21].

When the barrier strength \( \kappa \) is large, the split hard-wall trap can be considered as a double well. Similar to the case of optical lattices, the local Wannier functions \( W_{\kappa}^{L}(x) \) at the left (right) well with the energy band indices \( i \) can be defined as \( W_{\kappa}^{L}(x) = 1/\sqrt{2}(\psi_{\alpha}(x) + \psi_{\beta}(x)) \) and \( W_{\kappa}^{R}(x) = 1/\sqrt{2}(\psi_{\alpha}(x) - \psi_{\beta}(x)) \). From the symmetry of \( \psi_{\alpha}(x) \) and \( \psi_{\beta}(x) \), one observes that \( W_{\kappa}^{L}(x) = W_{\kappa}^{R}(-x) \). If we expand the bosonic field operator as \( \hat{\psi}(x) = \sum a_{i,R} W_{\kappa}^{L}(x) + \sum a_{i,L} W_{\kappa}^{R}(x) \), where \( a_{i,L(R)} \) is the bosonic annihilation operator for a particle at the left (right) well, the Hamiltonian can be written as the form of two-site BHM

\[
\hat{H} = \sum_{i,j} \left( J_{i,j}^{L,L} a_{i,R} a_{j,R} + J_{i,j}^{L,R} a_{i,L} a_{j,R} \right) + \sum_{i,j} \left( J_{i,j}^{R,L} a_{i,R} a_{j,L} + J_{i,j}^{R,R} a_{i,L} a_{j,L} \right) + \sum_{i,j,k,l} U_{i,j,k,l} a_{i,R} a_{j,L} a_{k,R} a_{l,L},
\]

where the integral \( J_{i,j}^{L,L} = \int D\psi \psi_{i,R}(x) \psi_{j,R}(x) \hat{H}_0 \psi_{i,L}(x) \psi_{j,L}(x) \), with \( \hat{H}_0 = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) + \kappa^2 \delta \) and the interaction integral \( U_{i,j,k,l} a_{i,R} a_{j,L} a_{k,R} a_{l,L} = c \int D\psi \psi_{i,L}(x) \psi_{j,L}(x) \psi_{k,R}(x) \psi_{l,R}(x) \). The subscripts \( i, j, k, l \in \{L, R\} \) are the well indices and the superscripts \( i, j, k, l \in \{1, 2, 3, \ldots\} \) are the energy band indices. Here, we note \( J_{i,j}^{R,R} = J_{i,j}^{L,L} \) for the symmetric double well. The Hamiltonian (4) can be divided into intraband and interband parts, that is

\[
\hat{H} = \sum_{i} \hat{H}_i + \hat{H}_{\text{interband}}.
\]

The \( i \)th intraband Hamiltonian can be written as

\[
\hat{H}_i = (\epsilon_{i,L} n_{i,L} + \epsilon_{i,R} n_{i,R}) + [J_{i} + 2(n_{i,L} + n_{i,R} - 1) J_{i}] \times (a_{i,L}^\dagger a_{i,R} + a_{i,R}^\dagger a_{i,L}) + U_{i}^0 [n_{i,L}(n_{i,L} - 1)],
\]

where \( n_{i,L} = a_{i,L}^\dagger a_{i,L} \) and \( n_{i,R} = a_{i,R}^\dagger a_{i,R} \). The interband hopping energy between the left and right wells, \( J_{i} = J_{i}^{L,L} = J_{i}^{R,R} \), is the on-site interaction energy and \( U_{i}^{0} = U_{i}^{RR} = U_{i}^{LL} \) is the intraband pair hopping energy. It is easy to check that \( \epsilon_{i,L} = \epsilon_{i,R} = (\epsilon_{i,s} + \epsilon_{i,\alpha})/2 \) and \( J_{i} = (\epsilon_{i,s} - \epsilon_{i,\alpha})/2 \).

The interband Hamiltonian reads

\[
\hat{H}_{\text{interband}} = \sum_{i,j} \sum_{\alpha,\beta,\gamma,\delta} U_{i,j}^{\alpha,\beta,\gamma,\delta} \times (a_{i,R}^\dagger a_{j,L}^\dagger a_{i,R} a_{j,L} + a_{i,L}^\dagger a_{j,R}^\dagger a_{i,L} a_{j,R}).
\]

Figure 1. (a) Single-particle energy levels for the split hard-wall trap with \( \kappa = 50 \). (b) The eigenenergy of two interacting bosons changing with the interaction strength \( \kappa \) in the split hard-wall trap with \( \kappa = 50 \).

+ \( n_{i,R}(n_{i,R} - 1) \] + \( U_{i}^{LR}(a_{i,L}^\dagger a_{j,L}^\dagger a_{i,R} a_{j,R} + a_{i,R}^\dagger a_{j,L}^\dagger a_{i,L} a_{j,R} + 4n_{i,L} n_{i,R}) \).

where \( n_{i,L} = a_{i,L}^\dagger a_{i,L} \) and \( n_{i,R} = a_{i,R}^\dagger a_{i,R} \). The interband hopping energy between the left and right wells, \( J_{i}^{L,R} = J_{i}^{R,L} \), is the on-site interaction energy and \( U_{i}^{LR} = U_{i}^{RR} \). The intraband pair hopping energy. It is easy to check that \( \epsilon_{i,L} = \epsilon_{i,R} = (\epsilon_{i,s} + \epsilon_{i,\alpha})/2 \) and \( J_{i} = (\epsilon_{i,s} - \epsilon_{i,\alpha})/2 \).

The interband Hamiltonian reads

\[
\hat{H}_{\text{interband}} = \sum_{i,j} \sum_{\alpha,\beta,\gamma,\delta} U_{i,j}^{\alpha,\beta,\gamma,\delta} \times (a_{i,R}^\dagger a_{j,L}^\dagger a_{i,R} a_{j,L} + a_{i,L}^\dagger a_{j,R}^\dagger a_{i,L} a_{j,R}).
\]
evolves, we shall use the revival probability

\[ F(t) = |\langle \Psi(t) | \Psi(0) \rangle|^2 = 1 - 4 \sum_{n,m} C_n^a C_m^a \sin^2[(E_n - E_m)t/2], \]  

(9)

the reduced single-particle density matrix

\[ \rho(x,x',t) = \langle \Psi(t) | \hat{\Psi}(x) \hat{\Psi}(x') | \Psi(t) \rangle \]  

(10)

and the pair correlation function

\[ g^{(2)}(x_1, x_2, t) = \langle \Psi(t) | \hat{\Psi}(x_1) \hat{\Psi}(x_2) \hat{\Psi}(x_1) \hat{\Psi}(x_2) | \Psi(t) \rangle \]  

(11)

after time \( t \) to describe the dynamics in the split hard-wall trap system.

3. Results and discussions

Before studying the quantum dynamics of many-body systems, we first recall the tunnelling dynamics of a single atom. If there is only one boson in this split hard-wall trap, the initial state is just the ground state of the left well, that is \( \Psi(0) = -\sqrt{2} \sin(\pi x) \) with energy \( \pi^2/2 \). After the barrier strength \( \kappa \) switches on to a finite but large strength, the weight coefficients of the ground and the first excited state of the final Hamiltonian \( H_f \) are \( C_1 \approx \sqrt{2}/2 \) and \( C_2 \approx \sqrt{2}/2 \). At time \( t \), the wavefunction reads

\[ |\Psi(t)\rangle \approx \frac{\sqrt{2}}{2} e^{-i\mu_1 t}[|\psi_1,S\rangle + \frac{\sqrt{2}}{2} e^{-i\mu_1 t}[|\psi_1,A\rangle = e^{-i\mu_1 t}[ \cos(J_1 t) |W_1^1\rangle + i \sin(J_1 t) |W_2^1\rangle], \]  

(12)

where \( \mu_1 = (\epsilon_{1,S} + \epsilon_{1,A})/2 \). It is obvious that the boson stays in the left well with the probability of \( \cos^2(J_1 t) \), whereas in the right well with the probability of \( \sin^2(J_1 t) \). Consequently, the boson oscillates back and forth between two wells with the period \( \tau = 2\pi/(\epsilon_{1,A} - \epsilon_{1,S}) = -\pi/J_1 \), which is influenced by the barrier strength \( \kappa \) through controlling the energy gap between the ground state and the first excited state. Correspondingly, the fidelity \( F(t) \approx \cos^2(J_1 t) \) oscillates periodically between 1 and 0.

For a many-body system, no analytical expression like equation (12) is available. Nevertheless, when the atom number is small, we can resort to the full exact diagonalization method to calculate the energy spectrum and eigenstates via directly diagonalizing the Hamiltonian (3). Consequently, the time-dependent wavefunction, revival probability, single-particle density matrix and correlation function are straightforward to calculate via equations (8)–(11). For a continuum system, we need to truncate the set of single-particle basis functions to the the lowest \( L \) orbitals (modes), and the basis dimension of an \( N \)-particle system with \( L \) orbitals (modes) is given by \( D = (N + L - 1)!/[N!(L - 1)!] \). In general, one needs \( L \gg N \), and it is a formidable task to get the full spectrum of the many-particle system as the particle number \( N \) becomes large. Therefore, despite the fact that the exact diagonalization method can be applied to deal with the interacting boson systems in a numerically exact way for all relevant interaction strengths, it is only restricted to small-particle systems. When the interaction strength is weak, the two-site Bose–Hubbard Hamiltonian under the single-band (two-mode) approximation is widely taken to be the model system for the study of the dynamics of the double-well system. One of the advantages of the two-site Bose–Hubbard Hamiltonian (4) is that every term in the Hamiltonian has a straightforward physical meaning, which can help us to understand the physical consequence of different terms. Furthermore, in the scheme of the two-site BHM, the system is much more tractable both analytically and numerically and a large system can be studied. In the following, we shall first present exact numerical results by exact diagonalization and then results based on the two-site BHM under two-mode (single-band) and multi-mode (multi-band) approximations.

3.1. Exact result by exact diagonalization

We first consider the two-boson case. If two bosons are initially prepared in the ground state of the left well as the initial state of the system, which can be obtained by the exact diagonalization method. Through diagonalizing the second quantized initial Hamiltonian \( H_0 \) in the Hilbert space spanned by the single-particle eigenstates, we get the initial state \( |\Psi(0)\rangle \). Similarly, the eigenenergy and eigenvectors for \( H_f \) can also be obtained. As an example, we plot the lowest five eigenenergies of two interacting bosons in the split hard wall with \( \kappa = 50 \) versus the interaction strength \( c \) in figure 1(b).

When the interaction is absent, bosons just oscillate back and forth between two wells and return to their initial state after a Rabi period \( \tau \), which is the same as that of one boson. For interacting bosons, there will be many differences. The revival probability \( F(t) \) as a function of time \( t \) is shown in figure 2 for various \( c \). When interaction strength \( c \) is very small, the revival probability \( F(t) \) still displays the oscillating feature and the system returns to their initial state with probability close to 1 after a longer period. The revival time becomes...
Figure 3. Reduced single-particle density matrix $\rho(x, x', t)$ of two interacting bosons for (a1–a3) $c = 0, t = 0, 5, 15$, (b1–b3) $c = 5, t = 0, 5, 15$ and (c1–c6) $c = \infty$, $t = 0, 5, 16, 21, 21, 32$. Each plot spans the range $-1 < x, x' < 1$.

Figure 4. The pair correlation function $g^{(2)}(x_1, x_2, t)$ for (a1–a3) $c = 0, t = 0, 5, 15$, (b1–b3) $c = 5, t = 0, 5, 15$ and (c1–c6) $c = \infty$, $t = 0, 5, 16, 21, 22.5, 32$. Each plot spans the range $-1 < x, x' < 1$.

The reduced single-particle density matrix $\rho(x, x', t)$ of two interacting bosons shows how the probability distribution changes over time. When $c$ reaches a certain value ($c \sim 5$), the fidelity $F(t)$ approaches 1 with tiny oscillations within a very large timescale, which is known as the self-trapping phenomena. In this regime, the tunnelling to the right well is dynamically suppressed and two bosons stay in the left well stably. As the interaction strength $c$ increases further to the stronger regime, $F(t)$ begins to decrease more quickly and two bosons can tunnel to the right well again. In the limit of $c \to \infty$, $F(t)$ approaches zero quickly and then oscillates between 0 and 0; finally, it approaches 1 after almost a Rabi period. We note that the dynamical problem in the limit of $c \to \infty$ is exactly solvable via the Bose–Fermi mapping [19, 25].

To see clearly how the atoms tunnel between the left and right wells, we display the corresponding time-dependent reduced single-particle density matrix $\rho(x, x', t)$ in figure 3 for several typical $c$. The diagonal contribution $\rho(x, x', t)$ along $x = x'$ is just the single-particle density distribution. In figure 4, the pair correlation function $g^{(2)}(x_1, x_2, t)$ is also displayed. The pair correlation function $g^{(2)}(x_1, x_2, t)$ shows the probability of finding one particle at point $x_1$ and another particle at point $x_2$ in one measurement. As shown in (a1)–(a3) of figures 3 and 4, the non-interacting bosons can tunnel from the left well to the right well, and then go back to the left well, which forms a period of Rabi oscillation. However, as shown in (b1)–(b3) of figures 3 and 4, the single-particle density distribution and the pair correlation function $g^{(2)}(x, x', t)$ have no obvious change within a Rabi period and no oscillation between the left and right traps is observed in this self-trapping regime with $c = 5$. While in the fermionization limit, the oscillation phenomenon appears again in (c1)–(c6). Both of the two bosons tunnel to the right well when $t = 21$ (see (c4)) and go back to the left well for $t = 32$ (see (c6)). Our results are consistent with results in [13] based on the multi-configuration time-dependent Hartree method.

Next, we consider the dynamics of systems with more bosons. The dynamics of the $N = 3$ system is similar to the $N = 2$ case, except that the system enters the self-trapping regime earlier than $N = 2$. As shown in figure 5, when $c = 0.5$, the system already displays the feature of self-trapping with the fidelity $F(t) \sim 1$ with tiny oscillations within a very large timescale. Similarly, in the TG limit, bosons can tunnel to the right well more easily and return to the left well approximately after a Rabi period. The tunnelling dynamics of hard-core bosons is very similar to their correspondence of free fermions [29]. In figure 6, we plot the revival probability $F(t)$ for systems with $N = 1–4$ in the TG limit. It is shown that there is an obvious peak around the Rabi oscillation periods for various $N$, which implies that the system can return to the left well with the probability close to 1 after a Rabi period. One can understand this from the Bose–Fermi mapping, i.e.
bosons in the TG limit can be mapped into a spinless-free Fermi system \[29\]. For the case of \(\kappa = 50\), we can check that \(J_i \approx i^2 J_1\) for \(i = 1, 2, 3, 4\). The \(N\) atoms initially occupy the \(N\)-lowest single-particle levels of the left well, and roughly speaking, each particle tunnels with the Rabi period \(\tau_i = -\pi/J_i\). However, when the particle number \(N\) becomes large, the relations of \(J_i \approx i^2 J_1\) break down and even the dynamics in the TG limit can be quite complex.

### 3.2. BHM approximation

Now, we consider the two-site BHM described by the Hamiltonian \((4)\). If the interaction strength is much smaller than the level spacing between the first band and the second bands defined as \(\Delta = \mu_2 - \mu_1\), one may expect that the system can be approximately described by the single-band BHM. Under the one-band approximation, the BHM is described by \((6)\) with \(i = 1\). We note that the pair hopping term \(U_{1,L,R}^i\) in \((6)\) is generally very small in comparison with the on-site interaction; for example, in this work we have \(U_{1,L}^i \approx 4948 U_{1,L,R}^1\). Therefore in many previous works, the pair hopping term is omitted and a simplified single-band BHM given by

\[
\tilde{H} = \mu_1 (n_{1,L} + n_{1,R}) + \tilde{J}_1 \left( a_{1,L}^i a_{1,R}^i + a_{1,L}^i a_{1,R}^i \right) + U_0^i [n_{1,L}(n_{1,L} - 1) + n_{1,R}(n_{1,R} - 1)]
\]

\((13)\) has been widely used \([8, 26-28]\). Here, \(\tilde{J}_1 = J_1 + 2(n_{1,L} + n_{1,R} - 1)J'_1\). Since \(U_{1,L,R}^i \ll U_0^i\) in the whole interacting regime, the pairing hopping term is not expected to significantly change the static properties. However, when the term \(U_{1,L,R}^i\) is comparable with the hopping amplitude \(J_1\), it may contribute significantly to the dynamics, which has been emphasized in \([14]\). In the weakly interacting regime, the term \(J'_1\) is also usually neglected as its revision to hopping energy can be attributed to \(J_1\). As we shall illustrate later, when the interaction strength is very large, the contribution of \(J'_1\) cannot be neglected since \(J'_1 \propto c\).

By using the single-band BHM approximation, we study the tunnelling dynamics of the two-site BHM described by \(\tilde{H}\) given by \((6)\) with all particles prepared in one site initially. The revival probability \(F(t)\), changing with time \(t\) under one-band BHM approximation, is shown in figure 7 for the two-boson system. As shown in figure 7(a), when the interaction strength is not very large, the single-band BHM gives quantitatively a consistent description of the dynamics in comparison with the exact results by exact diagonalization (see figure 2(a)). With a further increase in the interaction, as shown in figure 7(b), although the single-band BHM with the pairing hopping term can correctly describe the enhancement of tunnelling, it does not provide quantitatively consistent results in comparison with the results of exact
Figure 8. The revival probability $F(t)$ for the two-boson system changes with time $t$ under one-band BHM approximation with (a) $U_{1LR}^1 = 0$ and $J_1^1 = 0$. (b) $U_{1LR}^1 = 0$.

diagonalization in figure 2(b). In order to see clearly the effect of the pair-tunnelling term, we also study the dynamics governed by the simplified BHM of equation (13) without the pair-tunnelling term. To see the effect of the term $J_1^1$, we consider both cases for the Hamiltonian of equation (13) with or without the term $J_1^1$. When the interaction strength is not so strong (for example, $c < 5$), we find that the results are almost the same as that presented in figure 7(a). This means that the terms of pair tunnelling and $J_1^1$ are not important when the interaction is weak. However, as shown in figures 8(a) and (b), the dynamics in the strongly interacting regime shows quite different behaviours if the pair-tunnelling term is absent. Comparing figures 7(b) and 8, we can conclude that the pair-tunnelling term of $U_{1LR}^1$ gives an important contribution to tunnelling in the large interaction regime. Comparing figures 8(a) and (b), we find that the term $J_1^1$ also plays an important role in enhancing the tunnelling.

The dynamics for the three-boson system is shown in figure 9. Comparing with the exact dynamical results in figure 5, we find that the one-band BHM approximation can describe the dynamics well only when the interaction strength is small so that $U_0^1 \ll \Delta$. In contrast to the two-boson system, the pair-tunnelling term has less significant effect on the enhancement of the tunnelling. For a very large $c$, although the system can tunnel to the right well, it does not give quantitatively consistent results in comparison with the results of the numerical exact diagonalization.

From the above results, we know that one-band BHM approximation is not enough to give a quantitative description for the dynamics of interacting bosons in the large interaction regime. To get better results, we need to keep more band levels and use the multi-band BHM given by equation (4) in our calculation. In figure 10, we show the ground energy of the two bosons versus the interaction strength using the exact diagonalization method, one-band, two-band, three-band and four-band BHM approximations, respectively. It is shown that the one-band BHM approximation can describe the ground energy very well when the interaction $c < 1$, and the two-band BHM approximation can describe well in the region $c < 10$, while the three- and four-band BHM approximations are efficient to describe the ground energy of two bosons well even for $c = 100$. For the dynamics problem, in order to get a quantitatively consistent results with the exact diagonalization results, we find that more bands are needed in comparison with the static problem. In figure 11, we have displayed the results of $F(t)$ for the two-particle systems with various $c$ within the multi-band BHM approximation. As shown in the figure, the result based on a five-band BHM approximation for $c = 10$ already quantitatively agrees with the exact numerical result. For $c = 50$, a ten-band BHM approximation is required for a quantitatively consistent result. The result for $c = 300$ based on an 18-band BHM approximation is also given in figure 11. In comparison with figures 2(b) and 7(b), we find that there exists only a qualitative agreement with the exact diagonalization result, although it is much better than the result of the single-band BHM approximation.
Figure 11. The revival probability \( F(t) \) changes with time \( t \) under multi-band BHM approximations, including a five-band BHM approximation for \( c = 10 \), a seven-band BHM approximation for \( c = 20 \), a ten-band BHM approximation for \( c = 50 \) and an eighteen-band BHM approximation for \( c = 300 \).

4. Summary

In summary, we have studied the dynamical properties of a few bosons confined in a one-dimensional split hard-wall trap by both the exact diagonalization method and the approximate method based on the two-site Bose–Hubbard model (BHM). The system is initially prepared in the left well of the trap by setting the barrier strength of the split hard-wall trap to infinity, and then it is suddenly changed to a finite value. With the increase in the interaction strength of bosons, the system displays Josephson-like oscillations, self-trapping and correlated tunnelling in turn. Comparing results obtained by two different methods, we conclude that the one-band BHM approximation can quantitatively describe the dynamics in the weakly interacting regime, but the multi-band BHM approximation is needed if we want to describe the dynamics of bosons with large interaction quantitatively. We also validate that the form of correlated tunnelling gives an important contribution to the tunnelling dynamics in the large interaction regime.

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