The impact of spatial correlation on the tunneling dynamics of few-boson mixtures in a combined triple well and harmonic trap

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Abstract. We investigate the tunneling properties of a two-species few-boson mixture in a one-dimensional triple well and harmonic trap. The mixture is prepared in an initial state with a strong spatial correlation for one species and complete localization of the other species. We observe a correlation-induced tunneling process in the weak interspecies interaction regime. The onset of the interspecies interaction disturbs the spatial correlations of one species and induces a tunneling process between the correlated wells. The corresponding tunneling properties can be controlled by the spatial correlations with an underlying mechanism that is inherently different from the well-known resonant tunneling process. We also observe and analyze the correlated tunneling of both species in the intermediate interspecies interaction regime and the tunneling via higher band states for strong interactions.

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1. Introduction

Ultracold atoms in optical lattices have manifested themselves as a powerful and flexible tool for the study of quantum systems [1–3]. In particular, ultracold atoms in optical lattices possess a high degree of controllability. The geometry and strength of the optical lattice can be tuned by changing the frequency, amplitude and polarization of the involved lasers [4–6], while the contact interaction strength of the atoms can be tuned via Feshbach resonances [7–9] as well as through confinement-induced resonances in quasi-one-dimensional systems [10–14]. Moreover, their rich internal atomic properties offer the possibility to simulate a wide range of quantum systems, exploiting the atomic spin properties [15–18] and the diversity of atomic species [19–33]. This can lead to a plethora of quantum properties and phenomena that will deepen our understanding of quantum physics, as well as widen applications of the quantum system.

Atomic species could differ in mass, intraspecies interaction strength and intraspecies permutation symmetry, i.e. being bosons or fermions, which renders the study of mixed ultracold atomic systems highly attractive. In mixtures containing atoms of different masses, the heavier atoms can play the role of an effective potential for lighter atoms, and this has been theoretically predicted [19, 20] and experimentally observed [21]. Such an effective potential can even lead to Anderson localization of both species [22]. The interplay of intraspecies and interspecies interactions can give rise to correlated phase structures, such as phase separation [23], quantum emulsion phases [24] and a pair or counterflow superfluid [25–27]. In mixtures composed of bosons and fermions, various correlated phase structures have also been studied both theoretically [28, 29] and experimentally [30]. It has been demonstrated that the interspecies interaction can modify the phases of each species, inducing the formation of composite particles and various phase transitions between dual Mott-insulator phases, anti-correlated phases as well as phases of complete separation. Moreover, the interspecies interaction strength between the bosonic and fermionic species can rearrange the phase space [34], changing
the temperature of the system, and induce an enhanced condensate fraction of the bosonic species [31–33].

Quantum phase transitions represent a main focus of the study of cold atoms, and the theoretical prediction as well as the experimental observation of the superfluid and Mott-insulator phases manifested itself as a milestone in the field [35, 36]. An interesting finding concerning the phase diagram is the coexistence of domains composed of different phases, for instance, the domain structure of the Mott phase and superfluid phase in the optical lattice augmented by a harmonic trap [37, 38]. One of the important characteristics of such a domain structure is the spatial correlations between different lattice sites. Only the sites in the superfluid phase maintain nonzero correlations, while no correlations exist for the sites in the Mott phase. An open question concerning the domain structure is how the spatial correlations can affect the tunneling dynamics of the system.

The spatial correlations between different sites indicate the coherent coupling of bosons in the optical lattices. There have been extensive studies of the relation between the coherence and the quantum dynamics of ultracold atoms in various setups. In double-well systems [39–42], it has been theoretically shown that the coherent coupling of Bose–Einstein condensates (BECs) in the two wells can give rise to coherent atomic tunneling effects, such as the bosonic Josephson effect and the macroscopic self-trapping effect, which have also been observed in experiments [43–46]. The coherent tunneling behavior is also generalized to the triple well, where self-trapping and delocalization are predicted [47, 48], and the multiwell system, where the localization of BECs takes place even in the absence of disorder [49, 50].

In this work, we study the impact of spatial correlations of a mixture of ultracold atoms on the quantum dynamics of the system. We do so by exploring a few-body bosonic mixture consisting of two bosonic species confined in a one-dimensional triple plus harmonic (TPH) well. We will first show that this few-body ensemble can present spatial correlations of the wavefunction between selected wells in the multiwell system, which is a signature of the domain structure in many-body systems. We demonstrate how these spatial correlations can affect the tunneling dynamics of the bosonic mixture. In particular, it is shown that in the low interspecies interaction regime, this spatial correlation can induce tunneling between the correlated sites, which sheds new light on the common resonant tunneling mechanism. In addition, in the intermediate interaction regime, we observe correlated tunneling of both species in resonant windows of the interspecies interaction strength on top of delayed tunneling, and in the strong interaction regime, higher band states contribute to tunneling, and correspondingly, enhanced population oscillation via higher band states is encountered.

This paper is organized as follows. In section 2, we discuss our model and first-principle numerical method, the multi-configuration time-dependent Hartree (MCTDH) approach [51–53]. In section 3, we study the ground state transition of single-species bosons in the TPH well on varying the intraspecies interaction, and the occurrence of corresponding spatial correlations. Section 4 presents a study of the tunneling dynamics of a bosonic mixture in the TPH well for different interspecies interaction strengths. We identify three interspecies interaction regimes according to the tunneling behavior: the low interspecies interaction regime, where spatial correlation of the bosons induces the so-called correlation-induced tunneling, the intermediate regime with correlated tunneling of different spaces and the strong interaction regime, where higher band states come into play. Section 5 contains a summary of this paper.
2. The setup and computational method

2.1. The setup

Our aim is to study the tunneling dynamics of a bosonic mixture consisting of two bosonic species, \( A \) and \( B \), in a TPH well. The Hamiltonian reads

\[
H = \sum_{\sigma=A,B} \sum_{j=1}^{N_{\sigma}} \left[ -\frac{\hbar^2}{2M_{\sigma}} \partial_{x_{\sigma,j}}^2 + V_{\text{tr}}(x_{\sigma,j}) + \frac{1}{2} \sum_{k(k\neq j)} g_{\sigma,1D} \delta(x_{\sigma,j} - x_{\sigma,k}) \right] \\
+ \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} g_{AB,1D} \delta(x_{A,i} - x_{B,j}).
\]  

(1)

Here, \( V_{\text{tr}}(x_{\sigma}) = V_0 \sin^2(\kappa x_{\sigma}) + \frac{1}{2} M_{\sigma} \omega^2 x_{\sigma}^2 \) models the TPH trap, and we apply hard-wall boundary conditions at \( x_{\sigma} = \pm 3\pi/2\kappa \) to confine the bosons to the central three adjacent wells. As the harmonic trap will eliminate the occupation of bosons in the outer wells of higher potential, the effects discussed in this paper are independent of hard-wall boundary conditions. \( M_{\sigma} \) is the mass of the \( \sigma \)-species, and \( \kappa \) is the wave vector of the laser beams forming the optical lattice. We assume that the bosons of both species take the same mass, i.e. \( M_A = M_B = M \).

We model the interspecies and intraspecies contact interaction by a delta function with respect to the relative coordinate of two bosons, and the strength of the interaction is given by \( g_{AB,1D} \), \( g_{A,1D} \) and \( g_{B,1D} \) for the interspecies and the intraspecies interaction, respectively. In the one-dimensional system as considered here, these interaction strengths can be tuned by Feshbach [7–9] and confinement-induced resonances [11, 12].

In the following, we make use of the natural units \( \hbar = 1, M = 1 \) and \( \kappa = 1 \), which is equivalent to rescaling the Hamiltonian in units of the recoil energy \( E_R = \frac{\hbar^2 \kappa^2}{2M} \). The competing parameters we focus on are mainly the inter- and intraspecies interaction strengths, \( g_{AB} = g_{AB,1D}/E_R \) and \( g_{\sigma} = g_{\sigma,1D}/E_R \), \( \sigma = A, B \).

We aim to study the effects of spatial correlation on the tunneling dynamics. To identify the relevant mechanisms, we focus on a few-body mixture consisting of two bosons of \( A \) species and one boson of \( B \) species. The initial state is prepared as follows: first, the interspecies interaction \( g_{AB} \) is turned off, and the \( A \) bosons relax to the ground state, which is characterized by the occupation of the middle well and by spatial correlations between the occupied left and right wells, while the \( B \) boson is localized to the left well. To trigger the tunneling, we turn on the interspecies interaction and simultaneously set the \( B \) boson free to move, which would drive the system out of its initial state and initiates the tunneling process. In experiments, this setup could be realized by a sudden doping of a \( B \) boson into the left well of a TPH trap, where two \( A \) bosons have already relaxed to the ground state with spatial correlations between the left and right wells. Such an instantaneous doping is then accompanied by the release of the \( B \) boson to the TPH well as well as the onset of interspecies interaction. The doping of the \( B \) boson can be experimentally achieved by e.g. single-site addressability techniques, which are now available for ultracold atoms [54–56].

2.2. The computational approach: the multi-configuration time-dependent Hartree method

In this study, we apply the numerically exact MCTDH method [51–53], which is a wave packet dynamical approach to the \textit{ab initio} solution of multi-dimensional time-dependent Schrödinger...
problems. In MCTDH, the many-body wavefunction is expanded in terms of Hartree products of single-particle functions of a corresponding basis:

\[ \Psi(x_1, \ldots, x_N; t) = \sum_{j_1, \ldots, j_N} A_{j_1, \ldots, j_N}(t) \phi_{j_1}^{(1)}(x_1, t) \cdots \phi_{j_N}^{(N)}(x_N, t), \]

(2)

where \( \phi_{j_i}^{(i)}(x_i) \) are the single-particle functions for the degree of freedom \( x_i \). Applying the Dirac–Frenkel variation principle to this ansatz leads to a set of differential equations for the \( A \) coefficients and the single-particle functions, which provide us with the time evolution of the system. In this ansatz, both the expansion coefficients \( A_{j_1, \ldots, j_N} \) and the single-particle functions \( \phi_{j_i}^{(i)}(x_i, t) \) are time dependent and are optimized at each time step, which leads to a reduction of the total number of the necessary single-particle functions for achieving convergence, and manifests itself as a big advantage of MCTDH compared with other exact computational methods.

The multi-configurational expansion of the wavefunction in MCTDH intrinsically takes into account higher band effects, which is essential for the study of systems with a temporally varying Hamiltonian, where the system could be excited to higher band states. In our setup, the instantaneous onset of \( g_{AB} \) can give rise to higher band excitation beyond the single-band approximation and therefore renders MCTDH an appropriate tool for our investigation. As we study bosonic mixtures, permutation symmetry within a single species of the mixture should also be preserved during the propagation of the wave packet. This is done in MCTDH by symmetrizing the \( A \)-coefficients according to the permutation symmetry of each species.

To prepare our initial condition in MCTDH, we choose the interspecies interaction strength \( g_{AB} = 0 \), and we take the intraspecies interaction \( g_A \), such that the ground state of the two \( A \) bosons exhibits spatial correlations only between the left and right wells. The localization of the \( B \) boson in the left well is technically realized by applying an artificial hard wall boundary condition between the left and middle wells for the \( B \)-species boson only.

3. Ground state evolution of a single species in the triple well with a harmonic trap

A milestone of ultracold atoms in optical lattices is the Mott-insulator-superfluid phase transition \(^{[35, 36]}\) driven by the interaction strength, the hopping strength between neighboring sites and the chemical potential. In an optical lattice augmented by a harmonic trap, the atoms can also exhibit a domain structure consisting of different phases \(^{[37, 38, 57]}\). This domain structure is characterized by the spatial correlations of the atomic wavefunction between selected lattice sites. For instance, one can realize a domain structure consisting of a Mott domain around the minimum of the harmonic confinement, surrounded by two superfluid wings. The superfluid wings are characterized by strong correlations, while there is no spatial correlation between different sites in the Mott domain. In this section, we demonstrate that such spatially selective correlations can be also realized for few-body systems confined to a TPH trap.

We start with two single-species bosons in a TPH well and study the evolution of the ground state with increasing interaction strength. For the analysis of the ground state, we focus on the evolution of the mean occupation \( \langle n_\alpha \rangle \) and particle fluctuation \( \delta n_\alpha = \langle n_\alpha^2 \rangle - \langle n_\alpha \rangle^2 \) of each well, and the spatial correlations among different wells, defined as \( G_{\alpha, \beta} = 2 \text{Re}(\langle \Psi | a_\alpha^\dagger a_\beta^\dagger | \Psi \rangle) \), where \( \alpha \) and \( \beta \) label the three wells, \( | \Psi \rangle \) is the ground state and \( a_\alpha^\dagger (a_\alpha) \) is the creation (annihilation) operator of a Wannier state in the well \( \alpha \). The corresponding results for these quantities are
Figure 1. The evolution of the ground state of the system consisting of two A-species bosons in the TPH well, with respect to the interaction strength: (a) the mean occupation, (b) particle fluctuation and (c) the spatial correlation between different wells. All the figures show a two-plateau structure, marked as plateau I and II, and this two-plateau structure corresponds to the transition of the ground state from $|0, 2, 0\rangle$ to $|1, 1, 0\rangle + |0, 1, 1\rangle$ (see the discussion in text). The particle fluctuations and also the fluctuation-induced correlations between the left and right wells arise on plateau II. The calculations were performed by MCTDH, with a harmonic trap frequency of $\omega = \sqrt{0.01} = 0.1$ and the height of the triple well of $V_0 = 4.0$. The mean occupation is obtained by direct numerically exact integration of the wavefunction in equation (2), whereas for the particle fluctuations and the spatial correlations we first project the wavefunction onto the number-state basis and calculate these quantities in the number-state picture. In all the three figures, the lines related to the left and right wells lie on top of each other due to the symmetry between the two wells.

shown in figure 1. Figure 1(a) presents the evolution of the mean occupation, and we observe a two-plateau behavior, where the mean occupation of the middle well changes from two to one and that of the left and right wells changes from 0 to 1/2. The mean occupation of 1/2 implies here that a boson occupies the left and right wells equally, i.e. with the same probability, leading to particle fluctuation in the left and right wells on the plateau II, as confirmed by figure 1(b). The middle well exhibits particle fluctuations only in the transition regime between plateaus I and II (see figure 1(b)). In figure 1(c) the correlation function between different wells shows a nonzero correlation between the left and right wells on plateau II, and no correlations exist between the middle well and the others except in the transition regime between the plateaus.

In the TPH well the barrier of the triple well $V_0$ is high enough such that all the bosons are well localized in a certain well in the complete interaction regime, and this enables us to construct a number-state basis to analyze the results in figure 1. The number-state basis of two bosons in a triple well contains six number states: $\{|2, 0, 0\rangle, |1, 1, 0\rangle, |1, 0, 1\rangle, |0, 2, 0\rangle, |0, 1, 1\rangle, |0, 0, 2\rangle\}$. The number state $|n_L, n_M, n_R\rangle$ refers to the state with $n_L$, $n_M$ and $n_R$ bosons in the left, middle and right wells, respectively. The number states in the low interaction regime can be constructed via the Wannier states of the bosons in each well, while in the strong interaction regime the bosons in the same well become strongly correlated, and the number states can be calculated as the states of strongly correlated bosons within each well indicated by the particle.
Figure 2. The response of (a) the mean occupation, (b) particle fluctuation and (c) spatial correlation between different wells to the interaction strength, for the system of three $A$ bosons in the TPH well. A three-plateau structure shows up and illustrates that the ground state undergoes transitions from $|0, 3, 0\rangle_A$ (plateau I) to $|1, 2, 0\rangle_A + |0, 2, 1\rangle_A$ (plateau II) and $|1, 1, 1\rangle_A$ (plateau III) at different interaction strengths. The parameters of the calculation are the same as in figure 1.

occupations of the number states. For a more detailed account of this, see [58]. In the ground state transition shown in figure 1, when the interaction strength is low, all the bosons concentrate in the middle well, corresponding to the ground state $|0, 2, 0\rangle$, and this refers to the plateau I in figure 1. As the interaction strength increases beyond some critical value, one boson is repelled out of the middle well, and localizes to the left and right wells simultaneously with the same probability, relating to the ground state of $|1, 1, 0\rangle + |0, 1, 1\rangle$, and consequently the mean occupation of the left and right wells takes the value of 1/2, while spatial correlations between the left and right wells arise. This regime corresponds to the second plateau II in figure 1. Only around the ‘critical point’ of the transition, the ground state possesses significant contributions from all the three number states $|0, 2, 0\rangle, |1, 1, 0\rangle$ and $|0, 1, 1\rangle$, and the middle well gets correlated with the left and right wells, which corresponds to the peaks of the occupation fluctuation of the middle well and the spatial correlation of the middle well and the other wells in figures 1(b) and (c), respectively.

In the system of two bosons in the TPH well, we find the spatial site-selective correlations only between the left and right wells, and this system is the smallest system to realize such site-selective spatial correlations. In a system with more bosons, such a multi-plateau structure of the ground state evolution and site-selective correlations are also encountered. Taking three bosons in the TPH well for example, we calculated the ground state evolution with respect to increasing interaction strength, and figure 2 shows the behavior of the mean occupation, particle fluctuation as well as the spatial correlations. Similar to the case of two bosons, we observe a multi-plateau structure in the three domains, and finite spatial correlations of particular sites on the second plateau. Combining figures 1 and 2, it becomes clear that an increasing interaction strength drives the bosonic ensemble from localization to the central well to a spreading among several wells. During this spreading, bosons can occupy spatially symmetric wells simultaneously, and this gives rise to nonzero particle fluctuations and correlations between the related wells. This case corresponds to the formation of domain structures in many-body systems, and

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offers a microscopic explanation of the domain-structure formation in the harmonically dressed optical lattices.

4. Tunneling dynamics in different interspecies interaction regimes

Let us now study the tunneling dynamics of a two-species bosonic ensemble, containing two bosons of $A$ species and one of $B$ species, which are confined to a one-dimensional TPH trap. Initially, the interspecies interaction is turned off, and each species relaxes to the corresponding ground state. Following the discussion in section 3, we set the intraspecies interaction strength of the $A$ species in order to realize the second plateau of figure 1(a), and the ground state of $A$ bosons corresponds to spatial correlations only between the left and right wells. The single $B$ particle is initially localized to the left well. We trigger the tunneling by releasing the $B$ particle to the complete system, and simultaneously turning on the interspecies interaction $g_{AB}$ to a finite value. In this way the $B$ particle will tunnel in the triple well on top of the domain-like structure of $A$ species, while the tunneling of the $B$ particle will also drive the $A$ bosons out of equilibrium as a back action. We study the interplay between the spatial correlations of the $A$ species and the tunneling of the $B$ particle.

Generally speaking, we can divide the interspecies interaction into three regimes according to the tunneling properties. The first one is the low interspecies interaction regime, where the tunneling is dominated by the spatial correlations of the $A$ species, and we observe the correlation-induced tunneling of the $A$ species, while the $B$ particle remains practically localized to its initial well. In the intermediate regime of $g_{AB}$, the correlation-induced tunneling vanishes due to a strong energetic detuning, and we observe a correlated tunneling process of $A$ and $B$ species in narrow windows of $g_{AB}$ on top of delayed tunneling. Finally, when the interspecies interaction is strong enough such that the system is nonadiabatically excited to higher bands when turning on $g_{AB}$, we observe a tunneling process with enhanced population oscillation due to higher band contributions.

As all the bosons of the two species are well localized to the TPH well in the tunneling process, we can again construct a number-state basis to analyze the tunneling dynamics. The number-state basis of two $A$ bosons and one $B$ boson in the TPH well can be obtained by the direct product of the number-state basis of each species, as $\{|2, 0, 0\rangle_A, |1, 1, 0\rangle_A, |1, 0, 1\rangle_A, |0, 2, 0\rangle_A, |0, 1, 1\rangle_A, |0, 0, 2\rangle_A \rangle \otimes \{|1, 0, 0\rangle_B, |0, 1, 0\rangle_B, |0, 0, 1\rangle_B\}$.}

4.1. Correlation-induced tunneling in the low interspecies interaction regime

Firstly, we focus on the low interaction regime. The initial state can be expressed as $(|1, 1, 0\rangle_A + |0, 1, 1\rangle_A)|1, 0, 0\rangle_B$, which indicates that the $A$ bosons are in the ground state corresponding to the plateau II of figure 1(a), and the boson $B$ is in the left well. We explore the time evolution of the population of the $A$ and $B$ bosons in each well, see figure 3. In figure 3(a), we show the evolution of the population of the $A$ species, which oscillates coherently between the left and right wells, and remains almost constant in the middle well. The population of the $B$ boson is shown in figure 1(b), and we find the $B$ boson to be localized in the left well. The role of the $B$ boson is an effective tilt in the left well. From figure 1 we conclude that in the low interspecies interaction regime, the tunneling process is dominated by the $A$ bosons and occurs between the left and right wells, while the $B$ boson is strongly localized.
Figure 3. The population oscillations of a mixture composed of two A bosons and one B boson with the initial state \((|1, 1, 0\rangle_A + |0, 1, 1\rangle_A)|1, 0, 0\rangle_B\). (a) Population of A bosons in the TPH well, where the oscillation is mainly between the right and left wells. (b) Population of the B boson, which remains localized to the left well. The calculations are performed by the MCTDH method, with the interaction strengths \(g_A = 0.5\) and \(g_{AB} = 0.05\) and the TPH is the same as in figure 1. The inset (b1) shows the population of A bosons in the left (dotted line) and right wells for \(g_{AB} = 0.02\) (blue line), \(g_{AB} = 0.07\) (green line) and \(g_{AB} = 0.1\) (red line). These population oscillations show that the amplitude of the tunneling decreases while the frequency increases as \(g_{AB}\) increases. The inset (b2) shows the probability of the number states \(|1, 1, 0\rangle_A|1, 0, 0\rangle_B\) and \(|0, 1, 1\rangle_A|1, 0, 0\rangle_B\) with \(g_{AB} = 0.05\). The tunneling is mainly between these two number states.

In order to explain the numerical results calculated by the ab initio MCTDH method, we again rely on a number-state analysis. The initial state is essentially the superposition of two number states \(|\Psi(t = 0)\rangle = |1, 1, 0\rangle_A|1, 0, 0\rangle_B + |0, 1, 1\rangle_A|1, 0, 0\rangle_B\), named in the following as \(|a\rangle\) and \(|b\rangle\), respectively. The spatial correlation of the A species between the left and right wells is reflected by this superposition in terms of number states. The time evolution of the system is the linear superposition of two tunneling branches, one of which takes \(|a\rangle\) as the initial state and the other one takes \(|b\rangle\) as the initial state. The tunneling properties in terms of the expectation value of a local operator, e.g. the population operators of the three wells, with the state \(|\Psi(t)\rangle = |\Psi(t)\rangle\) can be expressed as

\[
\langle \Psi | \hat{A} | \Psi \rangle = \sum_{\alpha, \beta} \langle \alpha | \hat{A} | \beta \rangle (\langle \beta | a \rangle \langle a | \alpha \rangle + \langle \beta | b \rangle \langle b | \alpha \rangle + 2 \langle \beta | b \rangle \langle a | \alpha \rangle) e^{i(e_{\beta} - e_{\alpha})t},
\]

where \(\alpha, \beta\) label the eigenstates of the complete interacting mixture, and \(e_{\alpha}\) is the eigenenergy of the \(\alpha\) eigenstate. The first two terms in the expectation value are the separate contributions from the two branches, and the third term comes from the interference of the two branches. The expectation value of \(\hat{A}\) contains the separate contributions from both tunneling branches, as well as the interference of the two branches. The interference term comes from the superposition of \(|a\rangle\) and \(|b\rangle\) in the initial state, and it is equivalent to saying that the quantum interference is induced by the spatial correlations.

In the low interspecies interaction regime, only the two number states \(|a\rangle\) and \(|b\rangle\) contribute significantly to the tunneling process (as shown in the inset of figure 3(b2), which provides the time evolution of the probabilities of the occupation of these two number states), and we can
therefore employ the reduced two-state basis consisting of $|a\rangle$ and $|b\rangle$, while the two eigenstates in this reduced basis for weak $g_{AB}$ are $\cos(\pm \pi/4 + \delta \theta)|a\rangle + \sin(\pm \pi/4 + \delta \theta)|b\rangle$, where $\delta \theta$ refers to the deviation of the eigenstates from those at $g_{AB} = 0$ and depends on the value of $g_{AB}$. In the following, we denote these eigenstates by $|1\rangle$ and $|2\rangle$. A direct calculation shows that the first two terms in equation (3) cancel each other for weak $g_{AB}$, and the tunneling properties, such as the population oscillation in figure 3(a), results exclusively from the quantum interference of the two branches, which becomes $4\Re((1|\hat{A}|2\rangle\langle2|b\rangle\langle a|1\rangle)\cos(e_1 - e_2)t]$ in the reduced basis of $\{|a\rangle, |b\rangle\}$.

In the following, we demonstrate the impact of spatial correlations of the three wells on the quantum interference term. Here the spatial correlation is measured in terms of the single-boson correlation function as discussed in section 3. We focus on the population oscillation of the three wells, taking for $\hat{A}$ the density operators of the three wells, i.e. $\hat{N}_L$, $\hat{N}_M$ and $\hat{N}_R$. We start with the population oscillation in the middle well. Since there are no spatial correlations between the middle well and the outer wells, the eigenstates $|1\rangle$ and $|2\rangle$ are also eigenstates of $\hat{N}_M$, and the first factor of the above-mentioned interference term $(1|\hat{N}_M|2) = (1|2) = 0$, leading to the freezing of the population in the middle well. In figure 3(a), we indeed observe no significant oscillation in the middle well, and confirm the effects of the spatial correlations. Furthermore, the spatial correlation of the left and right wells also vanishes as $g_{AB}$ increases further, and $(1|\hat{A}|2) (\hat{A} = \hat{N}_L$ or $\hat{N}_R)$ turns to zero, leading to very small population oscillations in the left and right wells. This trend is shown in figure 3(b1), where it is shown that the amplitude of the population oscillation in the left and right wells decreases as $g_{AB}$ increases. We therefore conclude now that the spatial correlation can affect the value of the interference term and as a consequence the amplitude of the tunneling process between different wells. In particular, the tunneling only takes place between wells with nonvanishing spatial correlation. In this way we refer to such a tunneling process as a correlation-induced tunneling. The increase of the tunneling frequency seen in figure 3(b1) is due to the fact that $g_{AB}$ detunes the eigenenergies of $|1\rangle$ and $|2\rangle$ and consequently increases the frequency of the oscillations due to $\cos(e_1 - e_2)t$.

The spatial correlations not only determine the amplitude of the tunneling process, but also the direction of the tunneling. To demonstrate this, we calculate the population of the three wells with the initial state as $|a\rangle - |b\rangle$, the so-called dark state, which is equivalent to a $\pi$-phase shift of the $A$ bosons in the right well, and the correlation $G_{LR}$ becomes negative. As shown in figure 4, the profile of the evolution of the population is similar to that shown in figure 3, where the initial state is prepared as $|a\rangle + |b\rangle$, but the tunneling direction is now from the right well to the left well, opposite to that in figure 3. This can be directly understood from the interference term, as the $\pi$-phase shift gives a minus sign to the interference term, and therefore switches the tunneling direction.

From figures 3 and 4, it becomes clear that the onset of the interspecies interaction $g_{AB}$ perturbs the spatial correlation of the $A$ species, and this leads to population oscillations of the $A$ bosons between the sites that are correlated in the wavefunction, which are the left and right wells of our system. The population of the uncorrelated site, i.e. the middle well, is barely affected. Moreover, the correlation determines not only which sites participate in the tunneling, but also the direction of the tunneling, which offers the possibility to control the tunneling processes by spatial correlations. Such a correlation-induced tunneling strongly depends on the coherent correlations between the left and right wells, and could be used as a measure for the coherence between the two wells. To illustrate this point, let us suppose that the TPH well is coupled to some source of decoherence; for instance, the left well is connected to a classical
environment, which causes a randomly temporally fluctuating phase difference between the left and right wells. The random phase difference is then mapped to that between the states \( |a\rangle \) and \( |b\rangle \). Beyond a certain strength of the fluctuation the interference is destroyed, and the consequently correlation-induced tunneling is also destroyed. In this sense, the destruction of correlation-induced tunneling can measure the coherence between the left and right wells.

As a final remark, it is also worth mentioning that the correlation-induced tunneling is triggered by the perturbation of the correlations of the system, being certainly not restricted to a few-body system. We could also expect to observe such phenomena in many-body systems, for instance in a double well. It has been shown that an ultracold bosonic gas in a double well with vanishing interaction can be seen as a whole BEC, and the correlation between the left and right wells is preserved. Such a bosonic gas will fragment into two separate BECs localized to the two wells as the interaction increases \[59\]. During the fragmentation process, the spatial correlation in terms of the single-boson correlation between the left and right wells vanishes, and this fragmentation manifests itself as the prototype phase transition of the superfluid to the Mott-insulator phase. As the condensate that is delocalized in the double well exhibits correlations, a weak tilt of the system, which detunes the potential energy of the condensates in the different wells, can also result in such a correlation-induced tunneling between the left and right wells. The amplitude of the tunneling can be used to measure the strength of the correlation between the left and right wells, in other words, the coherence of the neighboring wells. In this way, the correlation-induced tunneling manifests itself as an alternative method to measure the coherence of two separate condensates, in addition to the interference fringes after the overlapping of the condensates.

### 4.2. Correlated tunneling in the intermediate regime

As we increase the interspecies interaction beyond the weak interaction regime, the order of magnitude of which has been provided in the previous section, the two number states contributing to the initial state become increasingly different with respect to their energies and do not contribute significantly to the same eigenstates, thereby destroying the interference of
A correlated tunneling between number states with their spatially symmetric counterparts. In the resonant windows, however, of the system is practically delayed, due to the extremely weak coupling between the initial state and ‘half’ species. Generally speaking, the number states \( |1, 1, 0\rangle_A |1, 0, 0\rangle_B \) and \( |0, 1, 1\rangle_A |0, 0, 1\rangle_B \) are energetically in resonance with their spatially symmetric counterparts \( |0, 1, 1\rangle_A |0, 0, 1\rangle_B \) and \( |1, 1, 0\rangle_A |0, 0, 1\rangle_B \), respectively, for almost any value of \( g_{AB} \) and in particular in the intermediate regime except for narrow resonant windows, where some other number states become resonant with one of the initial number states. Outside these narrow resonant windows, the tunneling of the system is practically delayed, due to the extremely weak coupling between the initial number states with their spatially symmetric counterparts. In the resonant windows, however, correlated tunneling between \( A \) and \( B \) species are observed, and we show an example in figure 5.

Figure 5. The population oscillation of (a) the \( A \) species, (b) the \( B \) species in the TPH well, with the initial state \( (|1, 1, 0\rangle_A + |0, 1, 1\rangle_A) |1, 0, 0\rangle_B \), and for the interspecies interaction strength \( g_{AB} = 0.209 \) in the intermediate regime, with \( g_A = 0.6, \ V_0 = 4.0, \ \omega = \sqrt{0.03} \). For the density oscillations we observe a correlated tunneling of \( A \) bosons and the \( B \) boson. The inset (b) shows the probability oscillation of the number states, with the red line of \( |0, 1, 1\rangle_A |1, 0, 0\rangle_B \), the green line of \( |0, 2, 0\rangle_A |0, 1, 0\rangle_B \), and the blue line of \( |1, 1, 0\rangle_A |0, 0, 1\rangle_B \).

In the tunneling, we can see that the populations of the \( A \) boson in the left and right wells oscillate in the intervals \([1, 1/2]\) and \([0, 1/2]\), respectively, indicating the ‘half’ \( A \) boson tunnels from the right to the left well. Simultaneously, an amount of approximately ‘half’ \( B \) tunnels from the left to the right well opposite to the direction of the ‘half’ \( A \) boson, illustrating the two tunneling branches. In this sense the correlation-induced tunneling process disappears. The tunneling evolution in terms of the expectation value, as shown in equation (3), is then approximately the direct summation of each branch separately without interference term.

Generally speaking, the number states \( |1, 1, 0\rangle_A |1, 0, 0\rangle_B \) and \( |0, 1, 1\rangle_A |1, 0, 0\rangle_B \) are energetically in resonance with their spatially symmetric counterparts \( |0, 1, 1\rangle_A |0, 0, 1\rangle_B \) and \( |1, 1, 0\rangle_A |0, 0, 1\rangle_B \), respectively, for almost any value of \( g_{AB} \) and in particular in the intermediate regime except for narrow resonant windows, where some other number states become resonant with one of the initial number states. Outside these narrow resonant windows, the tunneling of the system is practically delayed, due to the extremely weak coupling between the initial number states with their spatially symmetric counterparts. In the resonant windows, however, correlated tunneling between \( A \) and \( B \) species are observed, and we show an example in figure 5.

In figure 5, \( g_{AB} \) resides in the resonant window, where \( |0, 1, 1\rangle_A |1, 0, 0\rangle_B \) is in resonance with \( |0, 2, 0\rangle_A |0, 1, 0\rangle_B \). The initial state is again prepared as \( |1, 1, 0\rangle_A |1, 0, 0\rangle_B + |0, 1, 1\rangle_A |1, 0, 0\rangle_B \), and now the tunneling process can be divided into two separate branches. The first branch evolves from \( |0, 1, 1\rangle_A |1, 0, 0\rangle_B \) to \( |0, 2, 0\rangle_A |0, 1, 0\rangle_B \) and \( |1, 1, 0\rangle_A |0, 0, 1\rangle_B \), during which one \( A \) boson and one \( B \) boson tunnel in the opposite direction, relating to the counterflow of the \( A \) and \( B \) bosons. In the second branch, the number state \( |1, 1, 0\rangle_A |1, 0, 0\rangle_B \) remains practically self-trapped, due to the weak coupling to its resonant state \( |0, 1, 1\rangle_A |0, 0, 1\rangle_B \). The combined tunneling process of the two branches will exhibit a counterflow process between ‘half’ \( A \) and ‘half’ \( B \) bosons.

Figures 5(a) and (b) show the population oscillations of the \( A \) and \( B \) species, respectively. During the tunneling, we can see that the populations of the \( A \) boson in the left and right wells oscillate in the intervals \([1, 1/2]\) and \([0, 1/2]\), respectively, indicating the ‘half’ \( A \) boson tunnels from the right to the left well. Simultaneously, an amount of approximately ‘half’ \( B \) tunnels from the left to the right well opposite to the direction of the ‘half’ \( A \) boson, illustrating the
counterflow behavior. The inset of figure 5 gives the probability oscillation of the number states in the first tunneling branch, and we do observe the resonant tunneling of the three number states in the first branch with small amplitude fast oscillations. The fast oscillations of the profiles of the number states indicate the higher band excitation due to the sudden doping of a $B$ boson, which will be discussed in more detail in the following subsection.

In the above example, we encounter a counterflow tunneling of ‘half’ an $A$ boson and ‘half’ a $B$ boson. After half a period of the tunneling, $|\Psi\rangle$ evolves from $(|1, 1, 0\rangle_A + |0, 1, 1\rangle_A)|1, 0, 0\rangle_B$ to $|1, 1, 0\rangle_A(|1, 0, 0\rangle_B + |0, 0, 1\rangle_B)$, and the correlation of the $A$ bosons between the left and right wells vanishes, while the $B$ boson possesses spatial correlation between the left and right wells. In other words, in the course of the tunneling, the spatial correlations are transferred between the $A$ and $B$ species. With this example, we demonstrate an appealing mechanism of correlated tunneling in mixtures. During the tunneling process, the spatial correlations between the left and right wells are transferred back and forth between the two species, which could be used as dynamical writing and reading of quantum coherence between qubits, as well as gate operations of qubits, and could potentially find applications in quantum computing.

### 4.3. Higher band contributions in the strong interspecies interaction regime

Up to this point, we have focused on the situation when $g_{AB}$ is not large enough to excite higher band states during the onset of $g_{AB}$, and the main effect of the onset of $g_{AB}$ is to modify the onsite interaction of related number states. In this section we discuss the tunneling mechanisms, when $g_{AB}$ is large enough such that higher band states come into play, and this certainly cannot be covered by a standard single-band approximation.

In the strong interspecies interaction regime, the two tunneling branches with initial states $|1, 1, 0\rangle_A|1, 0, 0\rangle_B$ and $|0, 1, 1\rangle_A|1, 0, 0\rangle_B$, respectively, are not coupled to each other, and evolve separately. We can obtain the tunneling properties of the system by separately studying the tunneling of each branch. For the tunneling branch with the initial state $|0, 1, 1\rangle_A|1, 0, 0\rangle_B$, where the $A$ and $B$ bosons reside in different wells initially and cannot interact with each other, the onset of $g_{AB}$ will not affect this initial state, and the tunneling of this branch will remain practically self-trapped, due to a large onsite energy detuning. We can only observe tiny population fluctuations of the three wells from this tunneling branch, which arises from the finite coupling of $|0, 1, 1\rangle_A|1, 0, 0\rangle_B$ with other energetically detuned number states.

On the other hand, the part $|1, 1, 0\rangle_A|1, 0, 0\rangle_B$ of the initial state is also energetically detuned from all other number states except its spatially symmetric counterpart, and should remain practically self-trapped. However, an instantaneous onset of $g_{AB}$ will strongly affect the part $|1, 1, 0\rangle_A|1, 0, 0\rangle_B$ of the initial state, and higher band states could be excited, as the $B$ boson is in the same well together with one $A$-boson. The higher band states have a larger hopping strength between neighboring wells, as the wavefunction of the higher band states can penetrate further into the barrier and has a larger overlap among states in neighboring sites [60]. This can increase the coupling of $|1, 1, 0\rangle_A|1, 0, 0\rangle_B$ to other energetically detuned number states and consequently amplify the amplitude of the population fluctuations. In figure 6, we show the tunneling dynamics of $A$ and $B$ bosons for different interspecies interaction strengths $g_{AB}$. We observe that the tunneling is almost frozen at a relatively small $g_{AB}$ with only weak population oscillations, illustrating the self-trapping behavior, and the amplitude of the
population oscillations increases as $g_{AB}$ increases, verifying the higher band excitation-induced hopping enhancement.

In figure 7 we show the one-body density profile of the $A$ bosons and $B$ boson at different time instants during tunneling in order to visualize the higher band excitation. Figure 7(a) shows the one-body density profile of the $A$ bosons before and after the onset of $g_{AB}$, and we observe the reformation of the wave packet in the left well. Initially, the $A$ bosons occupy the ground level of all three wells, and are only partially excited in the left well by the onset of $g_{AB}$, resultingly, we observe the density of a superposition of the ground and excited states, which blurs the signature of a higher band excitation. The $B$ boson, however, is localized in the left well initially, and we observe a clear signature of a higher band excitation, when tunneling to a higher band state in the right well occurs. In figure 7(b), we observe the density profile of a ground state in the left and middle wells, while the first excited state is populated in the right well after a sufficient propagation time. This tunneling process therefore works like a filter, which separates the ground and excited states into different wells.
5. Brief summary and discussion

We have explored the mechanisms of tunneling dynamics of few-boson mixtures confined to a combined triple well and harmonic trap. The harmonic trap induces spatial correlations to one species, and we studied how such correlations affect the tunneling properties of the mixture. The tunneling dynamics is qualitatively different for different interspecies interaction regimes. In the weak interspecies interaction regime, we observe a so-called correlation-induced tunneling, and in the intermediate regime, correlated tunneling between different species is observed whereas in the strong interaction regime, higher band states come into play, and the population oscillations of different wells are enhanced due to an effective weakening of the optical lattice barriers.

Our main result is the correlation-induced tunneling in the weak interspecies interaction regime. Such a tunneling arises due to the exposure of spatial correlations to a weak perturbation, and is a novel mechanism different from the common resonant tunneling process. We demonstrate that the spatial correlations can well control the dynamics of the correlation-induced tunneling, including the participating wells and the tunneling direction. We also discuss possible applications of the correlation-induced tunneling, such as the measure of off-site coherence, and the generalization to many-body systems.

In the intermediate interspecies interaction regime, the correlation-induced tunneling effect disappears, as the high-energy detuning between the involved states contributing to the correlation destroys the interference of different tunneling branches. The tunneling of both species is now delayed except in some resonant windows of the interaction strength. For the latter we observe correlated tunneling of both species, which can dynamically transfer the correlation initially present in one species to the other species. We propose that such a correlated tunneling can work as writing and reading and gate operations between qubits.
Finally, in the strong interspecies interaction regime, higher band states are excited in the course of the onset of interspecies interaction, and we observe a tunneling with stronger amplitude via higher band states, where the tunneling amplitude increases with increasing interaction strength.

Our study can be directly generalized to a wider parameter regime, for instance, to the attractive interaction regime. We can accommodate a \( B \) boson to the triple well plus harmonic potential that shows attractive interspecies interaction, and explore the interplay between the spatial correlation and the strength of the attractive interspecies interaction. Following the discussion in section 4.1, it is clear that the correlation-induced tunneling will also take place in the weakly attractive interspecies interaction regime after the doping of the \( B \) boson, but the tunneling direction should be opposite to that of the repulsive interspecies interaction. In this way the correlation-induced tunneling is controllable not only by the sign of spatial correlation, but also by the sign of interspecies interaction. Furthermore, the attractive interspecies interaction can also tune various sets of number states into resonance and realize the interspecies correlated tunneling, with different tunneling processes from those in the repulsive interspecies interaction regime. For instance, in the initial condition of \(|1, 1, 0\rangle_A|1, 0, 0\rangle_B + |0, 1, 1\rangle_A|1, 0, 0\rangle_B\), one of the states \(|1, 1, 0\rangle_A|1, 0, 0\rangle_B\) (or its spatially symmetric counterpart \(|0, 1, 1\rangle_A|0, 0, 1\rangle_B\)) can be tuned into resonance with the state \(|0, 2, 0\rangle_A|0, 1, 0\rangle_B\), and resonant tunneling should take place between these three states. As the other state \(|0, 1, 1\rangle_A|1, 0, 0\rangle_B\) in the initial condition remains practically self-trapped, we observe in the tunneling process that ‘half’ an \( A \) boson and ‘half’ a \( B \) boson form a pair and tunnel together, i.e. we encounter the tunneling process of a ‘molecular complex’ composed of ‘half’ bosons.

In section 4.2 we have discussed the spatial correlation transfer from the \( A \) bosons to the \( B \) boson, and it is certainly of interest to study the mutual interplay between the spatial correlations of two species, which can be realized by adding more \( B \) bosons to the system and initially relaxing both species to the ground states with different spatial correlations. Ground states possessing different degrees of spatial correlations for each species can be achieved by tuning the intraspecies interaction of \( A \) and \( B \) species separately with the interspecies interaction turned off. After turning on the interspecies interaction the tunneling process will be triggered, and will show rich properties induced by the interplay between the spatial correlations of the different species and the interplay between the inter- and intraspecies interactions.

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