Interaction quench induced multimode dynamics of finite atomic ensembles

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Abstract
The correlated non-equilibrium dynamics of few-boson systems in one-dimensional finite lattices is investigated. Starting from weak interactions we perform a sudden interaction quench and employ the numerically exact multi-layer multi-configuration time-dependent Hartree method for bosons to obtain the resulting quantum dynamics. Focusing on the low-lying modes of the finite lattice we observe the emergence of density-wave tunneling, breathing and cradle-like processes. In particular, the tunneling induced by the quench leads to a ‘global’ density-wave oscillation. The resulting breathing and cradle modes are inherent to the local intrawell dynamics and connected to excited-band states. Moreover, the interaction quenches couple the density-wave and the cradle modes allowing for resonance phenomena. These are associated with an avoided-crossing in the respective frequency spectrum and lead to a beating dynamics for the cradle.

Finally, complementing the numerical studies, an effective Hamiltonian in terms of the relevant Fock states is derived for the description of the spectral properties and the related resonant dynamics.

Keywords: interaction quench, non-equilibrium dynamics, higher-band effects, density-wave tunneling, cradle mode, breathing mode, avoided crossing

(Some figures may appear in colour only in the online journal)

1. Introduction

Ultracold atoms in optical lattices are regarded as an ideal tool to study properties of quantum many-body systems in a controllable manner [1–4]. This is experimentally manifested by handling independently the lattice potential and the interaction strength between the atoms. The former is achieved by tuning counter-propagating lasers and the latter by means of optical, magnetic or confinement-induced Fano-Feshbach resonances [5–10]. Currently one of the main focus of many-body physics is to comprehend quantum phase transitions (QPTs) and to unravel their internal mechanisms. In this direction, the experimental progress yielded the realization and explanation of superfluid (SF) to Mott insulating (MI) states, complementing the theoretical efforts within the Bose–Hubbard (BH) framework [11, 12]. Furthermore, other exotic quantum phases like the Bose Glass phase or Mott shells have been realized in disordered systems [13–16]. These and other QPTs raise new prospects for theory and experiment, most notably the inescapable necessity of taking quantum effects into account.

Apart from the experimental efforts in the investigation of the ground state properties in many-body systems, recently it became possible, using trapped ultracold atomic gases, to explore the evolution of isolated strongly correlated systems [17] after being quenched. In a corresponding experiment, the system is originally prepared in the ground state $|\psi_0\rangle$ of the Hamiltonian $\hat{H}$, and then driven out of equilibrium at time $t = 0$ by a sudden change of either the trapping frequency or the interaction strength, yielding a new Hamiltonian $\hat{H}_f$ evolving the system in time. The resulting non-equilibrium situation triggers challenging conceptual questions concerning the unitary evolution, such as the not yet fully understood connection of quantum ergodicity to the integrability of a system [18, 19]. The experimental applications in this field includes the realization of a quantum version of Newton’s
cradle [20], the quenching of a ferromagnetic spinor condensate [21], the light-cone effect in the spreading of correlations [22, 23], as well as the collapse and revival of a BEC [24]. Also, a recent experiment on quenched atomic SFs reports the realization of Sakharov oscillations which are known to emerge from the large-scale correlations in galaxies [25].

From another perspective, the inclusion of higher-band contributions results in an additional orbital degree of freedom yielding novel phenomena such as unconventional condensation [26–28] and anisotropic tunneling. Indeed, excited-band populations caused by interactions have already been observed either by sweeping the magnetic field across a Feshbach resonance [29] or via Raman transitions which couple directly the zeroth band to the first excited \( p \)-band of the lattice [30]. Other experimental achievements indicate the observation of a 2D SF in the \( p \)-band [31] and the orbital excitation blockade [32] when exciting atoms to higher orbitals as well as supersolid quantum phases in cubic lattices [33, 34]. The aforementioned aspects have led, among others, to the construction of multiflavor and multiorbital models [35–38]. Motivated by the previous studies here we investigate the higher-band dynamics of interaction quenched SFs focussing on the resulting low-lying collective modes, which are nowadays of great experimental interest.

In the present study, we examine the response of a finite atomic ensemble confined in one-dimensional (1D) finite lattices subjected to a sudden change in the interaction strength. More precisely, we focus on highly non-perturbative situations by considering weak-to-strong interaction quenches with respect to the initial state. In this manner, we drive the system to a regime where the interparticle interactions dominate in comparison to their kinetic energy. For weak interactions, the single-band approximation, namely the BH model, provides quantitative predictions of the system dynamics; for strong interactions, however, it yields at most a qualitative description. In this manner, by considering strong quench amplitudes and examining representative few-body setups for incommensurate filling factors, our treatment goes beyond the validity of the BH model. The numerical method which we employ in order to study the dynamical properties of our 1D finite setups is the recently developed multi-layer multi-configuration time-dependent Hartree method for Bosons (ML-MCTDHB) [39, 40], based on MCTDHB which has been developed and applied successfully previously [41–44]. Both methods are very efficient in treating bosonic systems both for static properties and in particular their dynamics (see next section), while they are equivalent for the case of a single species treated here.

We demonstrate the emergence of higher-band modes, namely the breathing and the cradle modes as well as the rise of the density-wave tunneling, following interaction quenches. Especially the observation of the cradle mode which refers to a localized wave-packet oscillation is arguably one of our central results. The dynamical properties of incommensurable setups are investigated by examining the time-evolution of the corresponding one-body densities and their respective fluctuations. In addition, we analyze the Fourier spectra of representative intrawell observables and the variation of the center of mass coordinate for the cases of the cradle and breathing modes, respectively. More specifically, the occurrence of a resonance between the cradle and one of the tunneling modes, being manifested by an avoided crossing in the frequency spectrum, is observed here. This opens the possibility to control the interwell dynamics by triggering the intrawell dynamics via the quench amplitude in optical lattices. Additionally, the construction of an effective Hamiltonian describing the dynamical behaviour is provided and the minimal Fock space required to produce the cradle process is derived.

The work is organized as follows. In section 2 we introduce our setup, explaining also the ML-MCTDHB method, the quench protocol and the number state representation. In section 3 we report on the quench dynamics for different incommensurate filling factors and demonstrate the emergent modes that arise due to the interaction quench. We summarize our findings and give an outlook in section 4.

2. Setup and analysis tools

2.1. The model

Our system consists of \( N \) neutral short-range interacting bosons in a 1D trap. The many-body Hamiltonian reads

\[
H = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m} + V(x_i) \right) + \sum_{i<j} V_{\text{int}}(x_i - x_j),
\]

where the one-body part of the Hamiltonian contains the 1D lattice potential \( V(x_i) = V_0 \sin^2(kx_i) \) which is characterized by its depth \( V_0 \) and periodicity \( l \), with \( k = \pi/l \) being the wave vector of the lasers forming the optical lattice. Furthermore, in order to restrict the infinite trapping potential \( V(x_i) \) to a finite one with \( m \) sites and length \( L \), we impose hard wall boundary conditions at the appropriate positions. On the other hand, we model the short range two-body interaction potential as \( V_{\text{int}}(x_i - x_j) = g_{1D} \delta(x_i - x_j) \) with the effective coupling strength \( g_{1D} \) depending on the 3D s-wave scattering length \( a_0 \), the oscillator length \( a_\perp = \frac{\hbar}{\sqrt{2 M a_0}} \) of the transverse trapping potential and the mass \( M \) of the atom. From the above expression it is obvious that we can tune the interaction strength by the scattering length \( a_0 \) or the frequency of the confinement \( \omega_\perp \) via Feshbach resonances [8, 9] or confinement induced resonances [45–47] respectively. Additionally, for reasons of computational convenience we will rescale the above Hamiltonian in units of the recoil energy \( E_R = \hbar^2 k^2 / 2M \) by setting \( \hbar = M = 1 \). In this manner, the rescaled interaction strength can be rewritten as \( g = \frac{g_{1D}}{E_R} \), whereas the spatial and temporal coordinates are given in units of \( k^{-1} \) and \( E_R^{-1} \) respectively. Therefore, all quantities below are in dimensionless units.
In a BH model which we address here for reasons of comparison, the Hilbert space is truncated with respect to the localized lowest-band Wannier states which form a complete set of orthogonal basis functions. This represents an alternative and more convenient way for discussing phenomena in which the spatial localization of states plays an important role. Our \textit{ab initio} simulation goes beyond the single-band approximation and requires higher-band states to describe the real and site-independent \((d_j = J_j = J)\) tunneling strength. Notice also, that the hard wall boundaries we consider here imply zero tunnel coupling between the first and the last sites (in contrast to periodic boundary conditions which result in a certain coupling for all sites). In our \textit{ab initio} simulations we use a sufficiently large lattice depth \(V_0 = 4.5\) such that each well includes two localized single-particle Wannier states, i.e. the ground and first-excited states, while the higher excited states are taken into account as delocalized states.

2.2. The computational method : ML-MCTDHB

The ML-MCTDHB constitutes a variational numerically exact \textit{ab initio} method for investigating both the stationary properties and in particular the non-equilibrium quantum dynamics of bosonic systems covering the weak and strong correlation regimes. Its multi-layer feature enables us to deal with multispecies bosonic systems, multidimensional or mixed dimensional systems in an efficient manner. Also, the multiconfigurational expansion of the wavefunction in the ML-MCTDHB method takes into account higher-band effects which renders this approach unique for the investigation of systems governed by temporally varying Hamiltonians, where the system can be excited to higher bands especially during the dynamics. An important characteristic of the ML-MCTDHB approach is the representation of the wavefunction by variationally optimal (time-dependent) single particle functions (SPFs) and expansion coefficients \(A_{i_1...i_J}(t)\). This renders the truncation of the Hilbert space optimal when employing the optimal time-dependent moving basis. Also, the requirement for convergence demands a sufficient number of SPFs such that the numerical exactness of the method is guaranteed. Therefore, the number of SPFs has to be increased until the quantities of interest acquire the corresponding numerical accuracy. This constitutes a numerically challenging and time-consuming task especially for strong interactions where the use of more SPFs to ensure convergence is unavoidable.

Let us elaborate. In a generic mixture system consisting of \(N_{\sigma}\) bosons of species \(\sigma = 1, 2, ..., S\) the main concept of the ML-MCTDHB method is to solve the time-dependent Schrödinger equation

\[
i |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle
\]

\[
|\Psi(0)\rangle = |\Psi_0\rangle,
\]

as an initial value problem by expanding the total wavefunction in terms of Hartree products

\[
|\Psi(t)\rangle = \sum_{i_1=1}^{M_1} \sum_{i_2=1}^{M_2} \sum_{i_3=1}^{M_3} A_{i_1...i_J}(t) |\psi_{i_1}(t)\rangle \cdots |\psi_{i_J}(t)\rangle.
\]

Here each species state \(|\psi_{i_J}(t)\rangle\) corresponds to a system of \(N_{\sigma}\) indistinguishable bosons, which in turn can be expanded in terms of bosonic number states \(|n\rangle\) as follows

\[
|\psi_{i_J}(t)\rangle = \sum_{n} C_{\sigma}^{n} |\bar{n}(t)\rangle^\sigma,
\]

where each \(\sigma\) boson can occupy \(m_{\sigma}\) time-dependent SPFs \(|\varphi_{i_J}(n)\rangle\). The vector \(|\bar{n}\rangle\) contains the occupation number \(n_j\) of the \(j\)th SPF that obeys the constraint \(n_1 + n_2 + \ldots + n_{M_{\sigma}} = N_{\sigma}\).

Here we focus on the case of a single species in one-dimension where the ML-MCTDHB is equivalent to MCTDHB [41–44, 48]. To be self-contained, let us briefly discuss the ansatz for the many-body wavefunction and the procedure for the derivation of the equations of motion. The many-body wavefunction is a linear combination of time-dependent permanents

\[
|\Psi(t)\rangle = \sum_{\bar{n}} \tilde{C}\{\bar{n}\} |n_1, n_2, ..., n_{M}; t\rangle,
\]

where \(M\) is the number of SPFs and the summation is again over all possible combinations which retain the total number of bosons. Notice that in the limit in which \(M\) approaches the number of grid points the above expansion becomes exact in the sense of a full configuration interaction approach. On the other hand, the permanents in (5) can be expanded in terms of the creation operators \(a_{j}^\dagger(t)\) for the \(j\)th orbital \(\varphi_{j}(t)\) as follows

\[
|n_1, n_2, ..., n_{M}; t\rangle = \frac{1}{\sqrt{n_1!n_2!...n_{M}!}} \times \left(a_{1}^{\dagger}(t)^{n_1} \cdots (a_{M}^{\dagger}(t)^{n_{M}}} \right) |\text{vac}\rangle,
\]

which satisfy the standard bosonic commutation relations \([a_i(t), a_j(t)] = \delta_{ij}\), etc. To proceed further, i.e. to determine the time-dependent wave function \(|\Psi(t)\rangle\), we have to find the equations of motion for the coefficients \(C_d(t)\) and the orbitals \(\varphi_{j}(t)\) (which are both time-dependent). For that purpose one can employ various schemes such as the Lagrangian, McLachlan [49] or the Dirac–Frenkel [50, 51] variational principle, each of them leading to the same result. Following the Dirac–Frenkel variational principle

\[
\langle \delta | \hat{H} | \delta \rangle = 0,
\]

we can determine the time evolution of all the coefficients \(C_d(t)\) in the ansatz (5) and the time dependence of the orbitals \(|\varphi_{j}(t)\rangle\). These appear as a coupled system of ordinary differential equations for the time-dependent coefficients \(C_d(t)\) and nonlinear integrodifferential equations for the time-dependent orbitals \(\varphi_{j}(t)\). The aforementioned equations constitute the well-known MCTDHB equations of motion [41–44].

Note that for the needs of our implementation we have used a discrete variable representation for the SPFs (or...
oritals) $|q_n\rangle$, specifically a sin-DVR which intrinsically introduces hard-wall boundaries at both ends of the potential (i.e. zero value of the wave function on the first and the last grid point). For the preparation of our initial state we therefore relax the bosonic wavefunction in the ground state of the corresponding $m$-well setup via imaginary time propagation in the framework of ML-MCTDHB. Subsequently, we change abruptly the interaction strength and explore the time evolution of $\mathcal{H}(x_1, x_2, \ldots, x_N; t)$ using ML-MCTDHB. Finally, note that in order to justify the convergence of our simulations, e.g. for the triple well, we have used up to 10 SPFs finally confirming the convergence. Another criterion for convergence is the population of the natural orbital with the lowest population which is kept for each case below 0.1%.

### 2.3. Quantum quench protocol

Our approach to study the non-equilibrium dynamics follows a so-called quantum quench. According to this the system is originally prepared at $t = 0$ in the ground state $|\psi_0\rangle$ of some initial Hamiltonian $H_{in} = H(\zeta_{in})$, where $\zeta_{in}$ is a system parameter associated to the perturbation such as the interaction strength or the height of the barrier. Then for times $t > 0$ we suddenly quench the parameter $\zeta$ to a final value $\zeta_f$ and examine the subsequent evolution of the system under the new Hamiltonian $H_f = H(\zeta_f)$.

In the general case, the final Hamiltonian assumes the form $H_f = H_0 + \lambda H_1$, where $H_0$ is a dimensionless perturbing operator and $\lambda$, which possesses the dimensionality of an energy, is the so-called quench amplitude. In our case the quench protocol consists of tuning the interaction strength between the particles which appears in the two-body part $(V_{int})$ of the Hamiltonian (1). Therefore, we assume as the initial state $|\psi_0\rangle$ (at $t = 0$) the ground state of the Hamiltonian $H_{in} = H(\zeta_{in})$ and we explore its dynamical behaviour for $t > 0$ subject to the Hamiltonian $H_f = H(\zeta_f)$. Under this protocol the time evolution of the system according to the Schrödinger picture is $|\psi(t)\rangle = e^{-iH_f t/\hbar} |\psi_0\rangle$ while the evolution of the expectation value of a system operator $\hat{A}$ obeys

$$
\langle \psi(t) | \hat{A} | \psi(t) \rangle = \sum_{f,f'} C_f C_{f'} e^{-\frac{E_f-E_{f'}}{\hbar} t} \langle f | \hat{A} | f' \rangle,
$$

where $|f\rangle$ refers to the eigenstates and $E_f$ the respective eigenvalues of the final Hamiltonian $H_f = H(\zeta_f)$. Thus, for our system the new Hamiltonian governing the dynamics can be written as follows

$$
H(g_f) = H(g_{in}) + \frac{\Delta g}{\hbar} \sum_{\text{int}} (x_k - x_j),
$$

with $\Delta g_{in}$ being the corresponding quench amplitude.

### 2.4. Number state representation

Using ML-MCTDHB we calculate the wavefunction with respect to a time-dependent basis of SPFs. Therefore the expansion of the wavefunction in general reads $|\psi(t)\rangle = \sum_n A_n(t) |n(t)\rangle$. On the analysis side, however, it is preferable to analyze our results in a time-independent basis and make the connection with the multiband Wannier functions. In this respect, we have developed in the framework of ML-MCTDHB a fixed basis analysis package in terms of which we use a time-independent basis for the expansion of the wavefunction, i.e. $|\psi(t)\rangle = \sum_n A_n(t) |n\rangle$.

In addition, in order to interpret our results we will use as an explanatory tool the concept of a generalized number state representation with multiband Wannier functions. To use this representation we assume that the lattice potential is deep enough such that the Wannier functions belonging to different wells have very small overlap for not too high energetic excitation. Within this framework we can analyze the interband processes as well as the intraband tunneling. As a specific example, let us elaborate for the case of a triple well system the corresponding wavefunction in terms of these states which encode the allocation of the $n$ bosons among the individual wells

$$
|\psi\rangle = \sum_{n_I,n_J,n_K,n_L} C_{n_I,n_J,n_K,n_L} |n_I,n_J,n_K,n_L\rangle.
$$

Here $n_I, n_J, n_K, n_L$ are the number of bosons localized in the left, middle, and right well respectively which satisfy the condition $n_I + n_J + n_K + n_L = n$. The summation is over all the different arrangements of the $n$ bosons in the triple well as well as the different necessary excited states (index $f$) that we must take into account according to their energetical order. In this manner, we use an expansion in terms of the number states of the non-interacting bosons, i.e. products of non-interacting single particle Wannier functions. Finally, it is important to notice that such an expansion is valid also in the strong interaction regime but needs then a large number of excited configurations.

The notion of the generalized number states will be one of our basic tools for the analysis of the non-equilibrium dynamics. For illustration, let us analyze in some detail the case of four bosons in a triple well which will be one of the considered setups in the following. Here, in terms of the number states we can realize four different categories. The quadruple mode $\{0, 0, 0, 0\}$ and the single mode $\{1, 1, 0, 0\}$ and the double mode $\{1, 0, 0, 0\}$ that refers to four bosons in the same well, as well as the triple mode $\{1, 0, 0, 0\}$ and the single mode $\{1, 0, 0, 0\}$ that implies that three bosons are localized in the same well and the fourth resides in one of the remaining wells. In addition, there is the pair mode that can be separated into two categories: the double pair mode $\{0, 0, 0, 0\}$ and the single pair mode $\{0, 0, 0, 0\}$ which contains a pair and two separated bosons.

Let us comment on the relation between the different categories of number states and the eigenstates of the system. The number states of a particular category with the same intrawell energetical index $i$ share a similar ‘on-site’ energy and they will significantly contribute to the same eigenstates. In this manner, the eigenstates can be also classified with respect to the dominantly contributing number states, e.g. the single-pair (SP), the double-pair (DP), the triple (T) and the quadruple (Q) mode. To be concrete, in the following we will
use the notation $|i\rangle_{x,t}$ to characterize the eigenstates, where the index $\alpha$ refers to the spatial occupation, i.e. the SP ($\alpha = 1$), DP ($\alpha = 2$), $T$ ($\alpha = 3$) and $Q$ ($\alpha = 4$), the index $I$ denotes the respective energetical level and $i$ stands for the index within each group. For instance $\{|i\rangle_{1,0}\}$ represent the eigenstates which are dominated by the set of SP states $\{|2, 1, 1, 0, 1, 1, 2, 1, 0, 1, 1, 2\rangle\}$, where the index $i$ take values from 1 to 3.

Finally, note that for the second system which we consider, consisting of five bosons in ten wells, the same analysis in terms of number states is straightforward. More precisely, one can realize seven different categories of number states. Namely, the single mode $\{|1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0\rangle\}$, the SP mode $\{|2, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0\rangle\}$, the DP mode $\{|2, 2, 1, 0, 0, 0, 0, 0, 0, 0, 0\rangle\}$, the first triple mode $\{|2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0\rangle\}$, the second triple mode $\{|3, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0\rangle\}$ and the fifth mode $\{|5, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\rangle\}$. Here, each mode can be characterized using similar arguments as we did for the case of the triple-well.

3. Quench dynamics

The main characteristic of a system with incommensurate filling $\nu$ is the existence of a delocalized fraction of particles $[52]$. Therefore, the most important feature is the absence of a Mott insulating state since there is a SF fraction on top of a Mott insulator phase. Below we consider both the case $\nu > 1$ where on-site interaction effects prevail and $\nu < 1$ in which the main concern is the redistribution of particles over the sites as the interaction increases. In the following, we proceed for each case with a brief discussion of the ground state properties and then we focus on the quantum dynamics resulting after an interaction quench.

3.1. Filling factor $\nu > 1$

Our initial state is the ground state for a given interaction strength in the weak-interaction regime. Therefore, let us briefly summarize the ground state properties for weak interactions for a setup consisting of four atoms in three wells, i.e. one extra particle on a Mott background. For this case of incommensurability we encounter two main aspects: delocalization and on-site interaction effects. The particle density for the non-interacting case $g = 0$ is largest in the middle site and decreases for the outer ones due to the hard-wall boundary conditions that render the middle and outer sites non-equivalent. In the low-interaction regime we observe a tendency towards a uniform population for $g \approx 0.2$ due to the repulsion of the bosons. For further increasing repulsion such as $g = 0.8$ we note a trend towards the repopulation of the central well again.

In the following, we study the quench dynamics for $t > 0$ of the above setup by means of an abrupt change in the repulsive interaction strength at $t = 0$. In order to investigate out-of-equilibrium aspects in our system we first examine the response of the one-body density. Therefore, we perturb our system starting from a SF ground state with $g_{nn} = 0.05$ where the atoms are bunching in the central well. As a consequence of the quench the system gains energy. Figures 1(a) and (b) show the time-evolution of the relative density in the triple well trap for weak and strong quench amplitudes, namely $\delta g = 0.8$ and $\delta g = 2.0$ respectively. We define the deviation of the instantaneous density from the average value up to time $T$ for each grid point $x$ as $\delta \rho(x, t) = \rho(x, t) - \langle \rho(x) \rangle_T$ where the quantity $\langle \rho(x) \rangle_T = \int_0^T dt \rho(x, t)/T$ refers to the corresponding mean single-particle probability density. Therefore, $\langle \rho(x) \rangle_T$ refers to the average behaviour of the one-body density while $\delta \rho(x, t)$ is the respective fluctuating part. According to our simulations the ratio $\delta \rho(x, t)/\langle \rho(x) \rangle_T$ is of the order of $10^{-1}$.

As can be seen in figure 1, at each time instant $\delta \rho(x, t)$ exhibits a density-wave like spatial pattern. This density wave also evolves in time, changing between a peak-valley-peak and a valley-peak-valley pattern, where the peak and valley refer to a positive and negative relative density in a certain well, respectively. The evolution of this pattern reflects the tunneling dynamics under a quench, and will be termed in the following as density-wave tunneling. Note that the density-wave tunneling refers exclusively to the mode that transfers population among the middle and the outer wells. Additionally the inner-well dynamics which can be seen in figure 1(c) is described by two excited modes: the middle well exhibits a breathing mode due to the lattice symmetry, while in the left and right wells we observe the so-called cradle mode, manifested as a ’dipole-like’ oscillation of the localized wavepacket. A close comparison of figures 1(a) and (b) reveals a transition from a multifrequency to a single frequency spectrum for weak to strong interaction quenches respectively. In the following, we will discuss in some detail each of the aforementioned dynamical modes and their significant role in the overall non-equilibrium dynamics.

3.1.1. Density-wave tunneling and breathing mode

Let us first focus on the explanation of the density-wave tunneling as an effective breathing of the ’global wavepacket’ described by the envelope of the density distribution in the triple well. According to this, we illustrate in figure 2(a) some intersections of the one-body density for different time instants and define an envelope function for the triple-well which is the quadratic function that encloses the corresponding instantaneous peaks of the density. As we have already mentioned, the density-wave reflects the tunneling dynamics of bosons confined in the optical lattices, which is dominated in the present case by the states of the lowest-band. In turn, the dynamical tunneling is constituted by the contraction and expansion of the envelope in the course of the dynamics induced by the interaction quench. Intuitively, under an interaction quench the bosons tend to repel each other and the envelope will expand and then contract, which mimics the breathing dynamics of the bosons as known in the harmonic trap. In a recent study $[53]$ this mode has been examined in the framework of the BH model for a quench in the lattice frequency. This suggests that
Let us further investigate the properties of the tunneling modes due to their significance for the above-discussed effects. The tunneling properties can be identified in terms of the overlap of the instantaneous wavefunction during the tunneling process. Figure 1. The fluctuations $\delta \rho(x, t)$ of the one-body density caused by an abrupt quench of the inter-particle repulsion. The initial state of each setup is the ground state of $N = 4$ bosons confined in a triple-well trap with $g_{in} = 0.05$. The space-time evolutions of the density are depicted for different quench amplitudes (a) $\delta g = 0.8$, (b) $\delta g = 2.0$. In (c) we show an inset of (b) for the first $t = 50$ time units where we demonstrate the cradle, breathing and over-barrier modes. Note that the spatial extent of each well is $(-\pi/3; -\pi/2)$, $(-\pi/2; \pi/2)$, $(\pi/2; 3\pi/2)$ for the left, middle and right wells respectively. The vertical axis represents the spatial extent of the trap whereas the horizontal axis denotes the propagation time $t$.

Figure 2. (a) Evolution of the one-body density $\rho(x, t)$ induced by an abrupt change of the inter-particle repulsion with amplitude $\delta g = 2.8$. The initial state is the superfluid ground state of $N = 4$ bosons with $g_{in} = 0.05$ confined in a triple-well trap. We observe spatio temporal oscillations constituting the density waves (see also figure 1). Shown is also the envelope of the one-body density (dashed lines) at different time instants: $t = 1$ (blue), $t = 10.3$ (red), $t = 18.8$ (light blue) and $t = 26.2$ (brown). The spectrum of the interwell tunneling modes can be obtained from the spectrum of the fidelity $F(t) = \langle |\psi(t)\rangle |\psi(0)\rangle^2$ which is shown in (b) as a function of the quench amplitude $\delta g$. Here the vertical axis refers to normalized frequency units $\omega / \Delta \omega$, where $\Delta \omega = 2\pi / T$ and $T$ being the respective propagation time.

it also exists for many-body systems in optical lattices where instead of our hard-wall boundaries a weak harmonic confinement renders the sites of the optical lattice non-equivalent.
Figure 3. The time evolution of the one-body correlation function \(C_{ij}\) and the density correlations \(g^{(2)}_{ij}\) for a quench from \(g_{\text{in}} = 0.05\) to (a) \(g_f = 1.0\) and (b) \(g_f = 4.2\) (see text). For the density correlations we demonstrate the situation of (c) a weak quench \(\Delta g = 0.6\) and (d) a strong quench \(\Delta g = 4.0\).

The second branch refers to the next energetically closest different modes. The tunneling process is here from the energetically lowest state of a SP mode to the energetically lowest DP mode, e.g. from \([1, 2, 1, 0]\) to \([2, 2, 1, 0]\). Finally the third branch refers to a tunneling process from a SP mode to a T mode, e.g. from \([2, 1, 1, 0]\) to \([3, 1, 0, 0]\). The remaining tunneling branches as for instance a transition from a DP mode to a T mode do in principle exist but they are negligible in comparison to the above ones due to the respective energy differences and therefore we can hardly identify them in figure 2(b). Note that the same spectrum could also be found from the frequency spectrum of the local density of a certain well, e.g. from \(\rho_{1\alpha}(\omega)\).

According to the above the tunneling dynamics here is mainly an intraband phenomenon. To verify this we have also employed the respective single-band BH model where we have identified each branch in the weak interaction regime. Within this framework, we can observe the interwell tunneling processes but have to restrict ourselves to the weak interaction regime where the single-band approximation is valid. On the contrary, we can not observe either of the on-site breathing or cradle motion (see next section) which include higher-band contributions and are intrinsically linked to the intrawall structure.

Another important tool in order to explore the interwell tunneling is to examine how correlations among different sites react after an interaction quench. We examine two different types of correlations, the single particle correlations \(C_{ij}(t) = \langle \psi | b_i^{\dagger} b_j | \psi \rangle / N\) and the second order normalized correlation function (or coherence) \(g^{(2)}_{ij}(t) = \langle n_{i,n_j} \rangle / \langle n_i \rangle \langle n_j \rangle\). Here, \(b_i^{\dagger} (b_i)\) denotes the corresponding creation (annihilation) operator of a particle located at site \(i\) in the lowest-band, while \(n_i = b_i^{\dagger} b_i\) is the number operator for the site \(i\). Notice that we mainly focus on the lowest-band description as the present tunneling mode is dominated by the lowest-band contributions, thus filtering out the influence from higher-bands. In figures 3(a) and (b) we illustrate the time evolution for the various types of one-body correlations associated with the left well for different quench amplitudes \(\Delta g = 0.95\) and \(\Delta g = 4.15\) each time starting from the SF regime \(g_{\text{in}} = 0.05\). The single
particle correlations oscillate even for long time scales which can be attributed to the finite-size of our system. The diagonal term $C_{LL}$ reflects the density oscillations of the left well which are relatively small. Moreover, we observe the change in the periods $T$ of the tunneling, that is as we increase the interaction quench we obtain a decrease of the respective period denoted by rapid small amplitude oscillations. However, the non-diagonal terms $C_{ij}$ with $i \neq j$ exhibit a non-vanishing oscillatory behaviour with an amplitude much larger than the density oscillations, i.e. $C_{LL}$. The latter shows more frequencies than the density which illustrates the emergence of more dynamical structures. This indicates that even a weak tunneling can transport substantial off-site correlations in the system.

On the other hand, the two-body correlation function $g_{ij}^{(2)}$ can be used to measure density fluctuations in the system under consideration. A basic property of this function is that $g_{ij}^{(2)} > 1$ refers to bunching whereas $g_{ij}^{(2)} < 1$ indicates antibunching. Ensembles with $g_{ij}^{(2)} = 1$ are referred to as fully second order coherent whereas for bunched particles one can infer that they have the tendency to reside together and vice versa for the antibunched case. Figures 3(c) and (d) illustrate various components of the second order correlation function for different interaction quenches. For the diagonal terms that refer to the middle well we observe that $g_{MM}^{(2)} > 1$ for the whole propagation time while for the left (or right) well we find that $g_{LL}^{(2)}$ oscillates around unity. The latter indicates a dynamical transition from bunching to antibunching and vice versa which has an impact also on the $g_{MM}^{(2)}$ component. In particular, for small quenches we can see that $g_{MM}^{(2)}$ is almost unchanged during the dynamics while $g_{LL}^{(2)}$ oscillates around unity and spends more time below unity. This means that for small quenches we can not affect significantly the initial distribution and two bosons are more likely to reside in the middle well. Increasing the quench amplitude we observe that the two components are anticorrelated i.e. for the time intervals where $g_{LL}^{(2)}$ is smaller than unity the corresponding component $g_{MM}^{(2)}$ for the middle well is enhanced. Here the reduction of the $g_{LL}^{(2)}$ component is more pronounced than the enhancement of the $g_{MM}^{(2)}$, which might indicate an impact of the initial distribution. The off-diagonal terms $g_{LR}^{(2)}$, $g_{LM}^{(2)}$ with respect to the left well are always lower than 1 and anticorrelated. Also, for every time during the dynamics $g_{LR}^{(2)} > g_{LM}^{(2)}$ holds, indicating that it is more likely for two bosons to be one in the left and one in the middle site than one in the left and one in the right. On the other hand, the oscillatory behaviour of $g_{ij}^{(2)}$ can again be attributed to the finite size of our system. Concluding this part we can infer that the one-body and two-body correlations as shown in figure 3 demonstrate a rich phenomenology in terms of correlation dynamics. This might pave the way for further investigations on how a weak density-wave tunneling can transport significant correlation oscillations.

As the density-wave tunneling has been understood to lead to the ‘envelope breathing’ with the character of a breathing mode, let us now turn our attention to the study of the on-site or local breathing mode. In general, the breathing mode then refers to a uniform expansion and contraction of the local wavepacket. For a recent study concerning the dependence of the breathing mode frequency on the particle number as well as on the interaction strength see [54], while for further related and recent investigations we refer the reader to [55–58]. As we shall discuss briefly here, this local breathing mode can also be triggered by a quench of the interaction strength in a harmonic trap. To this end, figure 4(a) shows snapshots of the one-body density of a system consisting of two bosons in a single harmonic trap (with $g_{mm} = 0.05$) after an interaction quench $\delta g = 2.8$ which mimics the dynamics within the middle well of the triple-well system. Here, we observe the reshaping of the density

![Figure 4](image-url)
profile for different time instants as well as the formation of oscillatory structures which indicate the existence of higher-band effects.

Coming to the triple well, the local breathing mode refers to a contraction and expansion dynamics of the wavepacket in a single well, i.e. intrawell breathing induced by an interaction quench. In order to quantify the local breathing frequency in the triple-well setup we define the coordinate of the center of mass of the respective well

\[ X_{cm}^{(i)} = \frac{\int_{d_{i}}^{d_{i+1}} dx \left( x - x_{0}^{(i)} \right) \rho_{i}(x)}{\int_{d_{i}}^{d_{i+1}} dx \rho_{i}(x)}. \]

Here \( i = R, M, L \) stands for the right, middle and left well respectively whereas \( x_{0}^{(i)} \) refers to the middle point of the corresponding well. On the other hand, \( d_{i} \) are the coordinates of the edge points of an individual well and \( \rho_{i}(x) \) the corresponding single-particle densities. From this point of view the preferable quantity to identify the breathing process is the variance of the coordinate of the center of mass

\[ \text{var}\left[ X^{(i)}(t) \right] = \sigma_{\Delta x}^{2} = \int_{d_{i}}^{d_{i+1}} dx \rho_{i}(x) \left( x - X_{cm}^{(i)} \right)^{2}. \]

Therefore, the breathing frequency of the middle well can be obtained from the spectrum of the second moment

\[ \sigma_{\Delta x}^{2}(\omega) = \frac{1}{\pi} \int dt \sigma_{\Delta x}^{2}(t) e^{\text{int}(t)}. \]

In figure 4(b) we observe a dominant frequency, located at \( \omega \approx 50\pi \omega_{L} \) (with \( \Delta \omega = 2\pi/T \) and \( T \) the total propagation period) which is approximately two times the trapping frequency of a harmonic approximation to a single well. This frequency depends only weakly on the interaction quench and it is related to the breathing frequency. There occur additional low frequency branches in figure 4(b) which are related e.g. to the tunneling dynamics.

### 3.1.2. The cradle mode induced by the over-barrier transport

For a qualitative description of the cradle mode one has to rely on the intrawell dynamics of \( \delta \rho(x, t) \) for the left or right well as shown in figure 1. In particular, the generation of this mode is accompanied by a direct over-barrier transport as a consequence of the interaction quench. This results in a cradle mode which represents a dipole-like oscillation. In the following, let us first illustrate the main mechanism and then analyze in some detail the cradle mode.

Initially, in terms of its dominating spatial configuration our system consists of two bosons in the middle well and two others each of them localized in one of the outer wells. Then we perform a sudden change in the interaction strength which raises the energy as mentioned previously. As a consequence with high probability at least one particle from the central well gains enough energy to overcome the barrier (over-barrier transport), and directly moves to the outer wells where it performs an inelastic collision with the preexisting particle initially localized in the neighboring site. The two-particle collision leads to a cradle dynamics and to the dipole-like density oscillation as visualized in Figure 5. According to our simulations we observe significant over-barrier transport for \( \delta g > 0.24 \). This process is most significant for the first few periods of the cradle motion as for later times due to inelastic collisions in the left well the atom looses part of its initial energy and can predominantly tunnel through the barrier.

Therefore, the cradle mode as a localized wave-packet oscillation can be produced via a variation in the respective interaction strength. Moreover as already mentioned, is reminiscent of the dipole oscillation in the one-body density evolution while a detailed analysis demonstrates a major difference between the two. Indeed, the cradle mode which is of two-body nature possesses two intrinsic frequencies that refer to the center of mass and the relative frame of the harmonic oscillator. As we prove in the appendix up to a good approximation this can be modeled by a coherent state of the center of mass and relative coordinates. Finally, note that during the evolution we can identify regions of bright and dark cradles which are associated with an enhanced or reduced tunneling of the density from the respective well (see also figure 1).

Especially, as the cradle mode breaks the local reflection symmetry of the one-body density in each well, we divide for a further investigation of this mode (neglecting the breathing mode) each well into two equal parts left and right of the center with corresponding integrated densities \( \rho_{a,1}(t) \) and \( \rho_{a,2}(t) \). Here the index \( a \) refers to the corresponding well, i.e. \( a = L, M, R \) for the left, middle and right well respectively.

In the following, we use as a measure of the intrawell wavepacket asymmetry (referring to the cradle motion) the quantity \( \Delta \rho_{a}(t) = \rho_{a,1}(t) - \rho_{a,2}(t) \). Furthermore, in order to investigate the impact of different quenches on the system we compute the Fourier transformation of the quantity

\[ \Delta \rho_{a}(\omega) = \frac{1}{\pi} \int dt \Delta \rho_{a}(t) e^{\text{int}(t)} \]

which will provide us with the evolution of the frequencies of the respective modes for different quench amplitudes. Figure 6(a) presents the resulting frequencies from the \( \Delta \rho_{a}(\omega) \) versus the respective interaction quench \( \delta g \) for 110 different quenches from weak-to-strong interactions, where the amplitude \( \delta g \) varies from 0.04 to 4.5.

Firstly, from figure 6(a) we can identify one dominant branch which is insensitive to the quench amplitude and its frequency is that of the cradle mode. This branch corresponds to the cradle intrawell oscillation and will be referred to in the following as the cradle branch. A modulation of the frequency of the cradle motion can be achieved by tuning the barrier height, i.e. we can reduce its frequency using lower barriers and vice versa.

Besides the cradle branch, three interwell tunneling branches show up in the spectrum of \( \Delta \rho_{a}(\omega) \) with a relatively weak amplitude. Among them we can distinguish the contribution of the highest frequency tunneling branch. The latter together with the branch of the cradle experience an avoided-crossing at \( \delta g \approx 2.8 \) in the course of which both amplitudes are enhanced.

For a more detailed analysis of the above observations, let us assume that initially the state of the system in terms of the eigenstates of the final Hamiltonian is given by a linear superposition of the form

\[ |\psi(0)\rangle = \sum_{a} C_{a} |\psi_{a,1}\rangle_{\text{cradle}}. \]

Then at an arbitrary time instant \( t \) the expectation value of the
The intrawell asymmetry operator can be expressed as

\[ \sum_i \sum_{\Delta \rho} \psi_{\Delta \rho} \psi_{\Delta \rho}^{*} \Delta \rho \omega^{\alpha \beta} \neq 0 \]

\( i \) \& \( j \) \( \alpha \beta \) \( \gamma \delta \)

where \( \psi_{\Delta \rho} \) is the eigenstate of the cradle-like process (see text). Consequently, the corresponding oscillation frequency matches the energy difference between these eigenstates which is to a good approximation given by the energy difference (\( \Delta \epsilon \)) between \( |2, 1, 10 \rangle \) and \( |2, 1, 11 \rangle \). As a consequence we notice the occurrence of a beating (b) for the cradle in the region of the avoided crossing.

In conclusion, the avoided crossing and the accompanying enhancement indicate that the local intrawell dynamics can couple to the interwell dynamics. In turn, this induces a resonance between the two dynamical processes which can enhance the local and long-range dynamics. The fact that the cradle mode can be coupled with a mode of the interwell tunneling is remarkable. This gives rise to the possibility of controlling the 'global dynamics' by triggering the 'local

Figure 5. Visualization of the cradle process induced by the over-barrier transport. In this scenario, the system which is (a) initially in a superfluid ground state is subjected to an abrupt interaction quench. In this manner, a boson initiated in the middle well can overcome the barrier (b) and move to the neighboring well resulting in a cradle motion (c) due to the quench in the inter-particle repulsion.

Figure 6. (a) Fourier spectrum as a function of the interaction quench of the intrawell asymmetry \( \Delta \rho_{\omega}^{\alpha \beta} \) for the left well (see text). The same spectrum can be obtained for the right well. The frequency units \( \omega/\Delta \omega \) are normalized with \( \Delta \omega = 2\pi/T \) and \( T \) being the respective propagation period. An avoided crossing takes place between the tunneling and the cradle modes where we observe an enhancement of the mode amplitudes at least for finite time propagation periods. The full white dots in the tunneling branch correspond to the intraband frequency \( \Delta \omega_{01} \) between the states \( |2, 1, 1 \rangle_{0} \) and \( |3, 0, 1 \rangle_{0} \), whereas the empty circles in the branch of the cradle mode refer to the frequency \( \Delta \omega_{12} \) for the states \( |2, 1, 1 \rangle_{0} \) and \( |2, 1, 1 \rangle_{1} \), describing the cradle-like process (see text). As a consequence we notice the occurrence of a beating (b) for the cradle in the region of the avoided crossing.
dynamics’. Especially, we can tune the characteristic frequency of the tunneling mode to become resonant with the corresponding frequency of the cradle mode by means of tuning the quench amplitude. Increasing further the quench amplitude we can drive the system again out of resonance.

As a consequence of this avoided crossing the intrawell asymmetry \( \Delta \rho \) dynamics features a beating, as shown in figure 6(b), which corresponds to two dominant frequencies in the \( \rho_1(\omega) - \rho_2(\omega) \) spectrum. Indeed, let \( \Delta \omega_1(\delta g) = E_g - E_\delta \) be the frequency of the respective intraband tunneling \((1, 2, 1, 1)_0 \rightarrow (3, 0, 1)_0\). Assume further that \( \Delta \omega_2(\delta g) = E_\tau - E_r \) refers to a frequency of a process that includes a ground and the first excited state of the SP mode taking into consideration that we refer to one of the outer wells (left or right) so we need two particles there. In this manner, there exists a region of critical quench amplitudes \( \delta g_{\text{eff}} \) which corresponds to the avoided crossing where \( \Delta \omega_1(\delta g_{\text{eff}}) \approx \Delta \omega_2(\delta g_{\text{eff}}) \) and the system features a degeneracy between the states \((3, 0, 1)_0 \) and \((2, 1, 1)_1\).

From the above discussion, one can infer that a representative wavefunction describing the cradle process in terms of Fock states for the left well (and similarly for the right) can in principle be written as

\[
|\varphi_{\text{cradle}}\rangle_L = C_0(\delta g, t)|2, 1, 1\rangle_0 + C_1(t)|2, 1, 1\rangle_1 \equiv |2, 1, 1\rangle_L^\dagger,
\]

where the coefficients \( C_0 \) and \( C_1 \) denote the probability amplitudes for the corresponding state. Note also that the amplitude of the zeroth state \((2, 1, 1)_0\) depends on the quench while the one for the first-excited state \((2, 1, 1)_1\) is essentially constant, i.e. independent of \( \delta g \).

Taking advantage of the previous description we can construct an effective Hamiltonian for this process. Thus, if we denote by \(|\tilde{n}_0\rangle\) the corresponding truncated basis vectors, the effective Hamiltonian obtained from (1) in this subspace will be of the form

\[
H_{\text{eff}} = \sum_{\tilde{n}_0} \epsilon_{\tilde{n}_0} |\tilde{n}_0\rangle \langle \tilde{n}_0| + \sum_{\tilde{n}_0, \tilde{n}_1} J_{\tilde{n}_0, \tilde{n}_1} |\tilde{n}_0\rangle \langle \tilde{n}_0|,
\]

where \( J_{\tilde{n}_0, \tilde{n}_1} = \langle \tilde{n}_0| H_{\text{eff}} |\tilde{n}_1\rangle \) is the effective tunneling amplitude and \( \epsilon_{\tilde{n}_0} = \langle \tilde{n}_0| H_{\text{eff}} |\tilde{n}_0\rangle \).

Therefore the representative subspace providing the mode-coupling within a minimal model consists of the states \((2, 1, 1)_0, (3, 0, 1)_0, (2, 1, 1)_1\). In terms of the corresponding effective Hamiltonian the respective term for the cradle mode is \((2, 1, 1)_1 \rightarrow (2, 1, 1)_0\) whereas the term \((2, 1, 1)_0 \rightarrow (3, 0, 1)_1\) reflects the tunneling process. Thus from the Hamiltonian (16) one can realize a three-level system consisting of the states according to their energetic order: \((2, 1, 1)_0 \equiv |1\rangle, (3, 0, 1)_0 \equiv |2\rangle, (2, 1, 1)_1 \equiv |3\rangle\). In this manner, we take into account an energy detuning \( \Delta \) between the states \((2\rangle\) and \((3\rangle\) whereas due to the fact that the level \(|1\rangle\) is weakly coupled with the other levels we neglect the respective tunneling amplitudes, i.e. \( J_{22} = J_{23} = 0 \). Therefore, we can reduce our problem to a two level system realizing the Hamiltonian \( H_{\text{eff}} = \sum_{i=1}^3 \epsilon_i |i\rangle \langle i| + J_{32} |2\rangle \langle 3| + \text{h.c.} \) which is known to exhibit an avoided level crossing and can be solved analytically.

In the remaining part of this section, we proceed to the investigation of a system with filling factor \( \nu < 1 \) in order to generalize our findings. More precisely, among others we demonstrate that the cradle mode can also be found in the inner-well dynamics for a setup with ten wells, which reveals in particular that it is independent of the employed hard-wall boundaries.

### 3.2. Filling factor \( \nu < 1 \)

Let us consider here the case of five bosons in a ten-well finite lattice. Concerning the ground state analysis with filling factor \( \nu < 1 \), the most important aspect is the spatial redistribution of the atoms as the interaction strength increases. The non-interacting ground state \((g = 0)\) is the product of the single-particle eigenstates spreading across the entire lattice, while due to the hard-wall boundary conditions the two central wells of the potential are slightly more populated. As the expulsion increases within the weak interaction regime the atoms are pushed to the outer sites which gain and lose population in the course of increasing \( g \), while the particle number fluctuations are more pronounced for the wells with a lower population [52]. It is also important to notice that in such a setup the one-body density will not become uniform even for strong interactions. In addition, the particle number fluctuations saturate to a relatively high value (for \( g \approx 3.5 \)) in accordance with the existence of the delocalized phase. Also, in such a case of incommensurability due to the delocalized fraction of particles the long-range one-particle correlations do not vanish even for strong interactions.

In the following, we explore the dynamics following a sudden interaction quench at time \( t = 0 \) which is applied to the ground state in the weak interaction regime, \( g_{\text{ds}} = 0.05 \). Figure 7 demonstrates the response of the system on the one-body level namely \( \delta \rho(x, t) \) after a strong interaction quench \( \delta g = 4.0 \), from which we can easily identify the emergence of three modes. Initially we observe an over-barrier transport and then the cradle and the tunneling modes. The lattice symmetry (even number of wells) leads to the lack of the local breathing mode. Concerning the cradle mode, this would be a
superposition of the states $|1, 1, 2, 0, 0, 0, 0, ...\rangle + \text{permut}$ and $|1, 1, 2, 0, 0, 0, 0, ...\rangle + \text{permut}$ with $i \neq 0$, where \text{permut} stands for the spatial permutation of the occupations inside the ket vector. Here, one can consider the minimal subspace consisting of the above states with $i = 1$ in order to proceed in an effective approach as we did for the case $\nu > 1$.

Additionally, in order to visualize the cradle process from a one-body perspective we demonstrate in figure 8 for a specific quench $\delta g = 3.4$ the density fluctuations $\delta \rho(x, t)$ for different time instants. Figure 8(a) illustrates the evolution of the fluctuations for a specific time interval following up on the over-barrier transport, where we can observe the cradle process in each well. Subsequently, in figures 8(b) and (c) we show intersections of $\delta \rho(x, t)$ focusing on the second and the fourth wells in order to visualize the higher-band contributions to the mode. Indeed, in figure 8(b) we observe that the profile of the fluctuations corresponds to almost localized wave-packets inside the well which are spatially shifted with time. This process demonstrates the motion of the cradle and corresponds to the ground state of this mode. However, figure 8(c) illustrates the same profile $\delta \rho(x, t)$ but for a different well, where the appearance of at least one node indicates the occupation of the first excited Wannier state in the well. This behaviour together with the shift of the wave-packet indicates the first-excited state of the cradle mode.

Also, in the Fourier spectrum we can find the avoided crossing between the cradle and the tunneling frequency where the critical region of quench amplitudes is $\delta g_{\text{cr}} = 4.2 - 4.3$ with equal cradle frequency as for the triple well case due to the same barrier height $V_0 = 4.5$. In turn, the avoided crossing here, if we refer to the third well, can be explained from the dominant number states $|1, 1, 2, 0, 0, 0, 0, ...\rangle$ for the cradle and $|1, 1, 2, 0, 0, 0, 0, ...\rangle$ for the tunneling process. Therefore, we can conclude that by tuning the interaction quench we can again realize a resonance between the aforementioned modes.

An important observation is that as we increase the interaction quench the tunneling process can be altered. Indeed, this behaviour can be attributed to the fact that the higher the quench amplitude, the larger the energy of the system becomes. From this point of view we expect a strong link of the change of the spatial distribution of the atoms in the lattice and the quench amplitude. The above behaviour is a main characteristic of setups with filling factor $\nu < 1$ where on-site effects are not manifested. In order to quantify our arguments concerning the spatial redistribution process we will rely on an analysis of the one-body reduced density matrix $\rho^{(1)}(x, x'; t)$ of the dynamics provided by ML-MCTDHB. Its off-diagonal parts can be used as a measure of the coherence as they indicate off-diagonal long-range order in an infinite lattice. Although, for our finite setups we cannot conclude upon true off-diagonal long-range order this term refers to the appearance of short and long range one-body correlations. Thus, this quantity can be directly linked to the tunneling process. In figure 9, we depict the one-body density matrix for three different quenches namely $\delta g = 1.4$, 2.6, 3.8 at two different time instants $t_1 = 7.0$ (a), (b), (c) and $t_2 = 42.8$ (e), (f), (g) of the propagation in order to indicate the change in the tunneling process. The off-diagonal contributions fade out with increasing quench amplitude and a tendency for concentration close to the diagonal is observed at equal times which implies an alteration of the character of the tunneling process. In addition, the off-diagonal part cannot vanish completely even for strong quenches since the particles always remain delocalized. This is a main characteristic of incommensurate setups.

Going beyond the above examined finite setups, one can suggest a generalization for the wavefunction of the cradle state for a many-body system. Let $N$ be the number of sites and $n$ the total number of bosons. Then the corresponding generalized number state would be of the form $|n_1, n_2, ..., n_N\rangle$, whereas the minimum representative wavefunction for the cradle that refers to the first well can be written as

$$\psi^{\text{cradle}} = d_1(t)|2, n_2, ..., n_N\rangle_0 + d_2(t)|2, n_2, ..., n_N\rangle_1, \quad (17)$$

where $n_2 + n_3 + ... + n_N = n - 2$ with $n > 2$ and $d_1$, $d_2$ denotes the amplitudes for each contribution in the above expansion. An additional constraint is that for an even number

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure8.png}
\caption{The response of the fluctuating part $\delta \rho(x, t)$ of the one-body density after an abrupt change in the inter-particle repulsion. The setup consists of five particles in ten wells and the initial state corresponds to interaction strength $g_{\text{in}} = 0.05$. Shown are $\delta \rho(x, t)$ for (a) a given time period of the cradle-like process for $\delta g = 2.4$ and the respective fluctuating one-body density profiles at different time instants for (b) the second well indicating the ground state of the cradle state and (c) the fourth well demonstrating the first-excited state of the cradle process. The nodal structure indicates the occupation of excited Wannier states in the respective well whereas the oscillatory behaviour visualizes the cradle process.}
\end{figure}
of sites $N$ this relation holds for all permutations, while for odd $N$ the permutation that corresponds to a state with two particles in the middle well indicates the presence of the local breathing motion. The extension to cradles in the remaining wells is straightforward.

4. Summary and conclusions

We have explored the influence of sudden interaction quenches on small bosonic ensembles in finite 1D multi-well traps. In particular, we have mainly focussed on setups with incommensurate filling factors in order to avoid the suppression of tunneling due to MI phases for strong interactions. Starting from the SF regime, we change abruptly the effective coupling strength from weak to strong interactions. In this manner, we observe the emergence of tunneling, breathing and cradle processes. Furthermore for the explanation of the dynamical behaviour of our system in terms of a band structure we employ the concept of generalized multi-band Wannier number states which are meaningful for sufficiently large barrier heights $V_0$. Although these have been constructed numerically, such a treatment is valid even in the strong interaction regime where perturbative methods fail.

The density-wave tunneling has been linked to an effective breathing of the ‘global wavepacket’ that refers to the instantaneous density distribution of the trap. The local breathing mode has been identified as an expansion and contraction dynamics of bosons in the individual wells. Moreover, in terms of a number state analysis of the observed dynamics it is necessary to include higher-band contributions to describe it. On the other hand, the cradle process, as we have pointed out, exists in almost every site of the lattice and refers to a localized wave-packet oscillation. This mode is a consequence of the initial over-barrier transport of the particles from the central well to the outer ones due to the sudden import of energy into the system and the consequent inelastic collisions with the respective atoms in the outer sites. Therefore, we can describe this process via the coherent states of the harmonic oscillator refering here to the center of mass and the relative coordinate (see appendix). The aforementioned modes are always accompanied by a tunneling process which is mainly a lowest-band phenomenon. During the dynamical process, regions of density dips or dark cradles in the outer sites are accompanied by enhanced breathing dynamics on the middle site. Each of the above modes possesses different characteristic frequencies. In particular, we show that one can tune the frequency of the highest branch of the tunneling mode in resonance with the frequency of the cradle mode by varying the quench amplitude. In turn, this resonance is associated with an avoided crossing in the frequency spectrum of these modes resulting in an enhancement of both of them. In this case, the system features a dominant beating.

We have computed, the dominant Fock states in the expectation value of the asymmetry operator in order to describe the dynamics associated with the avoided-crossing. In this manner, we have found a representative cradle state which is a superposition of the first two bands, as well as the number state most responsible for the tunneling mode that couples with the cradle in the avoided crossing.

Figure 9. Off-diagonal one-body reduced density matrix $\rho^{(1)}(x, x'; t)$ for five particles in 10 wells for two different time instants $t_1 = 7.0$ (a), (b), (c) and $t_2 = 42.8$ (e), (f), (g) during the evolution. Shown are three values of the interaction quench (a), (d) $\delta g = 1.4$, (b), (f) $\delta g = 2.6$ and (c), (g) $\delta g = 3.8$. The elimination of the off-diagonal spots for strong quench amplitudes indicates the difference in the tunneling process.
There are at least two ways that one might pursue as a follow-up direction. A first possible extension is to consider smooth time-dependent interaction quenches in order to unravel the behaviour of the system in such a non-equilibrium continuously driven case or to find similarities with the so-called Kibble–Zurek mechanism [59–64]. A second path in this direction would be the study of mixtures consisting of different bosonic species.

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Appendix. Remarks on the cradle state

In this appendix we will briefly discuss the derivation of the cradle state. This state, as we have already mentioned in the main text, refers to an oscillation of two wavepackets of minimal uncertainty in a single well which we model as a harmonic trap. The creation of the two-particle cradle state in a single well corresponds to the collision between a particle injected to the well with another particle which is initially localized in the minimum of the well. We further model each particle as a localized one, where the first one is centered in the trap and the other one is displaced from the minimum by an amount \(x_0\). In this manner, taking advantage of the exactly solvable model of the harmonic oscillator, we can derive the initial wavefunction of the cradle state. In the following, we will use the natural units \(m = \hbar = 1\). Due to the harmonic potential approximation we can separate the motion into the relative \(X_t = (x_1 - x_2)/\sqrt{2}\) and center-of-mass \(X_c = (x_1 + x_2)/\sqrt{2}\) coordinates. Adopting these coordinates the initial wavefunction reads

\[
\psi_0(X_c, X_t; 0) = \left(\frac{\omega}{\pi}\right)^{1/4} e^{-\frac{1}{2}(x_1 - x_2)^2} \times \left(e^{-\frac{1}{2}(x_1 + x_2)^2} + e^{-\frac{1}{2}(x_1 - x_2)^2}\right). \tag{A.1}
\]

Thus, the intrawell oscillation can be separated into two parts: (a) the center-of-mass motion which is an effective one-body problem and (b) the relative motion that refers to a reduced two-body problem. Therefore, we can easily show that the wavefunction of the center-of-mass at any time \(t > 0\) is described by

\[
\psi(X_c, t) = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{2}(x_1 - x_0 \cos \omega t - x_2 \sin \omega t)}, \tag{A.2}
\]

which is the well-known coherent state solution of the harmonic oscillator. This wave-packet oscillates around the minimum of the potential in a simple harmonic trap without changing its shape while it satisfies the minimum-uncertainty, i.e. \(\Delta p \Delta x = \hbar/2\). On the other hand, the corresponding wavefunction of the relative frame reads

\[
\psi(X_t, t) = \sum_n C_{2n} e^{i\omega_{2n} t} \varphi_{2n}, \tag{A.3}
\]

where \(\varphi_{2n}\) are the even eigenstates of the trapping potential \(V(x) = \frac{1}{2} m \omega^2 x^2 + g \delta(x)\). These eigenfunctions are known as the Weber functions. Thus, we can conclude that the cradle state contains two characteristic frequencies: (a) the frequency \(\omega_c = \omega^2\) that refers to the motion of the center-of-mass and (b) the frequency \(\omega_t = \omega_{2n+2} - \omega_{2n} \approx 2\omega\) of the relative frame. The above comments lead us to the conclusion that the major difference between the cradle state that we have found here and the dipole state of a many-body system is that our state contains the two frequencies \(\omega_c\) and \(\omega_t\) while the many-body collective state has just one.

Comparing the analytical results with the exact numerical ones obtained from the ML-MCTDHB method we conclude that in our case we observe only the center-of-mass oscillation in the frequency spectrum. This is a consequence of the fact that the quantity \(\Delta \rho = \rho_1 - \rho_2\) that we have used to measure the intrawall asymmetry can describe only the motion of the center-of-mass.

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