Resonant quantum dynamics of few ultracold bosons in periodically driven finite lattices

S I Mistakidis¹, T Wulf¹, A Negretti¹,² and P Schmelcher¹,²

¹ Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany
² The Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany

E-mail: smistaki@physnet.uni-hamburg.de

Received 4 June 2015
Accepted for publication 4 September 2015
Published 3 November 2015

Abstract
The out-of-equilibrium dynamics of finite ultracold bosonic ensembles in periodically driven one-dimensional optical lattices is investigated. Our study reveals that the driving enforces the bosons in different wells to oscillate in-phase and to exhibit a dipole-like mode. A wide range from weak-to-strong driving frequencies is covered and a resonance-like behavior of the intra-well dynamics is discussed. In the proximity of the resonance a rich intraband excitation spectrum is observed. The single particle excitation mechanisms are studied in the framework of Floquet theory elucidating the role of the driving frequency. The impact of the interatomic repulsive interactions is examined in detail yielding a strong influence on the tunneling period and the excitation probabilities. Finally, the dependence of the resonance upon a variation of the tunable parameters of the optical lattice is examined. Our analysis is based on the ab initio multi-configuration time-dependent Hartree method for bosons.

Keywords: ultracold atoms, periodic driving, nonequilibrium quantum dynamics

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

1. Introduction

Ultracold atomic quantum gases in optical lattices have reached an unprecedented degree of control providing direct experimental access to a plethora of non-equilibrium phenomena [1–4]. This control includes the modulation of the interparticle interactions via confinement-induced, magnetic and optical Feshbach resonances [5–10], the design of arbitrarily shaped optical traps with variable lattice depths, and the ability to move time-periodically or even accelerate the entire lattice structure. This level of control and accuracy over the system parameters has opened the possibility to simulate and study quantum many-body phenomena in part inspired from condensed matter physics [11]. For instance, when accelerating an optical lattice, representative processes are Bloch-oscillations [12–16], Wannier–Stark ladders [17, 18], Landau–Zener tunneling [16, 18] and photon assisted tunneling [19], to name only a few. A promising technique is the lattice shaking which has been used in order to address, for example, the coherent control of the superfluid to Mott insulator phase transition [20], parametric amplification of matter waves [21], four-wave mixing [22, 23], topological states of matter [24], hybridized band structure [21, 25], and even the engineering of artificial gauge fields [26]. More recently it has been shown [27, 28] that one can use lattice shaking to probe coherent band coupling and realize the formation of ferromagnetic domains. Moreover, the dynamics induced by shaking an optical lattice can lead to an admixture of excited orbitals [29] and constitutes an emergent branch of modern quantum physics.

A substantial part of the previous studies has been primarily focused on the renormalization of the physics due to driving, the mean-field approach [14] for weak interactions, where the Gross–Pitaevskii equation is still valid, and a linear
response treatment [30]. However, a relatively large modulation of the strength or of the frequency of the driving as well as strong interactions calls for alternative methods which can take into account higher-orbitals. Indeed, the inclusion of higher-band contributions introduces new degrees of freedom and as a result additional physical processes come into play. Hereby, a sinusoidal shaking of the optical lattice is a natural starting point which induces an in-phase dipole mode on each site. An interesting and so far largely unexplored direction is the study of the interplay between higher bands for the intra-well mode and the inter-well tunneling dynamics with respect to the driving frequency, and the investigation of the effect of the interatomic interactions in the overall process. In this way, it is natural to start with the investigation of the few body analogue in order to achieve a more comprehensive understanding of the microscopic properties of the strongly driven interacting system. Although the major part of the presented results is devoted to the case of four bosons in a triple-well setup, we provide strong evidence that our findings are still applicable for larger lattice systems and larger particle numbers.

Motivated by the recent experimental progress [26, 27] we investigate in the present work the effects that a periodically driven one-dimensional optical lattice can introduce in a small ensemble of ultracold bosons. The dynamical response of the system for a wide range of driving frequencies is studied by means of the concept of fidelity or autocorrelation function. Even though we consider a scenario with a deep lattice such that the tunneling modes have a minor influence on the overall dynamics, a quite rich excitation spectrum is found. We note that such intra-band excitations, which lead to a coupling between the two lowest energy bands, have been exploited in order to realize single- and two-qubit gates, where the quantum bit has been encoded in the localized Wannier functions of the two lowest energy bands of each lattice site [31]. In order to analyze the intra-well dynamics we employ the one-body reduced density matrix. The Fourier spectrum of the local one-body density as well as of the on-site density oscillations are employed in order to obtain insights into the excited intra-well modes. We find a resonant behavior of the dipole mode indicating that the intra-well dynamics can be controlled by adjusting the driving frequency. Moreover, the magnification of the intra-well generated mode at resonance is also manifested in the population of additional lattice momenta. Our investigation of the resonances is supported by a Floquet analysis for the effective single-particle degree of freedom. This allows us to further explore the on-site dynamics and the inter-well tunneling that occur due to the driving. Including interatomic interactions for larger atom numbers, we analyze similarities and differences with respect to the single-particle description. The above outlined findings are confirmed for different filling factors, lattice potentials, and boundary conditions. To solve the underlying many-body Schrödinger equation we apply the ab initio multiconfiguration time-dependent Hartree method for bosons (MCTDHB) [32, 33] which is especially designed to treat the driven out-of-equilibrium quantum dynamics of interacting bosons.

This article is organized as follows. In section 2 we introduce our setup and the multi-band expansion. Section 3 contains the driven quantum dynamics first from a single-particle perspective, by performing a Floquet analysis, and second by inspecting the dynamics of a small bosonic ensemble including repulsive interactions. We summarize our findings and provide an outlook in section 4. The appendix briefly outlines our computational method.

2. Hamiltonian and multi-band expansion

This section is devoted to a brief presentation of the theoretical framework of our study. In particular, we shall briefly discuss the driven optical lattice, the underlying many-body Hamiltonian, and the concept of multi-band expansion. The latter will be a useful tool in order to understand the excitations involved in the dynamics.

2.1. Modeling the periodically-driven potential

The periodic driving of an optical lattice can be accomplished in two different ways. Retroreflecting mirrors that are used to form the lattice can be moved periodically in space or, alternatively, a frequency difference between counter-propagating laser beams can be induced by means of acousto-optical modulators [27] which renders the lattice time-dependent. Here, we model the driven optical lattice with a sinusoidal function of the form

$$V_{\text{dr}}(x, t) = V_0 \sin^2\left[ k_0(x - A \sin \omega_{\text{D}B}) \right].$$

Such a potential has been implemented in the experiment in [21]. It is characterized by the barrier depth $V_0$, a lattice wave-vector $k_0 = \frac{2\pi}{l}$, where $l$ denotes the distance between successive potential minima, the amplitude $A$ and the frequency $\omega_{\text{D}B} = 2\pi/T_{\text{D}B}$ of the driving field. In an experiment $k_0$ is the wave vector of the laser beams which form the optical lattice, while its depth $V_0$ can be tuned by adjusting the laser’s intensity.

2.2. The Hamiltonian

The Hamiltonian of $N$ identical ultracold bosons of mass $M$ confined in a driven one-dimensional $m$-well optical lattice reads

$$H = \sum_{i=1}^{N} \frac{\hbar^2}{2M} \frac{\partial^2}{\partial x_i^2} + V_{\text{dr}}(x_i, t) + \sum_{i<j} V_{\text{int}}(x_i - x_j),$$

(2)

where $V_{\text{int}}(x_i - x_j) = g_{1D} \delta(x_i - x_j)$ denotes the short-range contact interaction potential between particles located at position $x_i$, $i = 1, 2, ..., N$. In the ultracold regime the interaction is well described by $s$-wave scattering whose effective one-dimensional coupling strength [5] is given by

$$g_{1D} = \frac{2\hbar^2}{M c^2} \left(1 - \frac{|\omega_{s}^2/2|}{2a_{s}}\right)^{-1}.$$  

Here $a_{s} = \frac{\hbar}{\sqrt{2M\omega_{s}}}$ is the transverse harmonic oscillator length with $\omega_{s}$ the frequency of the two-dimensional confinement, while $a_{s}$ denotes the free space three-dimensional $s$-wave scattering length. In this way,
the interaction strength can be tuned either via \( a_0 \) with the aid of Feshbach resonances [9, 10], or via the transversal confinement frequency \( \omega_{x} \) [34, 35].

For the sake of simplicity and computational convenience, we rescale the Hamiltonian (2) in units of the recoil energy \( E_R = \hbar^2 k_0^2 / 2M \). Then, the corresponding length, time and frequency scales are given in units of \( k_0^{-1}, \omega_{R}^{-1} = \hbar E_R^{-1} \) and \( \omega_{x} \) respectively. In our simulations we have used a sufficiently large lattice depth with values ranging from \( V_0 = 4.5 E_R \) to 8.0 \( E_R \) such that each well includes three localized single-particle Wannier states. In particular, due to the deep optical lattice and small driving amplitudes (in comparison to the lattice constant) mainly used in our simulations highly energetic excitations above the barrier are excluded and as a consequence heating processes can be minimized. The confinement of the bosons in the \( m \)-well system is imposed by the use of hard-wall boundary conditions at positions \( x_0 = \pm m x \), where the potential is maximum. In addition, we set also \( \hbar = M = k_0 = 1 \) and the coupling strength becomes \( g = a_0 / A \), while \( A \) represents the dimensionless driving amplitude. The rescaled shaken triple well is given by \( V_{th}(x, t) = \hbar v_0 \sin^2 x_0 - A \sin \omega_{x} t \) with the hard wall boundaries located at \( x_0 = \pm 3 \pi / 2 \).

2.3. The multi-band expansion

The understanding of the spatial localization of states in lattice systems makes the use of multi-band Wannier number states crucial as it includes the information of excited bands and allows us to interpret both intraband and interband processes. In general, this representation is valid when the lattice potential is deep enough such that the Wannier states between different wells have a very small overlap for not too high energetic excitation. In the present case where the potential is periodically driven, the above description can still be used as long as the driving amplitude is small enough in comparison to the lattice constant \( l \), i.e. \( A \ll l \). In this way, each localized Wannier function can be still adapted and assigned to a certain well and the respective band-mixing is fairly small. For large displacements one should use a time-dependent Wannier basis in order to ensure that the corresponding on-site Wannier states are well-adapted to each well during the driving.

To introduce the formalism, let us consider a system consisting of \( N \) bosons, \( m \)-wells and \( k \) localized single particle bands [36, 37]. Then, the expansion of the many-body bosonic wavefunction in terms of the number states of non-interacting bosons reads

\[
|\Psi\rangle = \sum_{\{N\}} C_{\{N\}} |N_1, N_2, \ldots, N_m\rangle_I,
\]

where \( |N_1, N_2, \ldots, N_m\rangle_I \) is the multiband Wannier number state and the element \( N_i \) denotes the number of bosons being localized in the \( i \)-th well satisfying the constraint \( \sum_{i=1}^{m} N_i = N \). The summation is performed over the different configurations of the \( N \) bosons according to their energetic order denoted by the index \( I \). In particular, the index \( I \) corresponds to a high dimensional quantity \( I = (I_1, I_2, \ldots, I_m) \) which contains \( m \) elements each of them being a \( k \)-component vector. More precisely, the \( q \)-th element can be written as

\[
I_q = (I_q^{(1)}, I_q^{(2)}, \ldots, I_q^{(k)}),
\]

where \( I_q^{(k)} \) refers to the number of bosons located at the \( q \)-th well and \( k \)-th band, satisfying the constraint \( \sum_{q=1}^{m} \sum_{i=1}^{k} I_q^{(i)} = N \). Within the above notation one can investigate, among others, the probability of \( N_0 < N \) bosons to be in an excited band or to find a specific number state configuration. Indeed, suppose the case of \( N_0 < N \) bosons excited in the \( i \)-th band while the rest \( N - N_0 \) lie in lower bands. Then, it must hold \( I_i^{(i)} = I_i^{(j)} = \ldots = I_i^{(j)} = 0 \) for every \( j > i \), while \( I_i^{(i)} + I_i^{(j)} + \ldots + I_i^{(k)} = N_0 \) and \( I_i^{(i)} + \ldots + I_i^{(k)} = N - N_0 \) for every \( j < i \).

Let us consider an example of a system with four bosons \((N = 4)\) confined in a triple well \((m = 3)\) which includes three bands \((k = 3)\). Then, for instance, the state \([1, 2, 1]_I\) with \( I = (I_1, I_M, I_R) \), and \( I_1 = I_R = (0, 1, 0) \), \( I_M = (0, 1, 1) \) denotes a state for which in the left (right) well one boson occupies the first excited band, whereas in the middle well one boson is localized in the first excited and one in the second excited band. As a final attempt, here, we make a link between the ground state and its dominant spatial configuration in terms of the aforementioned multiband expansion. To do that, let us choose again a system consisting of four bosons in a triple well as it will be used extensively in the following. It is known that, in general, the ground state configuration depends on the interaction strength, while for the present system, i.e. \( N = 4 \) and \( m = 3 \), the on-site interaction effects will always be prominent. For the non-interacting case \((g = 0)\) the dominant spatial configuration of the system is \([1, 2, 1]_1\), with \( I_1 = I_R = (1, 0, 0) \) and \( I_M = (2, 0, 0) \) due to the hard-wall boundaries which render the middle and outer sites non-equivalent. In the course of increasing interaction a tendency towards a uniform population of each site, e.g. for \( g = 0.2 \), due to the repulsion of the bosons is observed. In this region the system is described by a superposition of lowest-band states which are predominantly of single-pair occupancy, e.g. \([1, 2, 1]_1, [2, 1, 1]_1, \) and double-pair occupancy, e.g. \([2, 2, 0]_1\). For further increasing repulsion, e.g. \( g = 0.4 \), a trend towards the repopulation of the central well is noted. As we enter the strong interaction regime, e.g. \( g = 1.5 \), the state consists of a particle in the first excited-band being on a commensurate background of localized particles which lie in the zeroth band and the dominant ground state configuration is \([1, 2, 1]_1\), with \( I_1 = I_R = (1, 0, 0) \) and \( I_M = (1, 1, 0) \). Finally, for strong interparticle repulsion, e.g. \( g = 3 \), the contribution from the higher-band states becomes more prominent and the corresponding ground state configuration is characterized by an admixture of zeroth- and excited-band states.

3. Driven quantum dynamics

This section is devoted to a detailed analysis of the bosonic dynamics in a driven optical lattice. At the beginning, a general overview of the effect of the driving on the finite bosonic ensemble with respect to the driving frequency is
regions (red sections in figure 1(a)) the evolved state is essentially unperturbed by the driving. In the first region, between 4.0 < \omega_D < 5.5, the minimal overlap in the course of the dynamics drops down to 0.1, whereas in the second (7.0 < \omega_D < 8.0) and third (10.0 < \omega_D < 15.0) regions the system maximally departs from the initial state with a percentage on the order of 50% and 65%, respectively. The emergence of these dynamical regions strongly depends on the parameters of the optical lattice. For instance, for smaller lattice depths the aforementioned regions will be wider, because of the smaller potential energy, which favors a possible deviation of the system from the initial state.

Let us inspect the time evolution of the total energy $E(t) = \langle \Psi(t) | \hat{H}(t) | \Psi(t) \rangle$. Figure 1(b) shows $E(t)$ for various driving frequencies $\omega_D$. For driving frequencies where $F_{\omega_D} \approx 1$ (e.g. $\omega_D \in \{1,3\}$, see also figure 1(a)) the dependence of the energy on the driving frequency is weak and it is essentially constant during the time evolution. On the other hand, for the regions where $F_{\omega_D} \ll 1$, $E(t)$ increases initially and it shows an oscillatory behavior. In particular, for $\omega_D = 4.5$ the total energy exhibits an oscillatory (almost periodic) pattern which can also be observed in the corresponding fidelity evolution. This driving frequency will be referred to in the following as critical and denoted by $\omega_C^{\text{D}}$, that is, the driving frequency for which $\min_{t \in [0,T]} F_{\omega_D}(t)$ is minimal. Indeed, as we shall see below, the most interesting dynamics of the system takes place close to this frequency.

Finally, let us inspect the response of the system to the driving from a one-body perspective via the single-particle density $\rho_1(x,t) = \int dx_2 ... dx_N |\Psi(x_1, x_2, ..., x_N; t)|^2$. Figure 2 illustrates the evolution of the one-body density for different driving frequencies $\omega_D$, but with the same amplitude $A$. The driving leads to oscillations of the particles densities in every site. As can be observed by having a glance at figure 2(a), the one-body density shows a weak response for driving frequencies away from the critical region $\omega_D \in [4, 5.5]$, while for $\omega_D = \omega_C^{\text{D}}$ (see figure 2(b)) we observe the periodic formation of enhanced density oscillations being accompanied by a broadening of each intra-well ensemble. The peculiar behavior of the bosonic ensemble observed for $\omega_D = \omega_C^{\text{D}}$ is characterized by three processes and time scales: (i) the internal fast oscillations of the density; (ii) the large amplitude oscillations of the density in each well of period $\sim 14$; (iii) the tunneling between the wells with a period of about 200. All these features will be analyzed in detail in the following subsections both at the single particle and many-body level.

3.2. Single particle dynamics

Here we investigate to what extent the previously presented results can be understood in the limit of zero interaction among the particles by means of Floquet theory. Specifically, we are interested in two distinct features of the dynamics observed in figure 2(b): first, the on-site dynamics and, especially, its resonance-like dependence on the driving frequency $\omega_D$, and second, the inter-well tunneling dynamics which are enhanced at certain values of $\omega_D$.

Figure 1. (a) Time evolution of the fidelity $F_{\omega_D}(t)$ as a function of the driving frequency $\omega_D$ (measured in units of $\omega_D$). (b) Time evolution of the expectation value of the Hamiltonian (2) (measured in units of the recoil energy $E_0$) for various driving frequencies $\omega_D = 0.4$ (green thin dashed line), $\omega_D = 4.0$ (black thick solid line), $\omega_D = 4.5$ (red thick dashed line), $\omega_D = 5.25$ (magenta thick dashed-dotted line), $\omega_D = 11.0$ (blue thin dashed-dotted line), and $\omega_D = 13.75$ (light-blue thin solid line). The driving amplitude is $A = 0.05$, while the initial state corresponds to the ground state of four weakly interacting bosons with $g = 0.1$ confined in a triple-well. Time unit is $\omega_D^{-1}$.

given. Subsequently, a Floquet analysis is employed in order to investigate the underlying single-particle physics. Finally, we focus on specific interaction effects.

3.1. Dynamical response

Let us explore the dynamical response or sensitivity of the system with respect to the driving frequency $\omega_D$. In order to investigate the stability of the system against the perturbations induced by the shaking (see equation (1)), we first analyse the fidelity $[38]$ between the initial state and the state evolved at time $t$: $F_{\omega_D}(t) = |\langle \Psi(0) | \Psi(t) \rangle|^2$, where the dependence on $\omega_D$ is implicit in the time evolved state $\Psi(t)$. Here we will consider a system of four bosons in a triple-well with $g = 0.1$, whose ground state (i.e. the initial state $\Psi(0)$) corresponds to a superfluid state, as the filling factor is not commensurable and we do not encounter the formation of a Mott insulating state. In terms of its dominant spatial configuration our system initially consists (see also section 2.3) of two bosons in the middle well and two others of them localized in one of the outer wells, i.e. the state $|1, 2, 1\rangle$, with $L = R = (1, 0, 0)$ and $J_M = (2, 0, 0)$ has the most prominent contribution. Figure 1(a) shows $F_{\omega_D}(t)$ as a function of the driving frequency $\omega_D$. The dynamics are characterized by three main regions with respect to $\omega_D$, where the system is driven far from the initial state, while for the remaining frequency...
3.2.1. Floquet theory. To be self-contained, we start by summing up the main notions of Floquet theory. Because of the temporal periodicity of the single particle Hamiltonian employed throughout this work (equation (2) with $g = 0$ and $N = 1$), every solution of the time-dependent Schrödinger equation (TDSE) takes the form of a Floquet mode (FM) $\Psi_\alpha(x, t)$ which in turn can be written as: $\Psi_\alpha(x, t) = e^{-i\epsilon_\alpha t/\hbar}\Phi_\alpha(x, t)$ with the real quasi energy (QE) $\epsilon_\alpha \in [-\hbar \omega_D/2, +\hbar \omega_D/2]$ and with $\Phi_\alpha(x, t) = \Phi_\alpha(x, t + T_D)$ respecting the temporal periodicity of the Hamiltonian \cite{39}. The FMs are eigenvectors of the time evolution operator over one driving period

$$U\left(T_D + t_0, t_0\right)\Psi_\alpha(x, t_0) = e^{-i\epsilon_\alpha T_D/\hbar}\Psi_\alpha(x, t_0). \tag{4}$$

This property is of particular interest as it allows for a stroboscopic time evolution of an arbitrary initial state $\Psi(x, t_0)$ once the FMs of a system are known. To show this, we exploit the fact that the FMs constitute an orthonormal basis for the solution space of the TDSE \cite{40} and expand $\Psi(x, t_0)$ at the initial time $t = t_0$ as

$$\Psi(x, t_0) = \sum_\alpha C_\alpha(t_0)\Psi_\alpha(x, t_0) \tag{5}$$

with the corresponding coefficients $C_\alpha(t_0)$. By applying the one period evolution operator $U(T_D + t_0, t_0)$ on both sides of equation (5) for $m$ times and by virtue of equation (4), we readily obtain the stroboscopic time evolution of $\Psi(x, t_0)$ as

$$\Psi(x, t_0 + mT) = \sum_\alpha C_\alpha(t_0)e^{-i\epsilon_\alpha mt_0/\hbar}\Psi_\alpha(x, t_0). \tag{6}$$

Numerically, we obtain the FMs for a given initial time $t_0$ by calculating the eigenvectors of the one period evolution operator $U(T_D + t_0, t_0)$ (see equation (4)). We refer the interested reader to \cite{41} for a detailed description of the employed computational scheme.

Finally, let us note that equation (6) already reveals some interesting features of the time evolution in periodically driven systems as we shall see in the following. Imagine that only a single FM, say $\Psi_\alpha(x, t)$, is populated. The stroboscopic evolution of the probability density is thus given as $|\Psi(x, mT_D)|^2 = |C_\alpha|^2|\Psi_\alpha(x, 0)|^2$. Hence, $|\Psi(x, t)|^2$ is again periodic with period $T_D$ and the only time dependence arises from the explicit time dependence of the FM, which is commonly referred to as ‘micro-motion’. This situation changes if the initial state populates multiple FMs. In this case one encounters interference terms in $|\Psi(x, mT_D)|^2$ between the different FMs in the form of $\sim e^{i\epsilon_\alpha(-t_0-t)}t_0/\hbar$. Thus, the quasi energies $\epsilon_\alpha$ in periodically driven systems play a comparable role in the time evolution as the energy eigenvalues do in time-independent setups.

3.2.2. On-site dynamics in the single well. To begin with, we shall investigate the observed on-site dynamics (see figure 2(b)), and in particular their dependence on the driving frequency $\omega_D$. To this end, we simplify the setup studied in section 3.1 to just a single well of the lattice potential. Hence, the potential is given by $V_0(x, t) = V_0 \sin^2(x - A \sin(\omega_D t))$ for $x \in (-\pi, +\pi]$ and we impose periodic boundary conditions at $x = \pm \pi$ in order to mimic the situation in an extended lattice. We choose as initial state $\Psi(x, 0)$ the single particle density as shown in figure 2(b) at $t = 0$ within the central potential well. The time evolution is then obtained by expanding $\Psi(x, 0)$ in terms of the FMs of the system and by making use of equation (6). As a result, we find that we can reproduce some of the main features of the on-site dynamics shown in figures 2(a) and (b), namely, we observe resonantly enhanced on-site oscillations in an interval of the driving frequencies around $\omega_D \approx 4.5$. Following the discussion in \cite{42}, further insight into this effect can be
The on-site dynamics as a function of the driving frequency \( \omega_D \) and tunneling dynamics \( \Psi \) according to their overlap with the initial state and label the \( \omega \) and \( C_0^2 \).

Figure 3. On-site dynamics for a single particle. (a) Populations \( |C_0|^2 \) and \( |C_1|^2 \) of the two most populated FMs. (b) QE spectrum as a function of the driving frequency \( \omega_D \) (measured in units of \( \omega_0 \)). Highlighted are the most (red) and second most (blue) populated FMs. The rectangular area indicates the narrow avoided crossings, while the circle highlights the area where a broad avoided crossing appears with respect to the driving frequency. For comparison, we depict again the black is again the QE spectrum as a function of the driving frequency \( \omega_D \).

second largest overlap as \( \Psi_1 \), etc. In figure 3(a) the coefficients of the two most populated FMs, \( |C_0|^2 \) and \( |C_1|^2 \) are shown as a function of the driving frequency. Apparently, both at small frequencies \( \omega_D \leq 4 \) and at large ones \( \omega_D \geq 5.5 \) only a single FM is notably populated, while \( |C_0|^2 \) and \( |C_1|^2 \) become comparable at distinct driving frequencies (e.g. at \( \omega_D \approx 5 \)). According to our discussion above, in cases when \( |C_0|^2 \) is close to one, and thus only a single FM is populated, the stroboscopic time evolution, as given by equation (6), becomes, to a good approximation, time periodic with the period of the driving \( T_D \). Note that this agrees with the observation of figure 2(a), that away from the resonance frequencies, the single particle density merely performs oscillations whose period matches \( T_D \). This corresponds precisely to the previously described micro-motion arising from the explicit time dependence of the FM \( \Psi_0(x, t) \).

On resonance, when \( |C_0|^2 \approx |C_1|^2 \), the evolution of \( |\Psi(x, 0)|^2 \) includes, besides the micro-motion, an interference term between \( \Psi_0 \) and \( \Psi_1 \), whose period is dictated by the corresponding quasi energies and is given by: \( T_{res}/T_D = \hbar \omega_D/(\epsilon_1 - \epsilon_0) \). Indeed, we find that this term is responsible for the observed on-site mode with a period of \( \sim 14 \) lattice oscillations (compare figure 2(b)). Up to now, however, it is not yet clear why \( \Psi_1 \) is resonantly populated at certain frequencies. In order to provide an answer to this question we follow the argumentation in [42] and consider the dependence of the QE spectrum on the driving frequency \( \omega_D \) as shown in figure 3(b). Highlighted are the two most populated modes at each \( \omega_D \) (blue and red dots) revealing avoided crossings of these two modes at the frequencies where a resonant enhancement of \( |C_1|^2 \) was observed in figure 2(b). Hence, at these values of \( \omega_D \) the FMs \( \Psi_0 \) and \( \Psi_1 \) are resonantly coupled by the driving which results in an increase of \( |C_1|^2 \) and ultimately to the section in 3.1 describing on-site dynamics.

In the following we provide insight into the question why we observe Floquet resonances at driving frequencies around \( \omega_D \sim 4.5 \). Let us start by noting that, by means of appropriate unitary transformations, the single particle Hamiltonian with a potential as given in equation (1) can be recast into the form:

\[
\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_0 \sin^2(k_0x) + V_D \sin(\omega_D t)x,
\]

where the amplitude of the oscillating term is given by \( V_D = mA\omega_0^2 \). That is, the transformed Hamiltonian takes the form of a static lattice plus a time-dependent perturbation whose strength is determined by \( V_D \). For the used parameters of \( m = 1 \) and \( A = 0.05 \) and for the range of considered frequencies of \( 3 \lesssim \omega_D \lesssim 6 \) we get that the amplitude \( V_D \) of the time-dependent term is of order one. Hence, it can be seen as a small perturbation compared to the static term of strength \( V_0 = 15 \) and we can expect that the QEs of the driven lattice setup can be estimated by the actual energies of the undriven lattice. Resonances would then be expected whenever the energy difference between two notably populated eigenstates of the static system matches an integer multiple of \( \hbar \omega_D \). In fact we find that the energies of the three energetically lowest
states of even parity are given by $E_0 \approx 2.6$, $E_1 \approx 11.6$ and $E_2 = 16.9$. Naively, we expect driving induced resonances whenever the ground state is resonantly coupled to one of the excited states. Indeed we find $E_1 - E_0 \approx 2 \times 4.5$ and $E_2 - E_0 \approx 3 \times 4.8$. Thus, following this line of argument, at driving frequencies of approximately $\omega_D = 4.5$ the ground state of the unperturbed lattice is coupled via a $2 \times 3$ photon process to the first (second) excited states. In order to justify this simplified picture we show the energies $E_0$ and $E_1$ on top of the QE spectrum of the driven lattice (see figure 3(c)). Away from any resonances, both energies are almost identical to the QEs of the corresponding Floquet states, so, for example, the red line is practically on top of an underlying black line. Closer to the resonance region, we see of course deviations of the QEs from the mere energies of the undriven lattice as the different states are coupled by the driving.

Finally, figure 3(d) provides an overview over the possibly observed frequencies in the on-site dynamics at various driving frequencies. Shown are the frequencies associated with all possible interference terms between the FMs weighted by their overlap with the initial state. More precisely, we calculate $\omega_{i,j} = (\varepsilon_i - \varepsilon_j) / \hbar$ for all pairs of FMs at a given driving frequency and determine the color coding by computing the product $|C_i^a C_j^b|$. Hence, the frequency $\omega_{i,j}$ appears in figure 3(d) only when both of the corresponding FMs $\Psi_i$ and $\Psi_j$ have appreciable overlap with the initial state. In agreement with the discussion concerning figure 3(b) we observe pronounced on-site oscillations only within an interval of driving frequencies $4.0 \lesssim \omega_D \lesssim 5.5$. In particular, the two narrow avoided crossings around $\omega_D \approx 4.5$ (see the rectangular in figure 3(b)) yield low frequency on-site dynamics, whereas the comparably broad avoided crossing at $\omega_D \approx 5$ (see the circle in figure 3(b)) results in a much faster on-site oscillation.

3.2.3. Tunneling dynamics in the triple well. Besides the on-site dynamics, figure 2(b) revealed a pronounced tunneling between the lattice sites at certain driving frequencies. Similar to the previous section, we analyze this effect in the following by applying Floquet theory for the single particle dynamics. We choose the same setup as before, that is, $V_0(x, t) = V_0 \sin^2(x - A \sin(\omega_D t))$, with the same initial state, i.e. essentially a Gaussian centered around the potential well at $x = 0$, but with the difference that the periodic boundary conditions are imposed at $x = \pm 2\pi$ (instead of at $x = \pm \pi$ as we did before). In this way we allow for tunneling of the wave packet into the two neighboring lattice sites. As for the on-site dynamics, we provide an overview over the observable frequencies in the temporal evolution in figure 3(e) (in close analogy to figure 3(d)). Note that, since the tunneling dynamics observed in section 3.1 occurs on much longer timescales as compared to the on-site dynamics, we only show the extract of the regime of small frequencies, i.e. $\omega_{i,j} \ll \omega_D$. Furthermore, because no on-site dynamics occur with timescales matching the extremely small frequencies of $\lesssim 0.02$, all the frequencies depicted in figure 3(e) are indeed associated with an inter-well tunneling mode. In accordance with the observation made in the many-particle simulations (see figure 2(b)) we observe a strong increase of the frequencies associated with the tunneling dynamics in the range of driving frequencies of $4 \lesssim \omega_D \lesssim 5.5$. Away from this resonance, for example at $\omega_D = 2.5$, the only notable tunneling mode corresponds to an interference term of two FMs which oscillates with a period of $T_{osc}/T_D \approx 3300$ and could therefore not be observed in the simulations performed in section 3.1. Within the regime of resonant driving, e.g. at $\omega_D = 4.5$, the frequency of the tunneling mode is increased strongly and the associated oscillation period becomes $T_{osc}/T_D \approx 200$ matching the observed tunneling mode in the weakly interacting regime (see figure 2(b)).

3.3. Interband tunneling and excitation processes

In the previous section we have shown that most of the features of the (effective) single-particle dynamics of figure 2 can be explained via a non-interacting Floquet theory. As we shall see now, however, the full dynamics presents a rich excitation spectrum ascribable to the particles interaction, especially in the strong interaction regime. Thus, we investigate the tunneling and excitation probabilities of the dominant particle configurations, for different driving frequencies $\omega_D$, by means of the multiband expansion introduced in section 2.3. More precisely, we compute and analyze the probabilities, during the dynamics, defined as

$$\left| C_{\{N_1, N_2 \}} \right|^2 = \left| \langle \{N_1, N_2 \} | \Psi(t) \rangle \right|^2.$$  (8)

The case $\omega_{in} = 0 \forall k > 1$ refers to the lowest-band inter-well tunneling dynamics. The initial state of the system corresponds to the ground state of four weakly interacting bosons with $g = 0.1$ in a triple well, while the dominant number state configuration (see also section 2.3) is $\{2, 1, 2, 1\}$ with $I_L = I_R = (1, 0, 0)$ and $I_M = (2, 0, 0)$. In this way, a lowest-band tunneling process can take place among the initial state and: (a) another state of single-pair occupancy, e.g. $\{2, 1, 1\}$ with $I_L = (2, 0, 0)$ and $I_M = I_R = (1, 0, 0)$; (b) a state with double-pair occupancy, e.g. $\{2, 2, 0\}$ with $I_L = I_M = I_R = (2, 0, 0)$ and $I_M = (0, 0, 0)$; (c) a state with triple occupancy, e.g. $\{3, 1, 0\}$ with $I_L = (3, 0, 0)$ and $I_M = (1, 0, 0)$, $I_R = (0, 0, 0)$; or (d) a state with quartic occupancy, e.g. $\{4, 0, 0\}$ with $I_L = (4, 0, 0)$ and $I_M = I_R = (0, 0, 0)$. However, from the system preferred tunneling processes form a hierarchy according to the energetical difference between the initial and final state. For instance, a tunneling process to another state of single-pair occupancy will be more preferable than to a state of double-pair occupancy, etc. Figure 4(a) shows the tunneling probability to the energetically closest number state, which is $\{2, 1, 1\}$ (or $\{1, 1, 2\}$) with $I_L = (2, 0, 0)$ and $I_M = I_R = (1, 0, 0)$ (or $I_L = I_M = (1, 0, 0)$ and $I_R = (2, 0, 0)$), i.e. $|P_{\{N_1, N_2 \}}|^2 = |\langle 2, 1, 1 | \Psi(t) \rangle |^2$ with $I_L = (2, 0, 0)$ and $I_M = I_R = (1, 0, 0)$, for various driving frequencies. As is shown, for $\omega_D < \omega_D^0$ this tunneling mode has a small amplitude and it is quite insensitive to $\omega_D$ as intuitively expected from the fact that the evolved-state is essentially unperturbed by the driving (see also figure 1(a)). For $\omega_D \approx \omega_D^0$, however, the amplitude of the oscillations is
Figure 4. (a) Tunneling probability (see main text) $|D_{N}^{[1]}|^{2} = |\Psi(t)|^{2}$ with $I_{L} = (2, 0, 0)$ and $I_{R} = I_{M} = (1, 0, 0)$ as a function of time for different driving frequencies $\omega_{D} = 0.5$ (blue solid line), $\omega_{D} = 4.5$ (red dashed line) and $\omega_{D} = 11.0$ (black dashed–dotted line). The most significant contribution of the interband tunneling mode is between the state $|2, 1, 1\rangle$ (with $I_{L} = (2, 0, 0)$ and $I_{R} = I_{M} = (1, 0, 0)$ and the initial $|1, 2, 1\rangle$ (with $I_{M} = (2, 0, 0)$ and $I_{R} = I_{L} = (1, 0, 0)$). (b) Inter-well tunneling probability $|D_{N}^{[1]}|^{2}$ at resonance for different values of the interatomic interaction $g = 0.1$ (black dashed–dotted line), $g = 0.5$ (blue solid line) and $g = 2.0$ (red dashed line). In all panels $A = 0.05$. The time evolution is expressed in units of $\omega_{D}$.

Firstly, let us consider the excitation dynamics. In this case it holds $I_{R}^{(k)} = 0$ for $k > 1$. To this aim, we have analyzed the probability of finding all the four bosons in the zeroth-band. The latter can be expressed via equation (8) as $|B_{N}^{[1]}|^{2} = \sum_{N_{1}, N_{2}, N_{3}}|\Psi(t)|^{2} = \sum_{N_{1}}|C_{N_{1}}|^{2}$, where the summation is performed over the excitation indices $I = (I_{L}, I_{M}, I_{R})$ which, in terms of the multiband expansion, obey the constraints $I_{L}^{(1)} + I_{M}^{(1)} + I_{R}^{(1)} = N$ and $I_{L}^{(j)} = I_{R}^{(j)} = I_{M}^{(j)} = 0$ for all $j > 1$. In particular, figure 5(a) shows the probability $|B_{N}^{[1]}|^{2}$ for all the bosons to reside in the zeroth-band for various driving frequencies $\omega_{D}$ and a fixed amplitude $A = 0.05$ during the time evolution. At the critical driving frequency a complete depopulation of the zeroth-band at some specific time intervals is observed. In particular, this probability exhibits revivals, which are connected with the enhancement of the (amplitude) oscillations of the single-particle density (see also figure 2(b)). On the other hand, for driving frequencies different from the critical frequency the respective probability of all the bosons occupying the zeroth-band is rather large and is indeed dominant. However contributions from excited configurations cannot be neglected, especially in the regions $7.0 < \omega_{D} < 8.0$ and $10.0 < \omega_{D} < 15.0$, where the system significantly departs from the initial state (see also figures 1(a) and 5(a) red dashed line). Furthermore, figure 5(b) presents the probability, at the critical driving frequency, of obtaining a state of $N_{0} \leq 4$ particles in the first-excited band and the remaining to be in the zeroth-band. The latter can be expressed as $|B_{N}^{[1]}|^{2} = \sum_{N}N_{1}|C_{N_{1}}|^{2}$, where the summation index $I = (I_{L}, I_{R}, I_{M})$ obeys the constraints $I_{L}^{(1)} + I_{R}^{(1)} + 2I_{M}^{(1)} = N - N_{0}$, $I_{L}^{(2)} = I_{R}^{(2)} = I_{M}^{(2)} = N_{0}$ and $I_{L}^{(j)} + I_{R}^{(j)} + 2I_{M}^{(j)} = 0$ for all $j > 2$. Indeed, the interplay between the four possible excitation scenarios from the zeroth to the first excited-band (i.e. one-particle excitation, two-particle excitation, etc) in the course of the dynamics is illustrated in a transparent way. It is observed that the complete depopulation of the zeroth-band is mainly accompanied by the excitation of three or all the four bosons in the first-excited band. For long evolution times, the zeroth-band possesses a low population and states with one or two bosons in the first-excited-band are mainly populated. The states with the most significant contribution are of the type $|1, 2, 1\rangle$ with $I_{L} = I_{R} = (0, 1, 0)$ and $I_{M} = (0, 2, 0)$ or $I_{M} = (1, 1, 0)$. We note that a small contribution comes from the state $|1, 2, 1\rangle$ with $I_{L} = I_{R} = (0, 1, 0)$ and $I_{M} = (0, 1, 1)$. This clearly shows
that the most prominent excitation process in our system originates from the energy difference between each of the above states and |1, 2, 1⟩ with \( I_a = I_R = (1, 0, 0) \) and \( I_M = (2, 0, 0) \), namely the (initial) ground state configuration.

Finally, in order to explore the impact of the interactions on the dynamics, figure 5(c) shows the probability \(|\mathcal{B}_{\omega}(t)|^2\) for long evolution times of all the bosons being in the zeroth-band for different interparticle repulsion at the driving frequency \( \omega_D = \omega_D^c \). For the non-interacting case the population of the zeroth-band shows revivals even for long time scales, while, as the interaction strength is turned on, the corresponding probability presents a decaying envelope. This envelope behavior is a pure effect of the interactions and reflects also the initial ground state configuration (see the discussion in section 2.3) which strongly depends on the interparticle interactions. As can be seen for increasing repulsion between the particles the probability of the system remaining in the zeroth-band, in the course of the dynamics, decays on increasingly shorter time scales and the system is dominated by different types of excitations, as expected intuitively.

3.4. Characteristics of the resonant behavior

To characterize the overall process with respect to the driving frequency, we compute the spectrum of the local one-body density

\[
\rho_i(\omega) = \frac{1}{\pi} \int_0^\infty dt \rho_i(t) e^{i\omega t},
\]

where \( \rho_i(t) = \int d^2 r \rho_i(x, t) \) denotes the spatially over a single well integrated single-particle density at every time instant \( t \). The index \( \alpha = L, M, R \) corresponds to the left, middle or right well respectively, whereas the limits of the wells are denoted by \( d_a, d_a' \). Note that in the present case all the components of \( \rho_i(\omega) \), i.e., \( \rho_L(\omega) \), \( \rho_M(\omega) \) and \( \rho_R(\omega) \), are equivalent due to the considered large lattice depths and the employed driving scheme which enforces the bosons among different wells to oscillate in-phase. Figure 6 shows the above spectrum, where five dominant branches (denoted as (1)–(5) in the figure) can be observed. The lowest branch denoted as (1) in figure 6 (in the range \( \omega \in [0, 0.02] \)) refers to the intraband tunneling being restricted to the energetically closest number states, e.g. from |1, 2, 1⟩ \( (I_M = (2, 0, 0), I_a = I_R = (1, 0, 0)) \) to |2, 1, 1⟩ \( (I_L = (2, 0, 0), I_M = I_R = (1, 0, 0)) \). This branch is hardly visible in figure 6 due to the presented wide range of frequencies that have been taken into account in order to visualize all the dynamical frequencies of the system. In addition, the next lowest branch (denoted as (2)) at \( \omega_D \in [4, 5] \) and \( \omega \in [0.05, 1] \) corresponds to the large amplitude density oscillations (see also figure 2(b)). These
mode frequencies have already been predicted via the Floquet analysis in section 3.2 (see figures 3(d) and (e)). To investigate in some detail the intra-well wavepacket dynamics, the quantity $\Delta \rho_{t}(t) = \rho_{1,1}(t) - \rho_{1,3}(t)$ is employed. Here, each well is divided from the center into two equal parts, namely left and right, with $\rho_{1,1}(t)$, $\rho_{1,2}(t)$ being the corresponding integrated densities at time $t$. The index $\alpha = L, M, R$ stands for the left, middle and right well, respectively. To determine the frequencies of this mode we calculate the spectrum $\Delta \rho_{t}(\omega)$.

The inset of figure 6 presents the corresponding spectrum, thus showing the emergent frequencies of the intra-well oscillations as a function of the driving frequency $\omega_D$. We observe that the spectrum $\Delta \rho_{t}(\omega)$ follows the evolution of the upper three branches (denoted by (3)-(5)) of the spectrum of $\rho_{t}(\omega)$, whereas in the region of the resonance the intra-well oscillation measured via $\Delta \rho_{t}(t)$ features a beating dynamics, as expected. Hence, away from the region around the critical driving frequency the generated dipole mode possesses three different frequencies, while close to $\omega_D$ the intra-well dynamics come into a resonance. Therefore, one can induce this resonant intra-well dynamics by adjusting the driving frequency. Finally, let us comment on the existence of some higher frequency components, e.g. branch (6) in figure 6, which correspond to very fast intrawell oscillations (i.e. $\omega \ll \omega_D$) and possess a low amplitude (in comparison to the previous branches (1)-(5)).

In turn, we shall visualize the above mentioned resonance and inspect how it depends on the lattice parameters. To this aim, the minimal occupancy, during the evolution time $T$, of the zeroth-band $\min_{t \in [0,T]} \rho_{t}(t) = \min_{t \in [0,T]} \sum_{\alpha} \{N_{1, N_{2}, N_{3}|\Psi(t)}\}$, with the energetical indices $I_{L}^{(1)} + I_{M}^{(1)} + I_{R}^{(1)} = N$ and $I_{L}^{(0)} = I_{M}^{(0)} = I_{R}^{(0)} = 0$ for every $j > 1$ is used. Employing the above quantity one can show that far from resonance there are regions with non-negligible excitations, i.e. $\min_{t \in [0,T]} \rho_{t} < 1$ (e.g. at $\omega_D = 11.0$; see also figure 1(a)) as well as regions where $\min_{t \in [0,T]} \rho_{t} \approx 1$ (e.g. $\omega_D = 2.0$ in figure 1(a)). Now let us analyze the dependence of $\min_{t \in [0,T]} \rho_{t}$ on the driving frequency around $\omega_D$. Firstly we study the dependence of the resonance on the driving amplitude. In figure 7(a) we show for an increasing driving amplitude the minimum of $\min_{t \in [0,T]} \rho_{t}$ as a function of the frequency $\omega_D$ which broadens and eventually reaches zero, meaning that the zeroth-band has been completely depopulated (see also figure 5(a)). On the other hand, for small amplitudes the value of the minimum of $\min_{t \in [0,T]} \rho_{t}$ is non-zero and in the limit $A \rightarrow 0$ its dependence on the driving frequency disappears. Instead, in figure 7(b) we show how the minimal population of the zeroth-band ($\min_{t \in [0,T]} \rho_{0}$) varies as a function of the lattice depth. For an increasing lattice depth it is known that the energy gaps among the different energy levels become larger. This phenomenon can intuitively be understood in terms of a tight-binding approximation. For simplicity let us assume only a nearest neighbor coupling $J \propto \int dx W_{s}(x) \left[\frac{\nu}{2m} + V_{0} \sin^{2}(x)\right] W_{s+1}(x)$ between the sites $s$ and $s + 1$, where $W_{s}(x)$ are the on-site localized Wannier states. Then, within this approximation, which is valid for a relatively deep potential, the resulting eigenvalues are $E_{k+1} = E_{0}^{\text{on-site}} - 2J \cos\left(\frac{k\pi}{N+1}\right) (k = 1, 2, \ldots, N)$, where $E_{0}^{\text{on-site}}$ are the on-site energies. Thus, the resonance can be tuned at will, i.e. for a decreasing lattice depth the $\omega_D$ is negatively shifted, as is confirmed by the numerical results of figure 7(b). Finally, let us comment on the dependence of the position of the resonance on the interparticle interaction strength $g$. Indeed, in order to investigate whether there is such a dependence, various interaction strengths (for the same particle number $N = 4$), e.g. $g = 0.1$, $g = 1.0$ and $g = 3.0$, have been considered (omitted here for brevity) and it was found that the position of the resonance is essentially unaffected.

In the following, let us inspect the momentum distribution with varying driving frequencies with the aim of understanding whether signatures of a parametric amplification of matter-waves can be observed. The momentum distribution is a routinely employed observable in atomic quantum gas experiments as it is accessible via time-of-flight measurements [4]. This quantity can be calculated as the
The momentum distribution of the one-body density as a function of time (measured in units of $\omega_k^g$) for $g = 0.1$ and different driving frequencies (a) before the critical frequency $\omega_D = 2.0$, (b) at the critical frequency $\omega_D = \omega_0 = 4.5$ and (c) at $\omega_D = 8.0$. (d) The case of strong interparticle repulsion for $g = 2.0$ and $\omega_D = \omega_0$. The horizontal axis represents the lattice momenta in units of the inverse lattice vector $k_0 = \pi/l$. In all panels $A = 0.05$.

Fourier transformation of the one-body reduced density matrix as

$$n(k, t) = \frac{1}{2\pi} \int \int dx dx' \rho_1(x, x'; t) e^{-i k (x-x')}.$$  \hspace{1cm} (10)

Here $\rho_1(x, x'; t)$ denotes the one-body reduced density matrix, being obtained by tracing out all the bosons but one in the density of the $N$-body system. The panels (a)–(c) of figure 8 present the time evolution of the momentum distribution for different driving frequencies before, on, and after the resonance. As can be noted, exactly at the resonance the momentum distribution exhibits a special pattern, that is, some additional lattice momenta are periodically activated during the dynamics. In particular, it is observed that the modes $\pm k_0 \approx \pm 1.57$, $\pm 3k_0 \approx \pm 3.14$, $\pm 5k_0 \approx \pm 4.713$ are populated, whereas out of resonance only the $\pm k_0$ modes are significantly populated. The population of the $\pm k_0/2$, $\pm 3k_0/2$ modes at $\omega_D = \omega_0$ is reminiscent of the parametric amplification of matter-wave phenomenon, as observed experimentally in [21]. However, an exact correspondence with [21] cannot be made due to the very different setup of our system, i.e. its finite size and the hard wall boundaries. A detailed study of this process, also for higher particle numbers and lattice potentials, would be desirable, but it is clearly beyond the scope of this work. Furthermore, figure 8(d) shows the momentum distribution at resonance, but for a strong interparticle repulsion $g = 2.0$. The expected periodic pattern for large evolution times is blunted as an effect of the strong interaction which decreases the degree of coherence.

Finally, in order to demonstrate that our findings are of general character we investigate a larger lattice system with a filling factor smaller than unity. Specifically, the case of five bosons in a twelve-well finite lattice has been considered. Concerning the ground state with filling factor $\nu < 1$, the most important aspect is the spatial redistribution of the atoms as the interaction strength increases. Indeed, as the repulsion increases from the non-interacting to the weak interaction regime the atoms are pushed from the central to the outer sites which gain and lose population in the course of increasing $g$.

In the following, the shaking dynamics applied at $t = 0$ to the ground state of the five bosons which are trapped in the twelve-well potential in the weak interaction regime ($g = 0.1$) is explored. The emergent non-equilibrium behavior shows similar characteristics as in the previous setup with filling $\nu > 1$, i.e. the occurrence of an intrawell dipole and an interwell tunneling mode. Interestingly, at the same frequency $\omega_D = \omega_0 = 4.5$ a resonance of the intra-well dynamics is observed. Figure 9 presents the one-body density evolution exactly at the critical point $\omega_0$. As in the case for setups with filling $\nu > 1$, the formation of enhanced density oscillations at each site is observed, which is in relation to the time periods where the zeroth-band is completely depopulated during the evolution. Employing a corresponding number state analysis the significant contribution of two kinds of number states has been confirmed: (a) either $I_1^{(1)} + \cdots + I_{12}^{(1)} = N - 1$, $I_3^{(1)} = \cdots = I_{12}^{(3)} = 0$ and one with $I_k^{(2)} = 1$ for $k = 1, \ldots, 12$ or (b) $I_1^{(1)} + \cdots + I_{12}^{(1)} = N - 1$, $I_k^{(2)} = \cdots = I_{12}^{(2)} = 0$ and a certain $I_k^{(3)} = 1$ for $k = 1, \ldots, 12$. Notice that the same kind of number states have been found to contribute significantly also in the dynamics of four bosons in the triple-well. The above mentioned observations suggest a generalization of the observed phenomena to larger systems as well. Indeed, the same shaken scheme has been tested in different systems (omitted here for brevity), e.g. ten bosons in a triple-well, six bosons in five wells, etc, confirming that the above observed resonant-like behavior of the bosonic ensemble occurs in each setup.

4. Conclusions and outlook

The correlated non-equilibrium quantum dynamics of few-body bosonic ensembles induced by the driving of a finite-size optical lattice has been investigated. Our work focuses particularly on the regimes of large lattice depths and small driving amplitudes. This choice has been made in order to limit the degree of excitations that would otherwise lead to heating processes. Starting from the ground state of a weak or strongly interacting small ensemble, we have examined in detail the time evolution of the system induced by periodically driving the optical lattice. We find that the dynamical evolution of the system is governed by two main modes: the inter-well tunneling and the intra-well dipole-like mode. The dynamical behavior of the system in the non-interacting regime has been firstly analyzed via Floquet theory, that is, at the single-particle level, providing an accurate interpretation of the observed processes. For large particle numbers and large interaction strengths, however, such a single-particle description was not sufficient anymore to provide an exhaustive explanation of the observed dynamics, and a multi-band Wannier number state expansion has been employed.
The inter-well tunneling mode is weak as a consequence of the deep optical lattice and the small driving amplitude. On the other hand, the local dipole mode has been identified from the intra-well oscillations of bosons in the individual wells. Remarkably enough, it has been found that by tuning the driving frequency the intra-well dynamics experiences a resonant-like behavior. This is manifested, for example, by the enhanced oscillations in the one-body density evolution or from the periodic population of additional lattice momenta in the momentum distribution of the one-body density. Additionally, on a single-particle level in terms of Floquet theory, it has been shown that in the proximity of the resonance the first two FMs possess the main contribution, while away from resonance the dynamics can be described with the inclusion of the first FM. To explain the enhanced population of the second FM at resonance the corresponding quasienergy spectrum has been employed, revealing avoided-crossings between the first two FMs at certain driving frequencies. To obtain the frequencies which refer to the on-site and tunneling dynamics, the corresponding frequencies associated with the interference terms between the FMs have been employed, revealing avoided-crossings of the local one-body density with respect to the driving frequency all the relative dynamical frequencies, e.g. on-site oscillations and tunneling period have been identified.

Finally, the occurrence of the above resonance seems to be universal in a periodically driven lattice as it is independent of the filling factor, the boundary conditions or the interparticle repulsion.

We would like to underline the fact that, contrary to related studies based, for example, on effective model Hamiltonians or lattice calculations with tensor network methods, our many-body analysis based on the \textit{ab initio} MCTDHB method has the advantage of providing the complete system wavefunction in space and time. Thus, it enables us to accurately identify the involved intra- and inter-well band excitations.

Let us comment on possible future investigations. Although in the present work we did not employ the multi-layer structure of the multi-layer multiconfiguration time-dependent Hartree method for bosons (ML-MCTDHB) method, our \textit{ab initio} approach is well suited to describe the dynamics of multi bosonic species. Given this, a first natural extension would be to study the driven dynamics of mixtures consisting of different bosonic species in order to unravel the induced excitation modes or to devise schemes for selective transport of an individual bosonic component. In relation to the present study, it would be interesting to simulate the parametrical amplification of matter-waves with interesting applications, like the generation of four-wave mixing, entanglement production, but also for fundamental tests of quantum mechanics with massive particles like the Hong–Ou–Mandel experiment, as recently performed with a Bose–Einstein condensate [23].

**Acknowledgments**

SM thanks the Hamburgisches Gesetz zur Förderung des wissenschaftlichen und künstlerischen Nachwuchses (HmbNFG) for a PhD Scholarship. PS gratefully acknowledges funding by the Deutsche Forschungsgemeinschaft (DFG) in the framework of the SFB 925 ‘Light induced dynamics and control of correlated quantum systems’. AN gratefully acknowledges discussions with Klaus Mølmer related to four-wave mixing.

**Appendix. The computational method: ML-MCTDHB and MCTDHB**

Our computational approach to solve the many-body Schrödinger equation of the interacting bosons relies on the ML-MCTDHB [43, 44] which constitutes an \textit{ab initio} method for the calculation of stationary properties and in particular the non-equilibrium quantum dynamics of bosonic systems of
different species. For a single species it reduces to MCTDHB which has been established in [32, 33, 45] and applied extensively [45–48]. The wavefunction is represented by a set of variationally optimized time-dependent orbitals which implies an optimal truncation of the Hilbert space by employing a time-dependent moving basis where the system can be instantaneously optimally represented by the corresponding time-dependent permanents. To be self contained let us briefly introduce the basic concepts of the method and discuss the main ingredients of our implementation.

Within the MCTDHB method the TDSE \((i\hbar \partial_t - H)\psi(x, t) = 0\) is solved as an initial value problem \(|\psi(0)\rangle = |\psi_0\rangle\). The many-body wavefunction which is expanded in terms of the bosonic number states \(|n_1, n_2, \ldots, n_M; t\rangle\), based on time-dependent single-particle functions (SPFs) \(|\phi_i(t)\rangle\), \(i = 1, 2, \ldots, M\), reads

\[
|\psi(t)\rangle = \sum_n C_n(t)|n_1, n_2, \ldots, n_M; t\rangle. \tag{A1}
\]

Here \(M\) is the number of SPFs and the summation \(\sum_n\) is over all the possible particle combinations \(n_i\) such that the total number of bosons is conserved and equal to \(N\). To determine the time-dependent wave function \(|\psi(t)\rangle\) we need to solve the equations of motion for the coefficients \(C_n(t)\) of the SPFs \(|\phi_i(t)\rangle\). Following the Dirac–Frenkel [49, 50] variational principle, i.e. \(\langle \dot{\psi} | i\partial_t - H | \psi \rangle = 0\) we end up with the well-known MCTDHB equations of motion [32, 33, 45, 51] consisting of a set of \(N\) nonlinear integro-differential equations of motion for the orbitals which are coupled to the \(\frac{N!}{(N - M)!} M^M\) linear equations of motion for the coefficients.

For our numerical implementation a discrete variable representation (DVR) for the SPFs and a sin-DVR, which intrinsically introduces hard-wall boundaries at both edges of the potential, has been employed. The preparation of the initial state has been performed by using the so-called relaxation method in terms of which one obtains the lowest eigenstates of the corresponding \(m\)-well setup. The key idea is to propagate some trial wave function \(\Psi(0)(x)\) by the non-unitary operator \(e^{-itH}\). This is equivalent to an imaginary time propagation and for \(t \to \infty\), the propagation converges to the ground state, as all other contributions (i.e. \(e^{-iE\tau}\)) are exponentially suppressed. In turn, we periodically drive the optical lattice and study the evolution of \(\Psi(x_1, x_2, \ldots, x_N; t)\) in the \(m\)-well potential within MCTDHB. To ensure the convergence of our simulations we have used up to nine single particle functions thereby observing a systematic convergence of our results for sufficiently large spatial grids. An additional criterion that confirms the achieved convergence is the population of the lowest occupied natural orbital kept in each case below 0.1%.

References

[1] Goldman N and Dalibard J 2014 Phys. Rev. X 4 031027
[2] Goldman N, Dalibard J, Aidselsburger M and Cooper N R 2015 Phys. Rev. A 91 033632
[3] Morsch O and Oberthaler M 2006 Rev. Mod. Phys. 78 179
[4] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[5] Olshanii M 1998 Phys. Rev. Lett. 81 938
[6] Grimm R, Weidemüller M and Ovchinnikov Y B 2000 Adv. At. Mol. Opt. Phys. 42 95–170
[7] Santos L, Baranov M A, Cirac J I, Everts H U, Fehrmann H and Lewenstein M 2004 Phys. Rev. Lett. 93 030601
[8] Inouye S, Goldenw J, Olsen M L, Tinknor C, Bohn J L and Jin D S 2004 Phys. Rev. Lett. 93 183201
[9] Köhler T, Gorali K and Julienne P S 2006 Rev. Mod. Phys. 78 1311
[10] Chin C, Grimm R, Julienne P and Tiesinga E 2010 Rev. Mod. Phys. 82 1225
[11] Lewenstein M, Sanpera A and Ahufinger V 2012 Ultracold Atoms in Optical Lattices: Simulating Quantum Many-body Systems (Oxford: Oxford University Press)
[12] Choi D I and Niu Q 1999 Phys. Rev. Lett. 82 2022
[13] Dahan M B, Peik E, Reichel J, Castin Y and Salomon C 1996 Phys. Rev. Lett. 76 4508
[14] Morsch O, Müller J H, Cristiani M, Ciampini D and Arimondo E 2001 Phys. Rev. Lett. 87 140402
[15] Peik E, Dahan M B, Bouchoule I, Castin Y and Salomon C 1997 Phys. Rev. A 55 2989
[16] Cristiani M, Morsch O, Müller J H, Ciampini D and Arimondo E 2002 Phys. Rev. A 65 063612
[17] Wilkinson S R, Bharucha C F, Madison K W, Niu Q and Raizen M G 1996 Phys. Rev. Lett. 76 4512
[18] Niu Q, Zhao X G, Georgakis G A and Raizen M G 1996 Phys. Rev. Lett. 76 4504
[19] Sias C, Lignier H, Singh Y P, Zenesini A, Ciampini D, Morsch O and Arimondo E 2008 Phys. Rev. Lett. 100 040404
[20] Eckardt A, Weiss C and Holthaus M 2005 Phys. Rev. Lett. 95 260404
[21] Gemelke N, Sarajlic E, Bidel Y, Hong S and Chu S 2005 Phys. Rev. Lett. 95 170404
[22] Hilligøt K M and Mølmer K 2005 Phys. Rev. A 71 041602
[23] Lopes R, Imanaliev A, Aspect A, Cheneau M, Boirond I and Westbrook C I 2015 Nature 520 7545
[24] Zheng W and Zhai H 2014 Phys. Rev. A 89 061603
[25] Lignier H, Sias C, Ciampini D, Singh Y, Zenesini A, Morsch O and Arimondo E 2007 Phys. Rev. Lett. 99 220403
[26] Struck J, Ölschläger C, Weinberg M, Hauke P, Simonet J, Eckardt A, Lewenstein M, Sengstock K and Windpassinger P 2012 Phys. Rev. Lett. 108 225304
[27] Parker C V, Ha L C and Chin C 2013 Nat. Phys. 9 769–74
[28] Choudhury S and Mueller E J 2014 Phys. Rev. A. 90 013621
[29] Sträßer C and Eckardt A 2015 Phys. Rev. A 91 053602
[30] Iucci A, Cazalilla M A, Ho A F and Giamarchi T 2006 Phys. Rev. A 73 041608
[31] Schneider P I and Saenz A 2012 Phys. Rev. A 85 050304
[32] Alon O E, Streltsov A I and Cederbaum L S 2007 J. Chem. Phys. 127 154103
[33] Alon O E, Streltsov A I and Cederbaum L S 2008 Phys. Rev. A 77 033613
[34] Kim J I, Melezhik V S and Schmelcher P 2006 Phys. Rev. Lett. 97 193203
[35] Giannakes P, Diakonos F K and Schmelcher P 2012 Phys. Rev. A 86 042703
[36] Mistakidis S I, Cao L and Schmelcher P 2014 J. Phys. B.: At. Mol. Opt. Phys. 47 225303
[37] Mistakidis S I, Cao L and Schmelcher P 2014 Phys. Rev. A 91 033611
[38] Gorin T, Prosen T, Seligman T H and Žnidarič M 2006 *Phys. Rep.* **435** 33

[39] Tannor D J 2007 *Introduction to Quantum Mechanics: A Time-Dependent Perspective* (Mill Valley, CA: University Science Books)

[40] Grifoni M and Hänggi P 1998 *Phys. Rep.* **304** 229–354

[41] Wulf T, Petri C, Liebchen B and Schmelcher P 2014 *Phys. Rev. E* **90** 042913

[42] Wulf T, Liebchen B and Schmelcher P 2015 *Phys. Rev. A* **91** 043628

[43] Cao L, Krönke S, Vendrell O and Schmelcher P 2013 *J. Chem. Phys.* **139** 134103

[44] Krönke S, Cao L, Vendrell O and Schmelcher P 2013 *New J. Phys.* **15** 063018

[45] Streltsov A I, Alon O E and Cederbaum L S 2007 *Phys. Rev. Lett.* **99** 030402

[46] Streltsov A I, Sakmann K, Alon O E and Cederbaum L S 2011 *Phys. Rev. A* **83** 043604

[47] Alon O E, Streltsov A I and Cederbaum L S 2007 *Phys. Rev. A* **76** 013611

[48] Alon O E, Streltsov A I and Cederbaum L S 2009 *Phys. Rev. A* **79** 022503

[49] Frenkel J (ed) 1934 *Wave Mechanics* 1st edn (Oxford: Clarendon Press) pp 423–8

[50] Dirac P A 1930 *Proc. Camb. Phil. Soc.* vol 26 (Cambridge: Cambridge University Press) pp 376–85

[51] Broeckhove J, Lathouwers L, Kesteloot E and van Leuven P 1988 *Chem. Phys. Lett.* **149** 547