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Bosonic quantum dynamics following a linear interaction quench in finite optical lattices of unit filling

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ABSTRACT

The nonequilibrium ultracold bosonic quantum dynamics in finite optical lattices of unit filling following a linear interaction quench from a superfluid to a Mott insulator state and vice versa is investigated. The resulting dynamical response consists of various inter and intraband tunneling modes. We find that the competition between the quench rate and the interparticle repulsion leads to a resonant dynamical response, at moderate ramp times, being related to avoided crossings in the many-body eigenspectrum with varying interaction strength. Crossing the regime of weak to strong interactions several transport pathways are excited. The higher-band excitation dynamics is shown to obey an exponential decay possessing two distinct time scales with varying ramp time. Studying the crossover from shallow to deep lattices we find that for a diabatic quench the excited band fraction decreases, while approaching the adiabatic limit it exhibits a non-linear behavior for increasing height of the potential barrier. The inverse ramping process from strong to weak interactions leads to a melting of the Mott insulator and possesses negligible higher-band excitations which follow an exponential decay for decreasing quench rate. Finally, independently of the direction that the phase boundary is crossed, we observe a significant enhancement of the excited to higher-band fraction for increasing system size.

1. Introduction

During the past two decades, ultracold atoms in optical lattices emerged as a versatile system to investigate many-body (MB) phenomena [1–4]. A prominent example is the experimental observation of the superfluid (SF) to Mott insulator (MI) quantum phase transition [5,6] which, among others, demonstrated a pure realization of the Bose-Hubbard model [7,8]. Moreover, lattice systems constitute ideal candidates for studying nonequilibrium quantum phase transitions [9–14], where a number of defects, induced by time-dependent quenches [15,16], appear in the time evolving state. The Kibble-Zurek mechanism of such defect formation [15,17–20], originally addressed in the context of classical phase transitions [21,22], has been tested in different ultracold MB settings [23–28] and refers to the rate of topological defect formation induced by quenches across phase transitions.

Quench dynamics of ultracold bosons confined in an optical lattice covering the MI-SF transition in both directions has been vastly used to examine both the Kibble-Zurek mechanism [19,25,26,29–32] and the approach to the adiabatic response limit [29,33–43,45]. Referring to the Kibble-Zurek mechanism, recent studies [30,31] of a linear quench across the MI-SF and back in the one-dimensional Bose-Hubbard model demonstrated that the excitation density and the correlation length satisfy the Kibble-Zurek scaling for limited ranges of quench rates. On the other hand and focussing on the slow quench dynamics across the MI-SF transition many recent works evinced the formation and melting of Mott domains [34,37–40], the growth of interparticle correlations [32,41–44] and the consequent equilibration process [16,35,45].

Despite the enormous theoretical and experimental efforts in this field, the response of such systems subjected to abrupt or quasi-adiabatic quenches has not been completely understood and deserves further investigation. In particular, a nonadiabatic quench inevitably excites the system, and a number of defects including higher-band excitations can be formed during the dynamics. The latter implies the necessity to consider a multiband treatment [46] of the nonequilibrium correlated dynamics and to obtain information about the higher-band excitation spectrum [47–52] being inaccessible by the lowest Bose-Hubbard model or mean-field (MF) methods. Promising candidates for such investigations constitute few-body systems [53,54] being accessible by current state of the art experiments [55–58]. In this context, it is possible to track the microscopic quantum mechanisms [59–62]

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consisting of intraband and interband tunneling, namely tunneling within the same or between energetically different single-particle bands respectively, and to avoid finite temperature effects. Such few-body systems do not serve as a platform to confirm the Kibble-Zurek scaling hypothesis due to their finite size [43]. However, they provide useful insights into the largely unexplored scaling of few-body defect density including the formation and melting of Mott domains and the excited to higher-band fraction participating in the dynamics.

In the present work we consider few bosons confined in an optical lattice of unit filling. Thereby, the ground state for increasing interaction strength experiences the few-body analogue of the SF to MI transition. We first analyze the MB eigenspectrum for varying interparticle repulsion, revealing the existence of narrow and wide avoided crossings between states of the zeroth and first excited band. Then, we apply a linear interaction quench (LIQ) protocol either from weak to strong interactions (positive LIQ) or inverserly (negative LIQ) covering in both cases the diabatic to nearly adiabatic crossing regimes. As a consequence we observe a dynamical response consisting of the lowest band tunneling and higher-band excitations. Overall, we find an enhanced dynamical response at moderate quench rates rather than in the abrupt or almost adiabatic regimes. The lowest band dynamics consists of first and second order tunneling [63–65]. These modes can be further manipulated by tuning either the interaction strength after the quench (postquench interaction) or the height of the potential barriers in the optical lattice. Furthermore, we show that following a positive LIQ the excited to higher-band fraction obeys a bi-exponential decay for varying ramp time. The latter decay law possesses two time scales being related to the width of the existing avoided crossings in the eigenspectrum. However, the interband tunneling [66,67], with varying height of the potential barrier exhibits a more complex behavior. For diabatic quenches it decreases, while for smaller quench rates it scales non-linearly possessing a maximum at a certain height of the potential barrier. The latter behavior manifests the strong dependence of the excited to higher-band fraction on the quench rate. Moreover, the excited fraction for a varying postquench interaction strength features different scaling laws. Approaching the region of the corresponding avoided crossing it exhibits a non-linear growth, while for stronger interactions it increases almost linearly. On the contrary, for a negative LIQ we observe the melting of the MI. Here, the lowest band transport (intraband tunneling) is reduced when compared to the inverse scenario, while the excited fraction is negligible obeying an exponential decay both with varying ramp time and potential height. Finally, for both positive and negative LIQs the higher-band fraction is significantly enhanced for increasing system size.

This work is organized as follows. In Section 2 we introduce our setup and outline the multiband expansion being used for a microscopic analysis of the dynamics. Section 3 presents the resulting dynamics induced by a LIQ connecting the weakly to strongly correlated regimes and back in a triple well of unit filling. To extend our findings in Section 4 we discuss the LIQ dynamics for larger lattice systems of unit filling. We summarize and discuss future perspectives in Section 5. Appendix A describes our computational methodology.

2. Setup and analysis tools

The Hamiltonian of N identical bosons each of mass M confined in a one-dimensional m-well optical lattice employing a LIQ protocol reads

$$H = \sum_{i=1}^{N}\left(\frac{p_i^2}{2M} + V_0\sin^2(kx_i)\right) + g(t,\tau)\sum_{i<j}\delta(x_i - x_j). \qquad (1)$$

The lattice potential is characterized by its depth V_0 and periodicity l, with $k = 2\pi/l$ being the wave vector of the counterpropagating lasers forming the optical lattice. To restrict the infinitely extended trapping potential to a finite one with m wells and length L, we impose hard wall boundary conditions at the appropriate positions, $x_m = \pm\frac{m\pi}{2k}$.

Within the ultracold regime, the short-range interaction potential between particles located at positions x_i, can be adequately described by s-wave scattering. To trigger the dynamics we follow a LIQ protocol. At $t = 0$ the interatomic interaction is quenched from the initial value g_i to a final one g_f in a linear manner for time $t \in [0,\tau]$ and then it remains a constant g_f. Therefore, our protocol reads

$$g(t,\tau) = g_i + \delta g\frac{t}{\tau}. \qquad (2)$$

Here, $\delta g = g_f - g_i$ denotes the quench amplitude of the linear quench, while g_i (g_f) is the effective one-dimensional interaction strength before (after) the quench. The effective one-dimensional interaction strength [68] is given by $g_{1D} = \frac{2\hbar^2 a_0}{Ma_\perp^2}\left(1 - |\zeta(1/2)|a_0/\sqrt{2}a_\perp\right)^{-1}$. Here $a_\perp = \sqrt{\hbar/M\omega_\perp}$ is the transverse harmonic oscillator length with $\omega_\perp$ the frequency of the two-dimensional confinement and a_0 denotes the free space 3D s-wave scattering length. Experimentally, the effective interaction strength can be tuned either via a_0 with the aid of Feshbach resonances [69,70] or via the corresponding transversal confinement frequency $\omega_\perp$ [68,71,72].

In the following, the Hamiltonian (1) is rescaled in units of the recoil energy $E_R = \frac{\hbar^2 k^2}{2M}$. Then, the corresponding length, time and interaction strength scales are given in units of $k^{-1}, \omega_R^{-1} = \hbar E_R^{-1}$ and $E_R k^{-1}$, respectively.

To simulate the nonequilibrium dynamics we employ the Multi-Configuration Time-Dependent Hartree method for Bosons (MCTDHB) [73,74] which exploits an expansion in terms of time-dependent variationally optimized single-particle functions (see Appendix A for more details). In contrast to the MF approximation, within this approach we account for the system's interparticle correlations and hence we will refer to MCTDHB simply as the MB approach. However, for the analysis of the induced dynamics in lattice systems, it is more intuitive to rely on a time-independent MB basis instead of a time-dependent one. Here, we project the numerically obtained wavefunction on a time-independent number state basis being constructed by the single-particle Wannier states localized on each lattice site. The MB bosonic wavefunction of a system with N bosons, m-wells and j localized single particle states [59,60] reads

$$|\Psi\rangle = \sum_{\{\vec{n}_i\}} C_{\{\vec{n}_i\}}\left|\vec{n}_1, \vec{n}_2, \ldots, \vec{n}_m\right\rangle, () \qquad (3)$$

where $|\vec{n}_1, \vec{n}_2, \ldots, \vec{n}_m\rangle$ is the multiband Wannier number state, the element $\vec{n}_i = |n_i^{(1)}\rangle \otimes |n_i^{(2)}\rangle \otimes \ldots \otimes |n_i^{(j)}\rangle$ and the Wannier orbital $|n_i^{(k)}\rangle$ refers to the number of bosons which reside at the i-th well and k-th band. For instance, in a setup with $N = 3$ bosons confined in a triple well i.e. $m = 3$, which includes $k = 3$ single-particle states, the state $|1^{(0)}, 1^{(1)}, 1^{(0)}\rangle$ indicates that in the left and right wells one boson occupies the Wannier orbital of the zeroth excited band while in the middle well there is one boson in the Wannier orbital of the first excited band. Below, when we refer to a boson that resides within the zeroth (ground) band we shall omit the zero index. Here, one can realize three different energetic classes of number states with respect to the interparticle repulsion. Namely, the triples $\{|3,0,0\rangle + \circlearrowleft\}$ (T), the single pairs $\{|2,1,0\rangle + \circlearrowleft\}$ (SP)