# Quantum Quenches and Off-Equilibrium Dynamical Transition in the Infinite-Dimensional Bose-Hubbard Model

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(Received 29 July 2010; revised manuscript received 17 September 2010; published 22 November 2010)

We study the off-equilibrium dynamics of the infinite-dimensional Bose-Hubbard model after a quantum quench. The dynamics can be analyzed exactly by mapping it to an effective Newtonian evolution. For integer filling, we find a dynamical transition separating regimes of small and large quantum quenches starting from the superfluid state. This transition is very similar to the one found for the fermionic Hubbard model by mean field approximations.

DOI: 10.1103/PhysRevLett.105.220401 PACS numbers: 05.30.Jp, 03.75.Kk, 67.85.De

Significant advances in the field of ultracold atoms have allowed one to engineer quantum many-body systems in almost perfect isolation from the environment. Thanks to the ability to rapidly tune different parameters, e.g., the interaction strength between the atoms or the creation of controlled excitations, the realm of nonequilibrium many-body physics of (almost) isolated quantum systems has thus been accessed and can now be studied experimentally. For example, Greiner *et al.* [1] studied the dynamics of interacting bosons loaded on an optical lattice. The physics of this system is well captured by the Bose-Hubbard model. By changing the intensity of the lasers, one can effectively tune the parameters in the corresponding Bose-Hubbard model. Rapid changes induce interesting non-equilibrium dynamics [1]. The activity in this field is booming: Several new experiments have been performed, including on fermionic systems [2,3]; questions about thermalization [4,5], its absence [6–8], and quantum dynamical phase transitions out of equilibrium [9,10] are currently addressed.

A protocol inducing an off-equilibrium dynamics, which has received a lot of attention recently, is the so-called quantum quench. It corresponds to preparing the system in the ground state of the Hamiltonian $\hat{H}_i$, to changing suddenly at time $t = 0$ a parameter of the Hamiltonian, for example, the interaction strength, and then letting the system evolve with the new Hamiltonian $\hat{H}_f$. Several studies have been performed for the Bose-Hubbard model, which as discussed above is relevant for experiments. There have been numerical analyses of one-dimensional systems by exact diagonalization and time-dependent density matrix renormalization group theory [4,5,7,8]. The saddle point approximation [11], Gross-Pitaevskii equations [12], and the Gutzwiller approximation [13,14] have been used to analyze higher-dimensional and realistic cases. The fermionic Hubbard model has also been studied by mean field theories recently [9,10]. In this work we present a complete analysis of quantum quenches in the Bose-Hubbard model (BHM) in the limit of infinite dimensions. The advantage of this limit is that the model can then be analyzed exactly even out of equilibrium. Its solution at equilibrium played an important role in determining the phase diagram and the properties of the Mott-superfluid quantum phase transition of the three-dimensional BHM [15]. Studying its off-equilibrium dynamics is therefore a natural route to follow. We will discuss in the conclusion the limitations of this approach and possible extensions. To obtain a well-defined infinite-dimensional limit, one has to scale the hopping amplitude as one over the dimension $d$ [16]. A complementary but in the bosonic case identical procedure [17], which we will follow for simplicity, consists in focusing from the start on the BHM defined on a completely connected lattice. The corresponding Hamiltonian reads

$$\hat{H} = -\frac{J}{V}\sum_{i\neq j}\hat{b}_j^\dagger \hat{b}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1), \qquad (1)$$

where $\hat{b}_i^\dagger$ and $\hat{b}_i$ are the bosonic creation and annihilation operators, respectively, $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ the occupation operator, and $V$ the total number of sites. In the following we take $J = 1$ and measure $U$ in units of $J$ and the time in units of $J/\hbar$. We shall study off-equilibrium dynamics induced by quantum quenches corresponding to a sudden change of the interaction strength from $U_i$ to $U_f$ at $t = 0$. Since $H$ is invariant under any permutation of sites, all eigenstates can be classified in terms of the corresponding symmetry classes. In particular, the ground state, whether Mott or superfluid, corresponds to a completely site permutation symmetric wave function. Since the time-dependent wave function also remains completely symmetric after the quench, one can restrict the analysis to the subspace of completely symmetric states. It is easy to convince oneself that these states can be parametrized by the fraction $x_0, x_1, x_2, \ldots$ of sites with $0, 1, 2, \ldots$ bosons and that they correspond to the flat normalized sum of all Fock states characterized by $Vx_i$ sites with $i$ bosons per site. In order to simplify the presentation, let us first focus on the simplified model where a maximum of two bosons per site are allowed ($n_b = 2$). We shall discuss later the generalization to any value of $n_b$. Since $x_0 + x_1 + x_2 = 1$ for $n_b = 2$ and because the number of particles $V(x_1 + 2x_2)$ is conserved by the dynamics, a generic symmetric state is identified by $x_1$ only and can be denoted $|x_1\rangle$ (henceforth we will drop the subindex 1). The evolution of the wave function $|\psi\rangle = \sum_x \psi_x |x\rangle$ is determined by the equation $\langle x| i\partial_t \sum_{x'} \psi_{x'} |x'\rangle = \langle x|\hat{H} \sum_{x'} \psi_{x'}|x'\rangle$. In this model, all matrix elements $\langle x|\hat{H}|x'\rangle$ are zero except $\langle x|\hat{H}|x \pm 2/V\rangle$ and the diagonal term $\langle x|\hat{H}|x\rangle$; the former corresponds to the physical process of one boson jumping from one site to another. The resulting Schrödinger equation for $\psi_x$ reads

$$\begin{aligned}\frac{1}{V} i\partial_t \psi_x &= D(x)\psi_x - W(x)(\psi_{x+2/V} + \psi_{x-2/V}) \\ &= [D(x) - 2W(x)\cosh(2\partial_x/V)]\psi_x \\ &= [D(x) - 2W(x)\cos(2\hat{p})]\psi_x, \end{aligned} \tag{2}$$

where $W(x) = x[(2 - x - n)(n - x)/2]^{1/2}$, $D(x) = U(n - x)/2 - x(2 + n - 3x)/2$, $n$ is the number of bosons per site, and subleading contributions in $1/V$ have been dropped. The initial wave function, which is the ground state at coupling $U_i$, is a wave packet of width $1/\sqrt{V}$; see [18] and below. Since $1/V$ plays the role of $\hbar$ in (2), the thermodynamic limit corresponds to the *classical* limit. As a consequence, the time evolution of the average particle position $x(t) = \langle\hat{x}\rangle$ and momentum $p(t) = \langle\hat{p}\rangle = \langle -i\partial_x/V\rangle$ is given by the Newton equations for the Hamiltonian $H = D(x) - 2W(x)\cos(2p)$, where $x(t)$ and $p(t)$ are classical canonical variables. The validity of this argument can be thoroughly established by a direct analysis [18]. In particular, one can show that on time scales less than $\sqrt{V}$, $\psi_x(t) \sim \exp\{V[x - x(t)]^2/2\sigma(t)^2 + iVp(t)x\}$; i.e., it is a sharp wave packet, centered at $x(t)$, of width of the order of $1/\sqrt{V}$ and has a very fast oscillating phase $e^{iVp(t)x}$, where $x(t)$ and $p(t)$ are the classical canonical variables defined above. In the following we will repeatedly make use of this mapping to a classical system. Similar mappings have been recently used in Refs. [10,19,20]. The first useful consequence is that the ground state is obtained, minimizing $H$ with respect to $p$ and $x$; the corresponding $p$ is actually always zero; as a consequence, the ground state is obtained by the value of $x$ minimizing $D(x) - 2W(x)$. The phase diagram is similar to the one derived by Fisher *et al.* [16] except that there is only one Mott lobe corresponding to $n = 1$. As we shall see, it is at integer filling $n = 1$, where the Mott state exists, that the off-equilibrium dynamics is most interesting. We shall consider this case first, for which the ground state (GS) corresponds to

$$x_{\mathrm{GS}} = \begin{cases} 1 & \text{if } U \geq U_c, \text{ Mott insulator GS} \\ (U/U_c + 1)/2 & \text{if } U < U_c, \text{ superfluid GS,} \end{cases}$$

with $U_c = 3 + 2\sqrt{2}$. In this simple model, the condensate fraction $|\Psi_0|^2$ is simply equal to $\frac{1}{V^2}\sum_{i\neq j} b_j^\dagger b_i$, which up to a sign coincides with the average value of the (intensive) kinetic energy. This can be easily obtained by subtracting the average value of the interaction term to the total energy and reads, for the ground state, $|\Psi_0|^2 = x_{\mathrm{GS}}(1 - x_{\mathrm{GS}})U_c/2$.

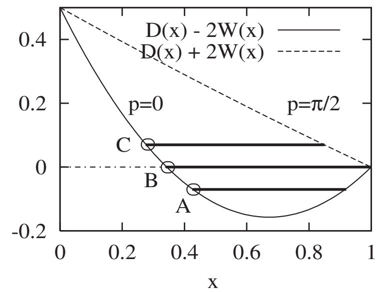


FIG. 1. Graphical solution for the value of $p$ at the turning points. The trajectories are full lines, and the position at $t = 0$ is indicated by a circle for the three trajectories $A$, $B$, and $C$. In case $A$ it is impossible to have a turning point at $p = \pi/2$. Case $B$ corresponds to the dynamical transition and $C$ to unbounded evolution of $p$. $A$, $B$, and $C$ are plotted in Fig. 2.

Let us now consider quenches starting from a superfluid ground state and increasing the value of $U$ from $U_i$ to $U_f$. A small increase of $U$ leads to oscillations of $x$ and $p$ as can be verified analytically and checked numerically; see Fig. 2(a). The turning points of $x(t)$, determined by $\dot{x} = 4W(x) \times \sin(2p) = 0$, correspond to $p = 0$. Actually, there would be the possibility to have $p = n\pi/2$, too. However, a $p$ starting from zero and reaching the value $\pi/2$ would imply, by energy conservation, a value of $x$ at the turning point such that $E = D(x) + 2W(x)$, where $E$ is the energy after the quench. This equation has no solution for small quenches as shown graphically in Fig. 1; see case $A$. It starts to have a solution for larger quenches, when $E$ becomes positive (cases $B$ and $C$ in Fig. 1). Actually, $E_d = 0$ corresponds to a *dynamical transition*: For $E < E_d$ the momentum $p(t)$ is bounded, whereas for $E > E_d$ it grows infinitely large. The condition $E = 0$ depends on $U_i$ and $U_f$. One finds that for a given $U_i$ the corresponding critical value is $U_f^d(U_i) = (U_i + U_c)/2$. Approaching $U_f^d$, the period of oscillation increases and diverges as $\tau = -c^{-1}\ln(|U_f - U_f^d|)$, where $c = \sqrt{(U_c - U_f)(U_f - 1/U_c)}$. Figure 2 shows the typical time evolution of $x$, $|\Psi_0|^2$, and $p$ for the three cases $A$, $B$, and $C$. Exactly at $U_f^d$, the system relaxes exponentially to the Mott state with a rate $c$. Approaching the transition, the system spends most of the time close to the Mott state, and therefore the time-averaged condensate fraction vanishes at $U_f^d$ in a singular way, proportional to $1/\tau$. This singularity is related to the fact that the Mott state is "absorbing": Classical trajectories falling into it cannot escape, and the period $\tau$ diverges when approaching $U_f^d$. Conversely, trajectories starting from the Mott state remain stuck to $x = 1$ on large times $t \sim \log V$. This is, however, a peculiarity of the infinite-dimensional limit; for a finite-dimensional system, spatial fluctuations will drive the system away from the

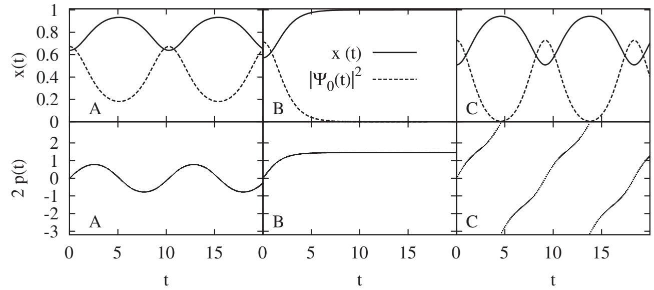


FIG. 2. Evolution as a function of time of $x$, $|\Psi_0|^2$ (top panels), and $p$ (bottom panels) increasing the amplitude of the quench. $U_f = 3.33$ is kept fixed and several $U_i$ are considered, with $A$, $B$, and $C$ corresponding to $U_i = \{1.62, 0.838, 0.1\}$ (unlike in the text where $U_f$ is varied). Case $B$ corresponds to the transition point.

Mott state [21,22]. In Fig. 3(a), as an example of singular behavior, we show $|\Psi_0|^2$ as a function of $U_f$ for quenches starting from the noninteracting case $U_i = 0$. Moreover, we compare $|\Psi_0|^2$ to its microcanonical average at the same energy. Clearly, the system is not thermalized. At $U_f^d$ the condensate fraction goes to zero after the quench, whereas the corresponding equilibrium state is still superfluid. The dynamical phase diagram in Fig. 3(b) summarizes our analysis for all kinds of quantum quenches [23]. Let us finally address the changes in the dynamical behavior when one quenches for noninteger filling. Since the absorbing Mott state disappears for $n \neq 1$, it is natural to expect, as indeed we find, that going away from $n = 1$ the dynamical transition disappears, too, and transmutes into a crossover that becomes more and more sharp approaching integer filling. Overall, the resulting physical picture is extremely similar to the one obtained recently for the fermionic Hubbard model by a time-dependent Gutzwiller approximation [10].

Clearly, a natural question is how much these results depend on the constraint of a maximum of two bosons per site. A complete analysis with an arbitrary number of bosons $n_b$ is very involved. The mapping to a classical system works also in this case. The classical degrees of freedom are the first $n_b - 1$ fractions $x_0, x_1, \ldots, x_{n_b-1}$ and their associated canonical momenta. Unlike in the case $n_b = 2$ where the classical motion is one-dimensional, these trajectories are no longer necessarily periodic. In order to study their regularity we have computed numerically for $n_b = 3$ the largest Lyapunov exponent $\lambda$ [25] of several trajectories. In this case $x_1$ and $x_2$ are the classical variables, and the expression of the Hamiltonian can be found in Ref. [18]. Depending on the initial condition, we find large values ($\lambda > 0.1$) characteristic of chaotic trajectories for large quenches and small, possibly zero, values characteristic of periodic or quasiperiodic trajectories for small quenches. We find again a dynamical transition, for $n = 1$ and $n = 2$, which are the only fillings for which the Mott ground state exists. At the transition line, the trajectories are chaotic. As in the previous case, the dynamical transition corresponds to a change in the form of the phase space trajectories: For $U_f > U_f^d$ the momentum $2p_1 - p_2$ becomes unbounded; see Fig. 4(a). The time evolution of the $x_i(t)$ is also similar and characterized by oscillations that take place on longer time scales close to the transition. Moreover, the qualitative evolution of the time-averaged $|\Psi_0|^2$ (and also $x_i$) with $U_f$ for a given $U_i$ resembles very much the one for $n_b = 2$. We have also analyzed higher values of $n_b$ up to $n_b = 5$ finding qualitatively and quantitatively similar results. Actually, the evolution of $\langle|\Psi_0|^2\rangle$ depends very little on $n_b$ for $n_b > 2$ as shown in Fig. 4(b) (the two curves $n_b = 4$ and $n_b = 5$ differ by less than 0.01%). The only issue that remains open is the form of the singularity at the dynamical transition for $n_b > 2$. Numerical solutions of the Newton equation are not precise enough to answer this question. Even in the case of two bosons per site, for which we know that $|\Psi_0|^2 = 0$ at the transition and the singularity is logarithmic, numerics alone would not be conclusive. For $n_b = 2$ the singularity

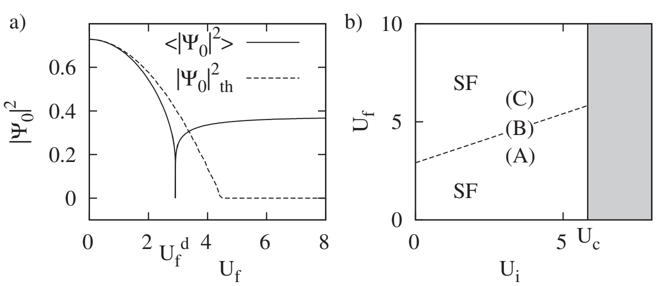


FIG. 3. (a) Evolution of the time average (continuous line) and microcanonical average (dashed line) of $\langle|\Psi_0|^2\rangle$ as a function of $U_f$ for $U_i = 0$. (b) Dynamical phase diagram for the model with a maximum of two bosons per site. Quenches from the Mott phase are not considered. Quenches from the superfluid phase are oscillating and similar to $A$ or $C$. The dynamical transition separating the two is displayed as a dashed line; it meets the Mott phase at $U_f = U_c$. The phase diagram for the case of more than two bosons per site is qualitatively similar.

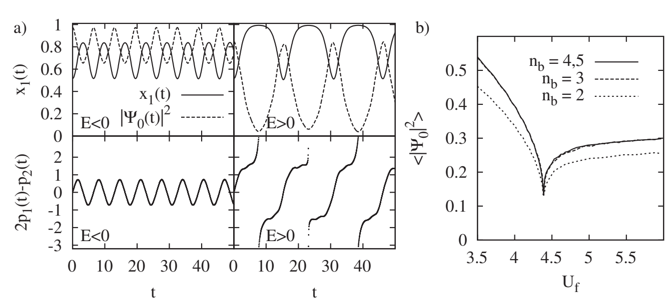


FIG. 4. (a) As in Fig. 2 but for $n_b = 3$ and $U_i = 1$. Left and right: $U_f = 2.5$ and 3.29, respectively, below ($E < 0$) and above ($E > 0$) the dynamical transition at $U_f^d = 3.21$. (b) Variation of $\langle|\Psi_0|^2\rangle$ as a function of $U_f$ for $n = 1$, $U_i = 3$, with $n_b = 2, 3, 4$, and 5. The plot of $n_b = 2$ is shifted of 0.025 along the $U_f$ axis for comparison.

was due to the fact that trajectories spend most of the time close to the Mott state. For $n_b > 2$, it is not clear whether trajectories starting with the same energy as the Mott state (energy zero) have to go arbitrarily close to it. Assuming that the classical dynamics is completely ergodic on the $E = 0$ hypersurface, one could argue that this should be the case. However, even in this case, time averages would not coincide with averages in the Mott state unless the recurrence time is of the same order as the trapping time, a difficult question to address. The conclusion of the analysis performed for a higher number of bosons is that the results for $n_b = 2$ are robust and expected to hold also for the BHM with an arbitrary number of bosons per site, except possibly the form of the singularity of $|\Psi_0|^2$ (and of the other observables).

Let us now discuss the implications and the limitations of our findings. Clearly, the infinite-dimensional limit neglects important dynamical and spatial fluctuations. This is manifest from the nondamped oscillatory evolution in time of the observables and the absence of thermalization. Certainly, $1/d$ corrections must be taken into account to lead to decoherence and thermalization. Nevertheless, we expect that our mean field approach should be able to qualitatively account for the short time dynamical behavior. As a consequence, the dynamical transition we find should transmute into a crossover in the short time dynamics for finite-dimensional systems. Indeed, results obtained for the one-dimensional BHM seem to be in agreement with our findings [26]. Moreover, we expect the dynamical transition we found to be quite general, at least within mean field treatments of the off-equilibrium dynamics. Actually, it is qualitatively identical to the one found for the fermionic Hubbard model within the Gutzwiller approximation [10] and very similar to the one obtained by out of equilibrium dynamical mean field theory [9], where some dynamical fluctuations are taken into account.

Including spatial and dynamical fluctuations would allow one to go beyond our mean field treatment. A good description of decoherence and thermalization for the BHM could be obtained in the future within a real time generalization of the equilibrium bosonic dynamical mean field theory [27,28].

We thank C. Kollath and M. Schirò for useful discussions. G. B. acknowledges partial financial support from ANR FAMOUS.

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