

Quantum quenches and off-equilibrium dynamical transition in the infinite dimensional Bose Hubbard model

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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.

Significant advances in the field of ultra cold 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 non-equilibrium 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], quantum dynamical phase transitions out of equilibrium [9, 10] are currently addressed.

A protocol which induces an off-equilibrium dynamics and 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 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 H_f . Several studies have been performed for the Bose Hubbard model, which as discussed above is relevant for experiments. There have been numerical analysis of one dimensional systems by exact diagonalization and t-DMRG [4, 5, 7, 8]. Saddle point approximation [11], Gross-Pitaevskii equations [12] and Gutzwiller approximation [14, 15] have been used to analyze higher dimensional and realistic cases. The fermionic Hubbard model has been also 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 [13]. 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 [24], 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:

$$H = -\frac{J}{V} \sum_{i \neq j} b_j^\dagger b_i + \frac{U}{2} \sum_i n_i(n_i - 1) \quad (1)$$

where b_i^\dagger , b_i are the bosonic creation and annihilation operators, $n_i = b_i^\dagger b_i$ 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 wavefunction. Since also the time-dependent wavefunction 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, \dots of sites with $0, 1, 2, \dots$ 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 maximum 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 wavefunction ψ_x is determined by the equation $\langle x|i\partial_t \sum_{x'} \psi_{x'}|x'\rangle = \langle x|H \sum_{x'} \psi_{x'}|x'\rangle$. In

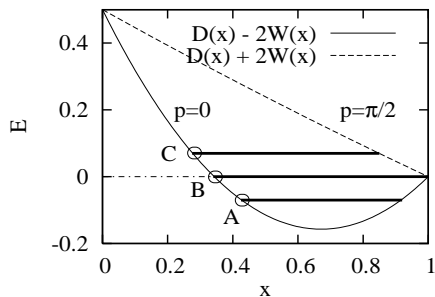


FIG. 1: Graphical solution for the value of p at the turning points. The trajectories are full lines, and the position at $t = 0$ is indicated by a circle for the three trajectories A, B and C. In case A it is impossible to have a turning point at $p = \pi/2$. Case B corresponds to the dynamical transition,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

this model, all matrix elements $\langle x|H|x' \rangle$ are zero except $\langle x|H|x \pm 2/V \rangle$ and the diagonal term $\langle x|H|x \rangle$; the former corresponds to the physical process of one boson jumping from one site to another. The resulting Schrödinger equation for ψ_x reads :

$$\begin{aligned} \frac{1}{\sqrt{V}} i \partial_t \psi_x &= D(x) \psi_x - W(x) (\psi_{x+2/V} + \psi_{x-2/V}) \\ &= (D(x) \psi_x - 2W(x) \cosh(2\partial_x/V)) \psi_x \end{aligned} \quad (2)$$

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. From the expression above, it is clear that $1/V$ plays the role of \hbar and, hence, the thermodynamic limit corresponds to the *classical* limit. The corresponding one dimensional Hamiltonian, with $\partial_x/N \rightarrow ip(t)$, is $H = D(x) - 2W(x) \cos(2p)$, and the dynamics after a quench is simply given by $\dot{x} = \partial_p H$ and $\dot{p} = -\partial_x H$. The validity of this intuitive argument can be established by a more detailed analysis of the large V limit [17], which shows that the wavefunction is peaked, with a width of order $1/\sqrt{V}$, around the value of $x(t)$ obtained from the classical limit and has a very fast oscillating phase $e^{iVp(t)x}$. In the following we will repeatedly make use of this mapping to a classical system. Similar semiclassical mapping have been recently used in [10, 18, 19]. 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; in 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)

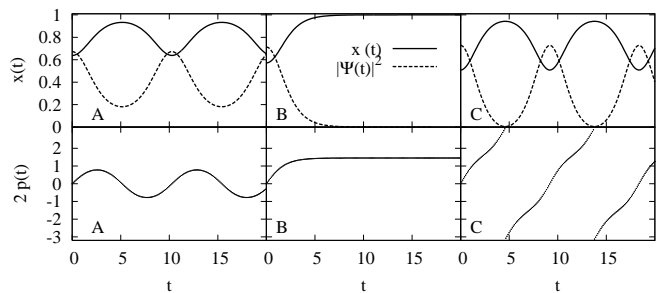


FIG. 2: Evolution as a function of time of x , $|\Psi|^2$ (top panels) and p (bottom panels) increasing the amplitude of the quench. $U_f = 3.33$ is kept fixed and several U_i are considered, with A, B, C corresponding to $U_i = \{1.62, 0.838, 0.1\}$ (unlike in the text where U_f is varied). The case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

corresponds to

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

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

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 2A. The turning points of $x(t)$, determined by $\dot{x} = 4W(x) \sin(2p) = 0$, 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, 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 $\tau = -c \ln(|U_f - U_f^d|)$, where $c = \sqrt{(1/U_f - 1/U_c)(U_c - 1/U_f)}/8$. Fig. 2 shows the typical time-evolution of x , $|\Psi|^2$ 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 spend 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, pro-

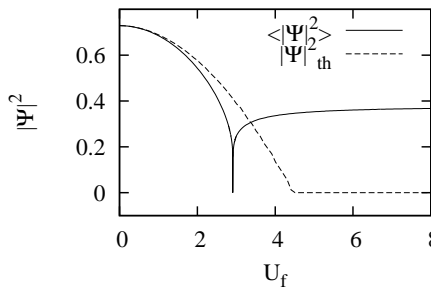


FIG. 3: Evolution of time average (continuous line) and microcanonical average (dashed line) of $\langle |\Psi|^2 \rangle$ as a function of U_f for $U_i = 0$.

portional to $1/\tau$. In Fig. 3 we plot the variation of the time averaged condensate fraction as a function of U_f for quenches starting from the non interacting case $U_i = 0$. We compare it to the microcanonical average of $|\Psi|^2$ at the same energy. They differ, thus showing that the system is not thermalized. The time averaged $|\Psi|^2$ has a clear singular behavior at U_f^d . This singularity is related to the fact that the Mott state is ‘absorbing’: classical trajectories falling into it cannot escape, and the period τ diverges when approaching U_f^d . Conversely, trajectories starting from the Mott state remain stuck to $x = 1$ [25]. As a consequence, quenches starting from the Mott state do not lead to any interesting dynamics. The dynamical phase diagram in Fig. 4 summarizes our analysis for all kinds of quantum quenches [26]. Let us finally address the changes in the dynamical behavior when one quenches for non integer 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 cross-over 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 maximum two bosons per site. A complete analysis with an arbitrary number of bosons is very involved. The main difficulties appear already for the case $n_b = 3$. In the following we shall focus on it and only cite results for $n_b > 3$. Taking into account the constraint $x_0 + x_1 + x_2 + x_3 = 1$ and $n = (x_1 + 2x_2 + 3x_3)$, one finds that the states completely symmetric under site permutations are identified by x_1, x_2 only. As before the study of the system in the thermodynamic limit can be reduced to the analysis of a classical system. The corre-

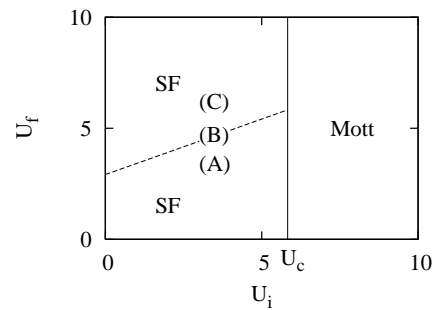


FIG. 4: Dynamical phase diagram for the model with maximum two bosons per site. Quenches from the Mott phase remain in the Mott phase. Quenches from the superfluid phase are oscillating and similar to A or C, and the dynamical transition separating the two is displayed as a dashed line. The phase diagram for the case of more than two boson per site is qualitatively similar.

sponding classical Hamiltonian reads:

$$\begin{aligned} H = & D - 2W_1 \cos(p_1 + p_2) - 2W_2 \cos(2p_1 - p_2) \\ & - 2W_3 \cos(p_1 - 2p_2), \quad W_1 = J(3x_0x_1x_2x_3)^{1/2} \\ W_2 = & Jx_1(2x_0x_2)^{1/2} \quad W_3 = Jx_2(6x_1x_3)^{1/2} \\ D = & x_2 + 3x_3 - J(x_0x_1 + 2x_1x_2 + 3x_2x_3) \end{aligned} \quad (3)$$

where $x_0 = 1 - x_1 - x_2 - x_3$ and $x_3 = \frac{1}{3}(n - x_1 - 2x_2)$. Now the trajectories $x_i(t)$ are no longer necessarily periodic. In order to study their regularity we have computed numerically the largest Lyapunov exponent [23] for trajectories with initial condition x_i^i, x_i^i . Depending on the initial condition we have found large values ($\lambda > 0.1$), characteristic of chaotic trajectories, for large quenches and small, possibly zero, values characteristic of periodic or quasi periodic trajectories for small quenches. Quenches to $E = 0$ lead to chaotic trajectories. The analysis of quantum quenches is more involved than in the previous case $n_b = 2$, but the results are qualitatively similar. We find a dynamical transition for $n = 1$ and $n = 2$, which are the only filling for which the Mott ground state exists. 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. 5a. The time evolution of the $x_i(t)$ is also similar and characterized by oscillations that take place on longer timescales close to the transition. Moreover, the qualitative evolution of the time averaged $|\Psi|^2$ (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 $\langle |\Psi|^2 \rangle$ depends very little on n_b for $n_b > 2$ as shown in Fig. 5b (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

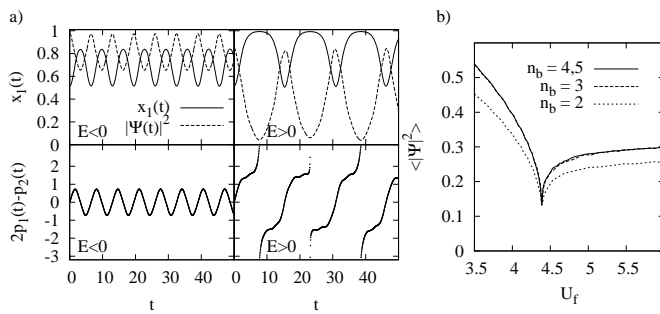


FIG. 5: a) As Fig. 2 but for $n_b = 3$ and $U_i = 1$. Left and right: $U_f = 2.5$ and 3.29 , respectively below ($E < 0$) and above ($E > 0$) the dynamical transition at $U_f^d = 3.21$. b) Variation of $\langle |\Psi|^2 \rangle$ as a function of U_f for $n = 1$, $U_i = 3$, with $n_b = 2, 3, 4$ and 5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

are not precise enough to answer this question. Even in the case of two bosons per site, for which we know that $|\Psi|^2 = 0$ at the transition and the singularity is logarithmic, numerics alone would not be conclusive. For $n_b = 2$ the singularity 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 of the trapping time, a difficult question to address. The conclusion of the analysis performed for 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 $|\Psi|^2$ (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 fluctuations. This is manifest from the non damped 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 cross-over 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 [20]. Moreover, the dynamical transition we found appears to be generic, 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. The first type of fluctuations certainly are important to obtain a good description of quenches from Mott to superfluid, where real space effects such as coarsening and vortex dynamics could play an important role. The second type of fluctuations are important to obtain a description of decoherence and thermalization for the BHM. Developing an off-equilibrium version of bosonic DMFT [21, 22] seems very promising from this point of view.

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- [26] Note that there is an additional dynamical transition obtained when quenching from the superfluid to very small U ($U_f < 1/U_c$) that we do not show since it is not robust: it disappears when one focuses on maximum three bosons per site ($n_b = 3$). Details will be shown in [17].