Dynamics-induced freezing of strongly correlated ultracold bosons

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Abstract - We study the non-equilibrium dynamics of ultracold bosons in an optical lattice with a time-dependent hopping amplitude \( J(t) = J_0 + \delta J \cos(\omega t) \) which takes the system from a superfluid phase near the Mott-superfluid transition \( (J = J_0 + \delta J) \) to a Mott phase \( (J = J_0 - \delta J) \) and back through a quantum critical point \( (J = J_c) \), and demonstrate dynamics-induced freezing of the boson wave function at specific values of \( \omega \). At these values, the wave function overlap \( F \) (defect density \( P = 1 - F \)) approaches unity (zero). We provide a qualitative explanation of the freezing phenomenon, show its robustness against quantum fluctuations and the presence of a trap, compute residual energy and superfluid order parameter for such dynamics, and suggest experiments to test our theory.

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In this work, we demonstrate that the periodically driven Bose-Hubbard model may exhibit dynamical freezing of the boson wave function by observing that after one cycle the wave function comes back to its original value \( \psi(T) = \psi(0) \) for specific values of the drive frequency \( \omega = 2\pi/T \). Our driving protocol constitutes a time-dependent hopping amplitude of the bosons \( J(t) = J_0 + \delta J \cos(\omega t) \) with \( J_0 \) and \( \delta J \) chosen such that the drive takes the system from a superfluid (SF) \( (J = J_0 + \delta J) \) to the Mott insulator (MI) state \( (J = J_0 - \delta J) \) and back through the tip of the Mott lobe where \( \mu = \mu_{\text{tip}} \). We provide a semi-analytical understanding of the freezing phenomenon using mean-field theory and compute the defect formation probability \( P = 1 - F \) (where \( F = |\langle \psi(t=0)|\psi(t=T) \rangle|^2 \) is the wave function overlap), the superfluid order parameter \( \Delta(T) = \langle \psi(T)|b|\psi(T) \rangle \) (where \( b \) denotes the boson annihilation operator), and the residual energy \( Q = E(t=T) - E_G \) (where \( E(t=T) \) is the energy of the system at the end of the drive cycle and \( E_G \) is the initial ground-state energy) as a function of \( \omega \). We also show, via inclusion of quantum fluctuation by a projection operator approach [11] and numerical mean-field study of a trapped boson system that the freezing phenomenon is qualitatively robust against quantum fluctuations and the presence of a trap. We also show that such a phenomenon persists for multiple drive cycles. We note that such a freezing behavior has two novel characteristics which distinguishes it from its counterpart

The theoretical study of non-equilibrium dynamics in closed quantum systems has seen great progress in recent years [1] mainly due to the possibility of realization of such dynamics using ultracold atoms in optical lattices [2,3]. For bosonic atoms, such systems are well described by the Bose-Hubbard model with on-site interaction strength \( U \) and nearest-neighbor hopping amplitude \( J \) [4,5]. Several theoretical studies have been carried out on the quench and ramp dynamics of this model [6–11]; some of them have also received support from recent experiments [3]. In contrast, studies on periodically driven closed quantum systems have been undertaken in the past mainly on driven two-level systems [12,13] or on weakly interacting or integrable many-body systems which can be modeled by them [14,15]. Among these, ref. [15] has predicted freezing of the time-averaged value of the order parameter (magnetization) of a periodically driven one-dimensional (1D) Ising or XY model, when the temporal average is performed over several drive cycles, at specific drive frequencies. Such a freezing occurs in the high-frequency regime and exhibits non-monotonic dependence on the drive frequency. However, to the best of our knowledge, the phenomenon of dynamics-induced freezing has never been demonstrated for dynamics involving a single drive cycle and/or for non-integrable quantum systems. Recent studies of periodic dynamics of the Bose-Hubbard model have not addressed this issue [16,17].
in ref. [15]. First it always occurs at low frequencies, i.e., \(\hbar\omega/U \ll 1\) for all \(\omega\) for which the freezing occurs. Second, it occurs for a single cycle of the drive. To the best of our knowledge, the dynamics-induced freezing phenomenon at such low drive frequencies and non-integrable models has not been studied in the context of closed quantum systems; our work therefore constitutes a significant advance in our understanding of periodic dynamics of closed non-integrable quantum systems.

The Hamiltonian describing a system of ultracold bosonic atoms confined by a trap and in an optical lattice is given by

\[ H = \sum_{(r,r')} -Jb_r^\dagger b_{r'} + \sum_r \left[ -\mu_r \hat{n}_r + \frac{U}{2} \hat{n}_r^2 (\hat{n}_r - 1) \right], \]

where \(\mu_r\) denotes the chemical potential at site \(r\), \(r'\) denotes one of the \(n\) nearest-neighboring sites of \(r\), and \(\hat{n}_r = b_r^\dagger b_r\). In the absence of a trap, \(\mu_r = \mu\) for all sites and for \(zJ < U\), the ground state of the MI state is the state with \(\hat{n}\) bosons per site with \(\hat{n} = 1\) for \(0 < \mu/U \leq 1\). For \(zJ > U\), the bosons are delocalized and the system, for \(d \geq 2\), is in a SF state. In between, at \(J = J_c\), the system undergoes a SF-MI transition. The equilibrium phase diagram model of the ground state constitutes the well-known Mott lobe structure [45].

To obtain an analytic insight to the freezing phenomenon, we first analyze the periodically driven Bose-Hubbard model in the absence of a trap and within mean-field approximation. The time-dependent mean-field Hamiltonian is given by

\[ \hat{H}_{\text{mf}} = \sum_r \left[ -\mu \hat{n}_r + \frac{U}{2} \hat{n}_r^2 (\hat{n}_r - 1) + (\Delta'_r(t) b_r^\dagger + \text{h.c.}) \right], \]

where \(\Delta'_r(t) = -J(t) \sum_{r'} (b_{r'}^\dagger b_r)\) and \(\Delta'_0 = \Delta'(t = 0)\). Within homogeneous mean-field theory, the Gutzwiller wave function for the bosons reads \(\psi(r_t, t) = \prod_n \psi_n(t) n\) [18]. The Schrödinger equation \(i\partial_t \psi(r_t, t)_{\text{mf}} = \hat{H}_{\text{mf}}(t)\psi(r_t, t)_{\text{mf}}\) yields the time-dependent mean-field equations for \(f_n(t) \equiv f_n^\prime\):

\[ (i\partial_t - E_n) f_n = \hat{\Delta}(t) \sqrt{n} f_{n-1} + \hat{\Delta}'(t) \sqrt{n+1} f_{n+1}, \]

where \(\hat{\Delta}(t) = -zJ(t) \sum_n \sqrt{n} f_{n-1} f_n\), and \(E_n = -\mu n + U(n-1)n/2\). In what follows, we shall choose \(J_0\) and \(\delta J\) such that the ground state of \(\hat{H}_{\text{mf}}\) with \(J = J_0 + \delta J\) is a SF state close to the QCP so that \(f_n(t = 0) \approx 0\) for \(n \geq 3\) and \(f_1(t = 0) \gg f_0(t = 0), f_2(t = 0)\).

Our strategy for solving these equations will be the following. First, we shall solve the mean-field equations numerically keeping states with \(n \leq 4\). Such numerics yields the result that in the MI and SF states close to the QCP all \(f_n(t)\) for \(n \geq 3\) remains small for all \(t\) during the dynamics. We shall then use this fact to develop semi-analytic understanding of the freezing phenomenon using equations for \(f_0, f_1\) and \(f_2\) (see footnote 1).

The equations for \(f_0, f_1\) and \(f_2\) then read (suppressing the time dependence of \(f_n(t)\) for clarity)

\[ i\partial_t f_0 = -zJ(t)[|f_1|^2 f_0 + \sqrt{2}f_2 f_0^2], \]
\[ i\partial_t f_2 = E_2 f_2 - zJ(t)[2|f_1|^2 f_2 + \sqrt{2}f_0^2 |f_2|^2], \]
\[ i\partial_t f_1 = E_1 f_1 - zJ(t)[2|f_2|^2 + |f_0|^2] f_1 + 2\sqrt{2}f_1 f_2 f_0. \]

Multiplying each of the equations for \(f_n\) in eqs. (4) by \(f_n^*\) and subtracting the equations thus obtained from their complex conjugates, it is easy to see that \(|f_n|^2\), for \(n \leq 2\), obeys the relation

\[ \partial_t |f_0|^2 = \partial_t |f_2|^2 = -\partial_t |f_1|^2/2. \]

Parameterizing \(f_n = r_n(t) \exp[i\phi_n(t)]\), with the choice that \(\phi_n(0) = 0\) and \(r_n(0) = f_n(0)\), one can write

\[ r_n^2(t) = -(r_1^2(t) - 1)/2 + [-\eta] \]

where \(\eta\) is a time-independent parameter whose value is fixed by the initial values \(r_n\) (see footnote 2). Note that \(\eta\) represents the magnitude of the particle-hole asymmetry since \(r_0 = r_2\) for \(\eta = 0\). Substituting eq. (6) in eq. (4), we get

\[ \partial_t r_1 = -\sqrt{2}zJ(t) \sin(\phi_1) r_1 g_1(\phi_1), \]
\[ \partial_t \phi_1 = -U + zJ(t)[g_1(r_1) - g_2(r_1) \cos(\phi_1)], \]
\[ \partial_t \phi_4 = -U + 2\mu + zJ(t) r_1^2 \left[1 - 4\sqrt{2} \eta \cos(\phi_1)/g_0(r_1)\right], \]

where we have suppressed the time dependence of \(r_1\) and \(\phi_4\) for clarity. \(\phi_4 = \phi_0 + \phi_2 - 2\phi_1\) and \(\phi_4 = \phi_2 - \phi_0\) are the sum and differences of the relative phases of the Gutzwiller wave function, and the functions \(g_i(r_1)\) are given by

\[ g_0(r_1) = \sqrt{1 - r_1^2}^2 - 4\eta^2, \quad g_1(r_1) = 6r_1^2 - 3 - 2\eta, \]
\[ g_2(r_1) = 2\sqrt{2} \left[r_1^2 - 1\right]/g_0(r_1) + g_0(r_1). \]

We note that the first two of the equations in eqs. (7) are coupled equations describing the evolution of \(r_1\) and \(\phi_1\), while the third describes the evolution of \(\phi_4\) in terms of \(r_1\) and \(\phi_1\). Furthermore, using a scaled variable \(t' = \omega t/(2\pi)\), we find that the relation between \(r_1\) and \(\phi_1\) can be written as

\[ dr_1/d\phi_1 = -\sqrt{2} \sin(\phi_1) r_1 g_1(\phi_1)/[g_1(r_1) - g_2(r_1) \cos(\phi_1)] - U/zJ(t'). \]

This allows us to symbolically write \(\phi_4 = \xi(r_1, t')\), where \(\xi\) is an unknown function, and thus establish an \(\omega\)-independent relation between \(r\) and \(\phi_4\) for any fixed \(t'\). of the freezing phenomenon: all numerical procedures were carried out keeping five states \((n = 0, 1, 2, 3, 4)\) states per site.

\[ ^1\text{We note that such a three level approximation is used in a subsequent discussion for obtaining a semi-analytic understanding}\]

\[ ^2\text{We note that within the single-site homogeneous mean-field theory, the system does not exhibit freezing for } \eta = 0. \text{ This behavior originates from the constraint of conservation of the particle number at each site and is not seen in realistic systems with traps where only the total particle number is conserved.}\]
which implies, via eq. (6), that $\omega/J_0 = 1$ (red dashed line) and $\phi_d(T)$ (blue solid line) with $\omega$. Finally, we note, from the panels (c) and (d) Plot $\phi_d(t)$ ($\phi_d(T)$) as a function of $t$ ($\omega$). For all plots $J_0 = 1.05 J_c$, $\delta J = 0.35 J_c$, and $\mu = 0.414 U$.

Equations (6), (7) and (8) constitute the central result of this work. They constitute a complete description of the evolution of $f_0$, $f_1$, and $f_2$ in the presence of the periodic drive and provide an understanding of the freezing phenomenon as follows. First, we find that a numerical solution of eq. (7), together with eq. (6), allows us to obtain $r_n$, $\phi_s$ and $\phi_d$ as functions of time. The plots of $1 - r_1(t)$ and $\phi_s(t)$ as functions of $t$ for $\omega/J_c = 0.52$ is shown in panel (a) of fig. 1. We find that $r_1$ changes appreciably when $J(t)$ is close to $J_c$; however, $r_1(T) \approx r_1(0)$ at the end of the evolution. Note that this also implies, via eq. (6), that $r_2(0) \approx r_2(0)$ holds for a significant range $\omega/J_c \leq 0.8$. Second, we note that, $\phi_s(t)$ undergoes rapid oscillation when $J(t) \leq J_c$; however, it also comes back close to its initial value at the end of the drive: $\phi_s(T) \approx \phi_s(0)$. Since $\phi_s$ and $r_1$ satisfies an $\omega$-independent relation, $\phi_s = \xi(r_1, t)$, we infer that $\phi_s$ must remain close to its initial value for the same range of $\omega$ for which $r_1(T) \approx r_1(0)$; this is verified numerically in panel (b) of fig. 1. Finally, we note, from the panels (c) and (d) of fig. 1, that $\phi_d(t)$ is a monotonic function of $\omega$. Thus, we may define $\omega = \omega^*_m$ for which $\phi_d(T) \approx 4\pi m$ $(m$ being an integer). Together with the fact that $r_1(T) \approx r_1(0)$ and $\phi_d(T) \approx \phi_d(0)$, we find that at $\omega = \omega^*_m$, both the relative phases satisfy $\phi_2 - \phi_1 = - (\phi_0 - \phi_1) \approx 2\pi m$ leading to $|\psi_{\text{mf}}(T)| \approx |\psi_{\text{mf}}(0)|$ up to a global phase. This constitutes the dynamics freezing of $|\psi_{\text{mf}}\rangle$.

To obtain an accurate estimate of the degree of freezing and to check the validity of the discussion above, we compute the defect density $P = 1 - F = 1 - |\langle \psi_{\text{mf}}(T)|\psi_{\text{mf}}(0)\rangle|^2$ via direct numerical solution of eq. (3) keeping $n \leq 4$ states per site. The plot of $P$ as a function of $\omega$ clearly shows that $P \rightarrow 0$ at $\omega = \omega^*_m$. A plot of $\log_{10} P$ vs. $\omega$ near $\omega^*_m/J_c \approx 0.47$, shown in panel (b) of fig. 2, reveals that $\log_{10} P \sim -4$ indicating that the overlap, up to a global phase, is exact within our numerical accuracy. We have checked for all $\omega^*_m \leq 0.8 J_c$, $\log_{10} P < -4$ which indicates a near perfect freezing. We also compute the residual energy $Q(T)$ and the SF order parameter

$$ \Delta = r_1 e^{i\phi_d/2} \left(r_0 e^{-i\phi_s/2} + \sqrt{2}r_2 e^{i\phi_s/2}\right), $$

at $t = T$ as a function of $\omega$. We find from eq. (10) that $|\Delta|$ is independent of $\phi_d$. Thus $|\Delta(T)|/|\Delta(0)|$ and $Q/U$ (which can also be shown to be independent of $\phi_d$) remain close to unity and zero respectively over the entire range of $\omega/J$ for which $r_1$ and $\phi_s$ remain close to their initial values as shown in panels (c) and (d) of fig. 2. Such a behavior distinguishes these quantities from $P$ which depends on $\phi_d$ and hence vanishes at discrete $\omega_m$. Finally, we find that for all values of $J_0$ shown in panel (b) of fig. 2, there is an appreciable range of $\omega/J_c$ within which the freezing phenomenon occurs and that $\omega^*_m$ decreases monotonically as a function of $J_0$ over this range.

A physical picture of the freezing phenomenon described above can be obtained as follows. The dynamics of the bosons in the MI and the SF phases near the transition constitutes change in both the amplitudes and the relative phases of the different components of the boson wave function. We find that the change in amplitudes after a complete cycle of the drive (at $t = T$) is close to zero over a range of $\omega \leq J_c$. Our treatment of the mean-field equations above brings out the crucial fact that this also means that the change in the sum of the relative phases,
projection operator for linear dynamics in where it provides a qualitative aspect. As shown in ref. [11], this formalism allows one to describe the dynamics of bosons by solving for the Shrödinger equation for $|\psi'|$:

$$\langle \psi'| \big( i\hbar \partial_t + \delta S[f_n]-\hat{J}(t) |\psi'\rangle = H^* [J(t)] |\psi'\rangle. \quad (14)$$

Using the expression for $|\psi'|$ and $E[[f_n]]$, one can convert eq. (14) to a set of equations for $\{f_n(t)\}$ [11]. Defining $\varphi_n = \sqrt{n + \hat{f}_n} f_{n+1}$, one gets

$$i\hbar \partial_t f_n = \delta E[[f_n(t)]] - \hat{J}(t) / \delta f_n + \frac{i\hbar \partial J(t)}{\partial t} \bigg|_{\n=1} \bigg( \sqrt{n+1} f_{n+1} - \delta_n \varphi_{n+1} - \delta_{n+1} \varphi_n \bigg) + \sqrt{n+1} \bigg( \delta_n \varphi_{n+1} - \delta_{n+1} \varphi_n \bigg). \quad (15)$$

A numerical solution of eq. (15) yields $f_n(t)$ and hence $|\psi'|$ using one which one can compute $|\psi(t)| = \exp[iS|\psi'(t)|]$ perturbatively to $O(J(t)^2/U^2)$. Similarly, the expectation value of any operator $O$ at any instant $t$ can be calculated in terms of $|\psi'(t)|$:

$$\langle O \rangle = \langle \psi'(t) | e^{-iS} O e^{iS} |\psi'(t)\rangle = \langle \psi'(t) | O |\psi'(t)\rangle - \langle \psi'(t) | iS |\psi'(t)\rangle + \ldots, \quad (16)$$

where the ellipsis indicate higher-order terms in $J(t)/U$. Note that the second term in the expression originates from quantum fluctuation and modifies mean-field result (first term). Using the above-mentioned procedure detailed in ref. [11], we compute $P(T), Q(T)$ and $|\Delta(\omega)|$ as shown in fig. 3. We find that key effects of the quantum fluctuations is to change numerical values of $\omega^*_m$ and the precise range of $\omega$ over which freezing occurs; however the mean-field results hold qualitatively in the sense that $P \rightarrow 0$ for several $\omega^*_m$ with $\log_{10} P \leq -4$ for all $\omega^*_m$. Further $\omega^*_m$ also decreases monotonically with $J_0$ as shown in panel (b) of fig. 3 for $\omega^* \approx 0.6 J_0$.

Next, we consider the effect of a harmonic trap on the freezing phenomenon. For this part, we numerically

3Note that the effect of quantum fluctuations which we incorporate through the projection operator method is particularly important at the critical point and in the superfluid phase due to the lack of adiabaticity originating from the presence of gapless excitations.
solve eq. (3) for \( d = 2 \) with \( \mu_r = \mu_0 + 0.01U[(r_x - 1/2)^2 + (r_y - 1/2)^2] \), for \( N_0 = 570 \) sites (linear dimension 24) and with fixed total particle number \( N_0 \). We choose the trap parameters so that the ground state of the bosons in the center of the trap at \( t = T/2 \) is MI phase with \( \bar{n} = 1 \). The evolution of the density profile of the bosons is shown in panel (a) of fig. 4 for \( t = 0 \) (left) and \( t = T/2 \) (right). Panel (b) of fig. 4 indicates value of \( \phi_d(T) \) as a function of the position of the bosons in the trap along the line \( y = 0 \). The plot shows that for all \( \omega \leq 0.3J_c \), \( \phi_d \) evolves coherently with negligible spatial variation. The plots for \( \phi_u \) and \( r_1 \) are similar in nature; thus, we expect the boson evolution to have the same qualitative properties as that found within a homogeneous mean-field approach. A plot of \( P(\Delta(T)|\Delta_0) \) as a function of \( \log_{10}(\omega/J_c) \) in the panels (c), (d) of fig. 4 confirms this expectation. We find that the main effect of the trap is to push the freezing phenomenon to lower frequencies leaving its qualitative nature unchanged. The largest freezing frequency occurs at \( \approx 0.2J_c^2 \), which is large compared to frequencies \( \approx 0.05J_c \) where momentum-conserving boson pair production at finite momenta, which is not captured within mean-field theory, is expected to become significant [19]. Figure 4 also demonstrates that the freezing phenomenon disappears at higher drive frequencies where the trapped bosons do not evolve coherently leading to spatial variation of \( \phi_d \).

Finally, we note that the freezing phenomenon persists for multiple periods of the drive. To show this explicitly, we revert to single-site mean-field theory and plot \( P \) around a freezing frequency \( \omega_m = 0.47J_c \) for several cycles of the drive in fig. 5. The plot shows that \( P(\omega^*) \) increases with number of drive cycles; however, even after \( t = 10T \), its value remains small \( (\leq 10^{-4}) \) which indicates that the freezing persists to a good degree of accuracy for longer drive times.

Fig. 4: (Color online) (a) Plot of the boson density profile in the trap at \( t = 0 \) and \( t = T \). (b) Variation of relative phase \( \phi_d(T) \) as a function of the position (along \( y = 0 \)) in the trap displaying coherent evolution of the bosons. (c) and (d): plots of \( P \) and \( |\Delta(T)|/|\Delta_0| \) as functions of \( \omega \) displaying the freezing phenomenon at \( \omega_m \). For all plots \( J_0 = 0.04U \), \( \delta J = 0.015U \), \( J_c = 0.041U \), and \( \mu_0 = 0.415U \).

For experimental verifications of our work, we suggest interference of two bosonic condensates in the presence of an optical lattice, near the QCP which are separated after creation by a double-well potential and allowed to evolve separately for a fixed holdout time. It is well known that recombination of such separated condensates can act as a readout scheme for their relative phases [20]. We propose such a readout when one of the condensates is driven periodically with a frequency \( \omega \) during the holdout for a single period \( T = 2\pi/\omega \). Our specific prediction is that the relative phase measured for such a drive with \( \omega = \omega_m^* \) is going to match the phase without any drive indicating dynamics-induced freezing. For all such experiments one needs to estimate an optimal temperature \( T_0 \) at which they can be carried out. The typical value of \( U \) deep inside the Mott phase is \( \approx 2 \) KHz = 200 nK leading to a melting temperature of \( T_m \approx 0.2U \approx 40 \) nK for \( d = 3 \). The SF phase near the Mott tip has a coherence temperature of \( T_c \approx \pi J_c \approx 35 \) nK [21]. Thus, a temperature of a few nano-kelvins \( (T_0 \ll T_m, T_c) \), which is currently within the experimental reach, would be ideal for testing our prediction.

In conclusion, we have demonstrated that periodic dynamics of the ultracold bosons described by the Bose-Hubbard model leads to dynamics-induced freezing of the boson wave function at specific drive frequencies which are determined by the condition \( \phi_d(T) = 4\pi m \). The freezing phenomenon manifests itself at discrete drive frequencies \( \omega_m^* \leq J_c \) via the presence of dips in the defect density and can be detected by suitable interference experiments. We have shown that this effect, which can be qualitatively understood using mean-field theory, is robust against quantum fluctuations, as incorporated using a
projection operator technique, and the presence of a trap. We note that designing assisted driving protocols for near-adiabatic drives in interacting many-body systems has been the subject of a plethora of theoretical and experimental studies lately [22]. Our work provides a rare example of near-adiabatic driving without assistance in an experimentally realizable non-integrable quantum many-body system.

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4The phrase “without assistance” means in the absence of the additional Hamiltonian $H_1$ as discussed in ref. [22].