Role of trap-induced scales in non-equilibrium dynamics of strongly interacting trapped bosons

Anirban Dutta\textsuperscript{1}, Rajdeep Sensarma\textsuperscript{2} and K Sengupta\textsuperscript{1}

\textsuperscript{1} Theoretical Physics Department, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032, India
\textsuperscript{2} Department of Theoretical Physics, Tata Institute of Fundamental Research, Mumbai-400005, India

E-mail: ksengupta1@gmail.com

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Abstract

We use a time-dependent hopping expansion technique to study the non-equilibrium dynamics of strongly interacting bosons in an optical lattice in the presence of a harmonic trap characterized by a force constant $K$. We show that after a sudden quench of the hopping amplitude $J$ across the superfluid (SF)-Mott insulator (MI) transition, the SF order parameter $|\Delta_r(t)|$ and the local density fluctuation $\delta n_r(t)$ exhibit sudden decoherence beyond a trap-induced time scale $\tau_0 \sim K^{-1/2}$. We also show that after a slow linear ramp down of $J$, $|\Delta_r|$ and the boson defect density $P_r$ display a novel non-monotonic spatial profile. Both these phenomena can be explained as consequences of trap-induced time and length scales affecting the dynamics and can be tested by concrete experiments.

Keywords: strongly correlated boson, non-equilibrium dynamics, Bose–Hubbard model

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(Some figures may appear in colour only in the online journal)
direction, follow the well known collapse and revival dynamics of the homogeneous system up to a trap induced time scale \( T_0 \sim K^{-1/2} \). Beyond this timescale, the oscillations decohere suddenly. We also look at the evolution of the system through a linear ramp-down of the hopping parameter \( J(t) \) with a rate \( \tau^{-1} \). We find that at the end of slow ramps \( (\tau U \gg 1) \), both \( |\Delta_n| \) and the local defect density \( P_r \) display novel non-monotonic spatial profile as a function of \( r \), which characterizes the highly non-equilibrium state produced at the end of the ramp. We provide a semi-analytic explanation for both the \( K \) dependence of \( T_0 \) and the non-monotonic spatial profile of \( |\Delta_r| \) and \( P_r \) after the ramp in terms of trap-induced length and time scales which affect the dynamics of these systems in the presence of a confining potential, and suggest concrete experiments to test our theory.

We note that the usual methods \([10–13]\) used to study equilibrium properties of the SI transition in the BH model cannot describe its non-equilibrium dynamics beyond Gutzwiller mean-field level or truncated Wigner approximation valid for large boson occupation per site \([14–16]\) for \( d > 1 \). Some progress has been made in this direction in the absence of the trap \([17–20]\); however, they do not describe the dynamics of non-uniform systems. To the best of our knowledge, attempts to address non-equilibrium dynamics of inhomogeneous BH model beyond Gutzwiller mean-field theory do not exist for \( d > 1 \); here, we aim to fill up this gap by develop a hopping expansion technique for strongly coupled trapped bosons which treats the equilibrium and non-equilibrium properties of the system on an equal footing. The BH model in the presence of a trap is given by

\[
H = -J \sum_{\langle r \sigma \rangle} (b^\dagger_r \sigma_r + h.c.) + \sum_r \left( \frac{U}{2} \hat{n}_r \hat{n}_r - 1 \right) - \mu_r \hat{n}_r, \tag{1}
\]

where \( b_r \) annihilates a boson at lattice site \( r \) and \( \hat{n}_r = b^\dagger_r b_r \). Here, \( \mu_r = \mu_0 - K|\tau|^2/2 \) is the effective chemical potential at site \( r \), \( K \) is the force constant of the harmonic trap potential, and the central value \( \mu_0 \) controls the total density. For concreteness, we will consider nearest neighbor hopping of bosons on a square lattice. Here, and in the rest of the work, we set the lattice spacing \( a \) and Planck’s constant \( h \) to unity.

The BH hamiltonian can be divided into a local part \( H_0 \), consisting of the Hubbard repulsion and the effective chemical potential term, and the kinetic hopping term \( T \). In the strong coupling regime, a perturbation expansion in the hopping terms is obtained in the following way: Consider neighboring sites \( r \) and \( r' \) with occupation numbers \( n_r \) and \( n_{r'} = n_r - \alpha + 1 \), where \( \alpha \) is an integer. When a boson hops from \( r' \) to \( r \), the energy change \( \Delta E_{r \rightarrow r'} = \alpha U - \mu_r + \mu_{r'} \). It is thus useful to consider the hopping terms corresponding to the same \( \alpha \) together and write:

\[
T = \sum_{\langle r \sigma \rangle} T_{r \sigma} = \sum_{\langle r \sigma \rangle \alpha} (T_{r \sigma}^\alpha + T_{r' \sigma}^{\alpha\dagger})
\]

\[
T_{r \sigma}^\alpha = -J \sum_{n_r} \sqrt{(n_r + 1)(n_r + 1 - \alpha)} \, \langle n_r + 1, n_r - \alpha \rangle \times \langle n_r, n_r - \alpha + 1 \rangle. \tag{2}
\]

encodes the hoppings which change the energy of the state by \( O(\alpha U) \). For a given pair of \( r \) and \( r' \), the low energy process corresponds to \( \alpha_{r \rightarrow r'} \), for which \( \Delta E_{r \rightarrow r'}^{\alpha} < \gamma J \), where \( \gamma \) is a number \( O(1) \). The rest of the terms are taken as high energy processes to be eliminated by a canonical transformation. Note that there can be pairs of sites where all hopping processes are high energy terms, and hence there are no terms \( O(J) \) in the effective Hamiltonian between these sites. A binary variable \( \eta_{r \rightarrow r'} \), which is 1(0) if the corresponding bond has (does not have) a low energy hopping term, is used to keep track of this.

Having identified the high-energy hopping processes for which \( \alpha_{r \rightarrow r'} = \alpha_{r' \rightarrow r} \), one can now design a canonical transformation \( S \) which eliminate these processes perturbatively to obtain an effective Hamiltonian \( H_{eff} = \exp(iS)H \exp(-iS) \).

To linear order in \( J \), and noting that \( H = H_0 + T \), this requires

\[
[H_0, iS] = \sum_{\langle r \sigma \rangle \alpha} (T_{r \sigma}^\alpha + T_{r' \sigma}^{\alpha\dagger}) \tag{3}
\]

and yields

\[
iS = \sum_{\langle r \sigma \rangle \alpha} \sum_{\alpha' = \alpha} (T_{r \sigma}^{\alpha} - T_{r' \sigma}^{\alpha\dagger}) \eta_{r \rightarrow r'} \tag{4}
\]

where we have used the fact that \( \alpha_{r \rightarrow r'} = -\alpha_{r' \rightarrow r} \).

Using the above \( S \), the effective low-energy Hamiltonian \( H_{eff} \) for the trapped bosons, to \( O(\gamma^2 J^2/\tilde{U}^2) \), is

\[
H_{eff} = H_0 + \sum_{\langle r \sigma \rangle \alpha} (T_{r \sigma}^{\alpha} + T_{r' \sigma}^{\alpha\dagger}) \eta_{r \rightarrow r'} \tag{5}
\]

where the terms in the last two lines of equation \( 5 \) represents \( 2 \)nd order virtual hopping of Bosons through intermediate states having high energy (difference). We first use this formalism to look at the equilibrium ground state of the trapped system. We use a variational wavefunction ansatz for the equilibrium state:

\[
|\psi_{eq}\rangle = \exp(-iS)|\psi_{eq}^0\rangle, \quad |\psi_{eq}^0\rangle = \prod_r \sum_{n_r} f_{n_r} |n_r\rangle \tag{6}
\]

giving a Gutzwiller wavefunction, \( n_r \) is the local boson occupation number basis, and the variational Gutzwiller coefficients \( f_{n_r} \) are determined by minimizing the ground state energy

\[
E_G = \langle \psi_{eq}^0 | H | \psi_{eq}^0 \rangle = \langle \psi_{eq}^0 | H_{eff} | \psi_{eq}^0 \rangle + \mathcal{O}(\gamma^2 J^2/\tilde{U}^2). \tag{7}
\]

The details of these calculations are presented in the supplementary material (stacks.iop.org/JPhysCM/28/30LT01/mmedia).\(^3\)

We note that in our approach, the system wavefunction \( |\psi\rangle \), unlike \( |\psi_{eq}\rangle \), retains spatial correlations due to the \( \exp(iS) \) factor; thus our method includes spatial correlation in the boson

\(^3\) We use a value of \( \gamma = 2 \); we have checked that our results are insensitive to the exact choice of \( \gamma \).

\(^4\) See supplementary materials for a detailed derivation.
wavefunction beyond Gutzwiller mean-field theory. In the present work, $S$ is evaluated to $O(F^2/U^2)$ which amounts to retaining short-range spatial correlations between second nearest neighbor sites. The ground state expectation value of any operator $\mathcal{O}$ to $\mathcal{O}(F^2/U^2)$ is then given by

$$\langle \psi | \mathcal{O} | \psi \rangle = \langle \psi | e^{iSF} \mathcal{O} e^{-iSF} | \psi \rangle + C \frac{2}{3} F^2/U^2.$$

(8)

The ground state density profile for a system of $51 \times 51$ lattice sites is shown in figure 1(a). It shows the wedding cake structure with the $n_r = (N_r)$ = 2 central Mott lobe surrounded by a SF ring and then the $N_r = 1$ Mott lobe, as we go towards the edge of the trap. To make quantitative comparison between this method, Quantum Monte Carlo (QMC) [21, 22] and mean-field theory [10], we plot in figure 1(b), the local compressibility $\kappa_r = \langle \psi | \nabla^2 \psi | \psi \rangle - n_r^2$ of the system as a function of $r_0 = |r|$ with $\mu_0 = 0.37U$ for which the central Mott lobe has $n_r = 1$. The comparison shows that our method provides a more accurate match with QMC data than the mean-field theory in the MI and MI-SF transition regions.

We now describe the non-equilibrium dynamics of this system as $J$ is changed according to an arbitrary protocol $J(t)$. The Schrodinger equation is given by $i\partial_t |\psi(t)\rangle = \hat{H}[J(t)] |\psi(t)\rangle$. Following [19], we use a time-dependent $\hat{S}(J)$, i.e. $|\psi(t)\rangle = \mathcal{O}^{SF(t)} |\psi(t)\rangle$. The basic idea is to keep the fast oscillating (high energy) terms within the canonical transformation, so that $|\psi(t)\rangle$ can encode the slow motion generated by the time-dependent effective Hamiltonian $\hat{H}_d[J(t)]$ (given by equation (5) with $J \rightarrow J(t)$). The Schrodinger equation then reduces to

$$(i\partial_t + \partial S/\partial t) |\psi(t)\rangle = \hat{H}_d[J(t)] |\psi(t)\rangle.$$  

(9)

We then use a time dependent Gutzwiller ansatz $|\psi(t)\rangle = \prod_{n} \sum_{\bar{\eta}_n} f_{\eta_n}(t) |\bar{\eta}_n\rangle$ and obtain the differential equations for $f_{\eta_n}(t)^5$. We note that for $S = 1$, equation (9) reduces to standard Gutzwiller mean-field equations [14]. These are solved numerically to obtain the time dependent state $|\psi(t)\rangle^5$.

First, we concentrate on the sudden quench of $J$ from $J_1$ to $J_2$ corresponding to SF ground state at the trap center to $J = J_2$ (MI ground state at the trap center with $\bar{n} = 1$). In figure 2(a), we plot the spatio-temporal profile of the local superfluid order parameter $|\Delta_r(t)| = \langle \psi(t) | \hat{n}_r | \psi(t) \rangle$. It shows oscillations with a frequency $\sim U^{-1}$, corresponding to the coherent collapse and revival of the superfluid state in the center. Around $T_0 \sim 1/R^{1/2}$, these oscillations suddenly die out; this decoherence is not the exponential decay due to hopping, but is precipitated by a catastrophic event which immediately causes loss of coherence$^7$. A similar pattern is seen in the local density fluctuations $\delta n_r(t)$, plotted in figure 2(b). In figures 2(c) and (d), we plot the spatio-temporal profile of $|\Delta_r(t)|$ and $\delta n_r(t)$, after smearing over a time grid $\delta t \sim U^{-1}$ to clearly visualize long time-scale dynamics of the system, showing the decoherence of the oscillations. A comparison of these results with those obtained from the mean-field theory is given in the supplementary materials$^9$.

To obtain a qualitative understanding of this phenomenon, we note that the trap leads to actual mass (particle) transport with a typical velocity $v_0 \approx J_1/\hbar$ affecting the dynamics of the system [15, 16]. When a boson hops outwards from a site $r$ along the radial direction, it encounters the boundary between the SF and the $n = 0$ MI phase at $\mu_0 = 0$ or $\tau = \tau = \text{Int}(|\sqrt{2\mu_0}/K|)$. Since the latter phase is analogous to the boson vacuum, the bosons get reflected back from this boundary. When the reflected wave reaches a given point inside the boundary, it interferes with the coherent oscillation and causes it to decohere. To see this process clearly, we plot in figures 3(a) and (b), the SF order parameter $|\Delta_r(t)|$ and the time derivative of the boson density, $\bar{n}$, at the trap center as a function of time. We clearly see that the sudden decoherence of $|\Delta_r|$, coincides with an increase in $\bar{n}$. The reflection of the bosons leads to inhomogeneous boson flux at a given site leading, via continuity equation, to finite

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$^5$ See footnote 4.

$^6$ This procedure is justified as long as $z(t)/U \ll 1$ for all time and thus can be used to study the dynamics of the bosons in the SF region near the critical point.

$^7$ The emergence and decay of the coherent oscillations repeat themselves several times at a longer time scale. See supplementary materials for a more detailed discussion of this phenomenon.

$^8$ See footnote 4.
For the central trap site, we expect this to happen around $t_0 \approx 2\tau_{\text{max}}/J_f$. Our reasoning above predicts $t_0 \sim 1/\sqrt{K}$ and $t_0 \sim \sqrt{\mu_0}$, which is roughly consistent with our qualitative argument. We note that this behavior is distinct from that obtained using mean-field theory; a detailed comparison is presented in the supplementary material.

Finally, we study the effect of a linear ramp-down of the hopping $J(t) = J_f + (J_f - J) t/\tau$ in this system. We choose $J_f(0) = 0.1(0.02)U$ so that the bosons start from the SF ground state and pass through the equilibrium MI-SF transition for $r < 14$. For $14 \leq r \leq 20$ ($r > 20$), the equilibrium state of the bosons are SF ($n = 0$ MI) state throughout the dynamics. We look at the system at the end of the ramp ($t = \tau$) and study the local order parameter $|\Delta_r(\tau)|$ and the local defect density $P(\tau) = 1 - |\langle \psi_\tau(r) | \psi_\tau(0) \rangle|^2$, where $|\psi_\tau(r)\rangle$ is the ground state with $J = J_f$ and $|\psi_\tau(0)\rangle$ is the non-equilibrium state right after the ramp. As shown in figures 4(a) and (b), $|\Delta_r(\tau)|$ and $P(\tau)$ display non-monotonic spatial profiles for large $\tau$ (close to adiabatic limit); they have a maximum at $r = 0$ followed by an initial reduction and later enhancement as $r$ increases. We note that such spatial profiles have no analog for trapped bosons in equilibrium; for monotonically increasing trap profile one can use a Kibbel-Zurek type argument to estimate the deviation of the final wavefunction from the initial one [23]. Since the evolution starts from the SF phase, which has gapless excitations, the initial evolution is diabatic at least till the equilibrium critical point is reached. Beyond that, the dynamics goes into the adiabatic regime when the instantaneous Mott gap $\varepsilon(t)$ satisfies $d\varepsilon/dt \leq \varepsilon(t)^2$.

Near the trap center, we can use LDA to define a local gap, $\varepsilon_{ij}(t) = \text{Min}[E_i^f(t), E_j^0(t)]$, where $E_i^f(t) = U - \mu_r - 2zJ(t)$ and $E_j^0(t) = \mu_r - zJ(t)$ are energies of particle/hole production.

The time at which the system enters the adiabatic regime, $t_1$, can be obtained by solving $d\varepsilon(t)/dt = \varepsilon^2(t_1)$ and yields $t_1(r) = \tau|J_f - J_0(\tau)|(J_f - J_0)^{-1} + \sqrt{\tau/(J_f - J_0)}$, where $J_0(\tau) = \text{Min}[U - \mu_r, 2z_\tau \mu_r, \varepsilon_z]$ is the equilibrium critical value of $J$ (estimated to $O(K/J(U))$ at the local effective potential $\mu_r$).

However, the effect of larger time spent in the non-adiabatic regime is offset by the slower evolution due to the presence of the trap as we move outward from the trap center. To understand this, consider the Gutzwiller mean-field theory of trapped boson with $J = J(t)$. Using a minimal model of three boson states near SI transition, $n = 0, 1, 2$ per site [24], the wavefunction $\psi_{\text{MF}} = \prod_r \sum_{\psi_r} e^{i\psi_r} \psi_r(t)|n\rangle$. In this limit, $\Delta_r(t) = \Delta_{g}(t)e^{-\varepsilon_{ij}t} + \Delta_{e}(t)e^{-\varepsilon_{ij}t}e^{-U/\mu_r}t^{1/2}$, where, within a rotating wave approximation,

$$\Delta_{[2]eff}(t) = -i\langle f\rangle \sum_{(r')} |c_{1f}\rangle |A_{rr'}(t)|B_{rr'}(t)|e^{i\theta_{rr'}t}$$

Here $\theta_{rr'}$ is the chemical potential difference across the bond between $r$ and $r'$, which increases linearly with distance from the center of the trap, while the coefficients $A_{rr'} = e^{i\varepsilon_{rr'}t}$ and $B_{rr'} = e^{-i\varepsilon_{rr'}t}$.
$B_{rr} = \sqrt{2} c_1 r^2 c_2'$. It can be seen from equation (11) that for $t > t_0$, where $t_0$ is defined by $J(t_0) = \delta \mu_{rr}$, the oscillatory terms would wash out the dynamics of $|\Delta|$ (in principle leaving a slow dynamics due to higher order terms in $J/U$). As we go outward from the center of the trap, $\delta \mu_{rr}$, and consequently $J(t_0)$ increases, which reduces the time $t_0$, beyond which the slow dynamics occurs. It is easy to see numerically that $t_0 = \tau$ or $J(t_0) = J_1$ for $r \approx 9$. Beyond this point, the sites experience the slow dynamics of $\Delta(t)$ for larger and larger time as we move further outwards. It is approximately around this point that the slow nature of the evolution overcompensates for larger time spent in the impulse region and one finds an upturn of the order parameter; i.e. $|\Delta(t)|$ increases with $r$ for $8 < r < 19$. A similar behavior is seen for the defect density $P_d$.

In conclusion, we have presented a novel hopping expansion techniques which allows us to address the non-equilibrium dynamics of trapped bosons in the strong coupling regime beyond mean-field theory. We have identified a trap-induced length scale $r_{\text{max}} \sim 1/\sqrt{K}$, which acts as a reflection boundary for the dynamics of the bosons after the quench leading to a sudden decoherence of the collapse revival oscillations at $t_0 \sim K^{-1/2}$. In evolution under a slow linear ramp of $J$, we have found a novel non-monotonic spatial profile of the defect density and order parameter amplitude which is qualitatively different from its counterpart in equilibrium and can be measured easily by available experiments.

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