Quench induced Mott insulator to superfluid quantum phase transition

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Mott insulator to superfluid quenches have been used by recent experiments to generate exotic superfluid phases. While the final Hamiltonian following the sudden quench is that of a superfluid, it is not apriori clear how close the final state of the system approaches the ground state of the superfluid Hamiltonian. To understand the nature of the final state we calculate the temporal evolution of the momentum distribution following a Mott insulator to superfluid quench. Using the numerical infinite time-evolving block decimation approach and the analytical rotor model approximation we establish that the one and two dimensional Mott insulators following the quench equilibrate to thermal states with spatially short-ranged coherence peaks in the final momentum distribution and therefore are not strict superfluids. However, in three dimensions we find a divergence in the momentum distribution indicating the emergence of true superfluid order.

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Introduction Systems of ultra-cold atoms provide us with many-body systems with tunable Hamiltonians that may potentially be used to realize various quantum phases of matter. However many of the interesting phases that have been predicted require extremely low temperatures that have not been reached in experiments. One new phase of matter that has been realized in cold atomic systems is the Mott-insulator (MI) phase, which is a gapped collective phase and therefore has the special property of a low entropy-density. This low entropy density makes the MI a favorable starting point for creating other low-temperature phases of atoms. In particular, a recent set of experiments [1] uses an effective Mott phase as a starting state and suddenly ramps up the tunneling to create potentially exotic low temperature superfluid-like (SF) states with \(p\) and \(f\)-orbital symmetries that have never been realized before. While such a sudden change or quench of the Hamiltonian from an initially known state to a desired Hamiltonian is a promising way to realize new states of matter [2,3], it is not clear whether a system following the quench evolves to a state near the desired ground state phase in any sense. Since the quenching process is manifestly non-adiabatic and very far from equilibrium, it is certainly possible, perhaps even likely, that the final state has only a small overlap with the ground state of the final Hamiltonian! Measurements of the momentum density using time-of-flight imaging do indeed show that the initial uniform momentum distribution, which characterizes the MI phase, develops coherence peaks that are characteristic of the superfluid phase. However, this evolution where the momentum density bunches up into peaks instead of spreading out is counter-intuitive and suggests dissipation of energy similar to evaporative cooling that is used to create Bose-Einstein condensates (BECs). Therefore, to understand the utility of this approach to realizing new phases of ultra-cold atoms, it is necessary to understand both the origin and extent of the superfluid state that is formed following similar quenches.

A natural approach to understanding these quenches is to consider an analogous quench in the most studied and simplest phases. While the final Hamiltonian following the sudden quench is that of a superfluid, it is not apriori clear how close the final state of the system approaches the ground state of the superfluid Hamiltonian. To understand the nature of the final state we calculate the temporal evolution of the momentum distribution following a Mott insulator to superfluid quench. Using the numerical infinite time-evolving block decimation approach and the analytical rotor model approximation we establish that the one and two dimensional Mott insulators following the quench equilibrate to thermal states with spatially short-ranged coherence peaks in the final momentum distribution and therefore are not strict superfluids. However, in three dimensions we find a divergence in the momentum distribution indicating the emergence of true superfluid order.

In this letter we develop an understanding of the peak formation in momentum distribution following an MI-SF quench by calculating this distribution for bosonic atoms trapped in an \(s\)-wave optical lattice. Since the initial MI phase is completely incoherent between sites, the momentum distribution is uniform. To reach a SF state, the tunneling is instantaneously quenched to a finite value on the SF side of the ground-state phase diagram. We find that the final momentum distribution after the quench depends strongly on the dimensionality of the lattice under consideration. The simplest case is the zero-dimensional (0D) lattice, where the momentum density following the MI-SF quench continues to oscillate in time and thus does not appear to equilibrate. In contrast, the one-dimensional (1D) MI chain, whose dynamics we calculate numerically using the systematically exact infinite time-evolving block decimation (iTEBD) [13] approach yields a momentum distribution which approaches equilibrium. Furthermore, the dynamics of the momentum density qualitatively agrees with the distribution calculated from the quantum rotor model (exact in the large filling limit) [14,15] studied within the semi-classical truncated Wigner approximation (TWA) [16]. Moreover, the equilibrium momentum density estimated from iTEBD quantitatively agrees with the result from the classical rotor model. Using this fact, which we verified in 0D and one dimensions (1D), we estimate the equilibrium momentum density using the classical rotor approximation in two di-
dimensions (2D) and three dimensions (3D) following a quench, which are relevant to the recent experiments [1]. We find that such an MI-SF quench in the 2D limit leads to a classical thermal gas state with short-ranged momentum correlations (and no condensate fraction). On the other hand, an MI-SF quench in the 3D limit leads to a classical thermal distribution (defined in Eq. 3) following a quench in a 0D (2 site) Mott insulator from a MI ground state with \( n_{\text{initial}} = 0 \) to \( n_{\text{final}} = J \) at various fillings \( n \) as a function of \( J/U \). Equilibrium is assumed to be thermal. Results at large filling \( n \) agree well with the rotor value.

Quenches in the Bose Hubbard model: Ultra-cold bosonic atoms in a deep optical lattice can be described by the Bose-Hubbard model which is written as

\[
H = -\zeta \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c) + \frac{U}{2} \sum_j n_j (n_j - 1),
\]

where \( \langle i,j \rangle \) are nearest neighbor sites on the optical lattice, \( b_i^\dagger \) is the boson creation operator on site \( i \), \( n_j = b_j^\dagger b_j \) is the number operator of bosons on site \( j \) and \( U \) is the charging energy per site. The inter-site tunneling matrix element \( \zeta \) between the sites is taken to vanish in the initial state so that the system is initially in a MI ground state with \( n_j = n \) (integer) atoms per site. The momentum distribution of the bosons, that is measured by time-of-flight images, is the fourier transform of the off-diagonal density matrix \( n_{jk} = \sum_i e^{i k j} (b_i^\dagger b_j) \). When the state following the quench reaches a thermal equilibrium, the correlations can be calculated from the free energy

\[
F[\beta, \mu] = -\frac{1}{\beta} \log \text{Tr}(e^{-\beta H - \mu N})
\]

where the inverse final temperature \( \beta \) and chemical potential \( \mu \) are determined by the conserved initial energy \( \langle E \rangle = -\partial_\beta \langle F \rangle = 0 \) and \( \langle N \rangle = -\beta \partial_\mu F = n \).

0D quenches: Let us start by considering the simplest MI-SF quench of a 0D MI which has two sites connected by a bond forming a two-well Josephson junction [15]. The Hamiltonian \( H \) for such a system can be numerically diagonalized exactly to obtain both the equilibrium value and dynamics of the momentum distributions \( n_{jk} \), which we plot in Fig. 1. For convenience we focus on the “visibility” of the momentum distribution,

\[
\text{Visibility} = \frac{2(n(k=0) - n(k=\pi/a))}{(n(k=0) + n(k=\pi/a))}
\]

which is a measure of how peaked the momentum distribution is at its maximum at \( k = 0 \) compared to its minimum at \( k = \pi/a \) (a being the lattice constant of the optical lattice). The visibility following a quench in the 0D MI-SF quench (Fig. 1(a)) oscillates as has been found in previous results [4, 7] and does not equilibrate in contrast to higher dimensional MIs where we find that \( n_{jk} \) reaches the equilibrium distribution calculated from Eq. 2. Therefore it is useful to consider the results of the thermal distribution in Fig. 1(b).

Consistent with previous theoretical studies [7, 15], the results in Fig. 1 show that for reasonably large filling factors \( n \) (other than \( n = 1 \)), the time-scale for dynamics and maximum visibility attain universal values for intermediate \( J/U \) corresponding to the quantum rotor model:

\[
H_{\text{rot}} = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j) + \frac{U}{2} \sum_j \pi_j^2
\]

where \( \pi_j = -i \partial_{\phi_j} \) is the angular momentum canonically conjugate to \( \phi_j \) [14, 15] and \( J = 2n\zeta \) is the Josephson coupling. The free-energy \( F \) is approximated by replacing \( H \rightarrow H_{\text{rot}} \) in Eq. 2. At values of \( J \) comparable to the Mott-gap \( U \), the system equilibrates to a sufficiently high temperature \( \beta^{-1} \), so that the free-energy \( F \) in the classical limit [7] is a combination \( F = \frac{-\log Z_{XY}}{\beta} + \frac{\log \beta}{2\beta} \) of charge fluctuations with energy \( 1/\beta \) and phase fluctuations described the classical XY model

\[
H_{XY} = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j)
\]

where \( Z_{XY} = \int \prod_j d\phi_j e^{-\beta H_{XY}} \) is the partition function of the XY model. In this approximation, \( \beta^{-1} \) is determined by the energy conservation equation

\[
Z_{XY}^{-1} \int \prod_j d\phi_j e^{\int J \sum_{\langle j,k \rangle} \cos(\phi_j - \phi_k)} = \frac{1}{2dJ}
\]
The classical equilibrium visibility from Eq. 3 at the equilibrium phase with a true SF component. This is consistent with the high-temperature expansion for a 3D MI on a 2D lattice with periodic boundary conditions to determine the equilibrium final temperature satisfying Eq. 6. We find the equilibrium temperature $\beta^{-1} = 1.51 J$ to be larger than the Kosterlitz-Thouless temperature $\beta_{KT}^{-1} = 0.89 J$ [19]. As seen in Fig. 3, the momentum density $n_k$ at $J = 0.662$ calculated using MC shows a peak (Fig. 2b) at $k = 0$ which is 3 times higher than the 1D case and is qualitatively similar to the momentum distributions observed in experiment for $p$-wave superfluids [1]. However, the equilibrium momentum distributions of the quenched MI both in 1D and 2D remain finite and smooth around $k \sim 0$ indicating a boson correlator that is exponentially decaying in real space.

**3D Mott Insulator:** The classical rotor approximation can also be applied to the 3D case as well. In contrast to the lower dimensional MI-SF quenches, we find that in 3D, the energy density $\epsilon_{\text{final}} = -0.988$ at MI-SF transition calculated using MC [23] is slightly higher than the equilibrium value following the quench given by Eq. 6, indicating an equilibrium phase with a true SF component. This is consistent with the high-temperature expansion for a 3D MI on a

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**Fig. 2:** (a) Quantum dynamics (iTEBD) simulations of visibility for 1D system and TWA show equilibration following a quench in a MI from $J_{\text{initial}} = 0$ to $J_{\text{final}} = J$ at various fillings $n$ and $J/U$. The thermal equilibrium visibility determined from the XY model is in good agreement with the iTEBD and TWA results. (b) Time-evolution of the momentum distribution for $J = 0.5 U$ and $n = 1$ shows evolution of the momentum distribution to one that is in good agreement with the classical thermal distribution.
simple-cubic lattice which estimates the equilibrium temperature $\beta^{-1} \approx 2.10 J$ to be below the critical temperature $T_c = 2.202 J$. Since the equilibrium temperature is close to the critical temperature, we can use scaling relations around the critical point to estimate the momentum distribution and the equilibrium temperature below $T_c$. Using the scaling relations for the energy density around $\beta^{-1} \sim T_c$, we obtain the equilibrium temperature $\beta^{-1} = T_c - 0.077 J$. The momentum distribution in the vicinity of $\beta^{-1} \approx T_c$ has a universal form at small $k$ which is given by

$$F(k) \approx w(\beta)^2 [(2\pi)^3 \delta(k) + \frac{\xi_T}{k^2}] + f_0. \quad (10)$$

Since the critical fluctuation contribution to $n_k$ is only accurate near $k \sim 0$, we have added a $k$-independent background $f_0 = [1 - w(T)^2(1 + \xi_T/2\pi)]$ to restore the total spectral weight to unity. Here $w(\beta) = B \left( \frac{T_c - \beta^{-1}}{T_c} \right)^{\beta_0}$ is the condensate fraction of the system. The parameters in Eq. (10) have been calculated to be: the critical amplitude $B = 1.245$, the critical exponent $\beta_0 \approx 0.35$, the transverse correlation length $\xi_T(T) = \xi_T(0) \left( \frac{T_c - T}{T_c} \right)^{-\nu}$ with $\xi_T(0) \approx 1.65$ and $\nu \approx 0.67$. To resolve the singularity at $k \sim 0$ we have broadened the momentum distribution by a width $\sigma \approx 0.05\pi/a$. The resulting singular momentum distribution is plotted in Fig. 3 as a function of $k_x = k$, with $k_y = k_z = 0$ has a peak near $k \sim 0$ with total weight of $1 - f_0 \approx 0.3$.

The recent MI-SF quench experiments in the 3D limit, can be thought of as a 3D MI-SF quench where the initial state is the ground state of the 3D XY Hamiltonian (Eq. 5) with tunneling $\xi_T$ turned on only along $z$. This corresponds to a lower initial energy density which in turn leads to a reduced equilibrium temperature $T_c - \beta^{-1} \approx 0.16 J$ because of energy dissipated in the phase-fluctuations along $z$. This results peak near $k \sim 0$ in the momentum distribution with total weight $1 - f_0 \approx 0.6$ which is twice as large as the peak obtained from quenching from the 3D MI state.

**Conclusion:** We have calculated the formation of peaks in the momentum distribution of bosonic atoms in an optical lattice following a quench from deep in the MI phase to an SF phase within the classical XY model approximation. The classical results are in semi-quantitative agreement with exact iTEBD calculations for the 1D MI. Understanding such MI-SF quenches is particularly important in the context of recent experiments that use such quenches to reach superfluid-like states. From our calculations we find that in 1D, 2D and 3D MIs, the initially uniform momentum distribution develops a peak at momentum $k = 0$ following the quench that is qualitatively similar to the one in experimental time-of-flight images. However in 1D and 2D the resulting momentum distributions are non-singular at $k = 0$ and represent phases without long-range phase order. In contrast, we find a true condensate in the 3D MI corresponding to the recent experiments with a divergent momentum distribution at $k = 0$. One interesting way to verify our theoretical predictions is to use the recently developed quantum gas microscope technique to look directly at the time evolution of the MI to SF quenches in systems of different dimensionalities.

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