Nature of Intermediate States between Superfluid and Mott insulator for Interacting Bosons in One-dimension with a Harmonic Trapping Potential

Shijie Hu,¹ Yuchuan Wen,¹,² Xiaoqun Wang,³,¹ and Yue Yu¹

¹Institute of Theoretical Physics, CAS, Beijing 100080, China
²Interdisciplinary Center of Theoretical Studies, CAS, Beijing 100080, China
³Department of Physics, Renmin University of China, Beijing 100872, China

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Successive quantum transitions in an intermediate regime are shown to exist between the superfluid and Mott insulating states for interacting bosonic atoms in one dimension with a trapping potential. These transitions, which are caused by the interplay of the trapping potential with the competition between the kinetic energy and the interaction, reveal novel many-body effects as reflected by low-lying excitation behavior, unconventional long-range correlations and an even-odd alternating squeezing process of superfluid bosons into the Mott insulating state. These features, most likely being generic for all dimensions when a trapping potential is involved, are relevant for both experimental observations and physical interpretation of the Mott insulator transition.

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Rapid developments in ultracold atom experiments on interacting bosons¹,², fermions³,⁴, and their mixtures⁵,⁶ in recent years have greatly stimulated a full exploration of various fundamental properties of strongly correlated systems. One of the most important progress has been made with the experimental observation of the Mott insulator transition from the superfluid phase of interacting bosonic atoms in optical lattices with a harmonic trapping potential². The bosonic Mott insulator mimics the conventional Mott insulator with electron correlations, which has been challenging condensed matter physicists for several decades. It was shown theoretically that bosons are uniformly distributed and the Mott insulator transition occurs only at sufficiently strong interactions⁷,⁸,⁹,¹⁰,¹¹. In experiments²,¹²,¹³, when a trapping potential is introduced to confine ultracold atoms, a shell structure for the local density shows up with a phase separation of Mott insulating and superfluid atoms¹⁴.

Experimentally, the Mott insulating state is exhibited by the vanishing of the interference pattern and the appearance of resonances in the excitation spectrum. The Mott transition occurs when the visibility of interference pattern and its derivatives changes sharply with respect to the lattice depth. The larger quantum fluctuations in one dimension (1D) than those in 3D are shown from the Bragg spectroscopy¹⁵. Most recently, the microwave spectroscopy with atomic clock shifts which precisely measures the fluctuation of the atomic number at each site allows to identify the superfluid layers between the Mott shells¹⁴, while the formation of a distinct shell structure and its incompressibility are shown for the in-trap density distribution by spatial selective microwave transitions and spin flip collisions. Numerical simulations, while verifying the shell structure of the local density¹⁶, show additionally a kink structure of the visibility¹⁷. All these findings raise an interesting issue whether and how the critical behavior of the Mott transition of the homogenous case is affected by the trapping potential. It seems that the single critical point for the homogenous case is expanded into an intermediate regime owing to the trapping potential. In this regime, we will show that those bosons in the central superfluid region are compressed one by one into the Mott insulating plateau with increasing the interaction such that a series of successive quantum transitions take place due to the interplay of the trapping potential with the competition between the kinetic energy and interaction.

In this study, we focus on exploring the nature of the intermediate states between the perfect superfluid and Mott insulating states. For this purpose, we investigate the one-dimensional Bose-Hubbard model with a harmonic trapping potential, which can be realized properly by interacting bosons trapped in an optical lattice with one dominant recoil energy in experiments. The Hamiltonian can be generally written as¹⁷,¹⁸:

\[ \hat{H} = -t \sum_i \left( \hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i \right) + \frac{U}{2} \sum_i n_i (n_i - 1) + V_T \sum_i n_i [i - (L + 1)/2]^2 \] (1)

where the lattice spacing has been set to one, \( t \) a hopping integral set as the energy unit, \( V_T \) the strength of the trapping potential with a center at \( x_o = (L + 1)/2 \), and \( U \) the on-site interaction. Here we employ density matrix renormalization group (DMRG) method¹⁸,¹³,²⁰ which has proved very successful for studying several kinds of physical properties in quasi-1D strongly correlated systems. For the present system, we modify the finite-size algorithm in order to obtain a given accuracy for low-lying energy states and recover the spatial inversion symmetry with the trapping potential under open boundary conditions. The sweeping is conducted from

\[ \sum_{\mathbf{r}} \hat{c}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}} \]
the middle to the two ends gradually rather than immediately and the convergence is reached for each sweeping length $l \in [4, L]$ and three lowest eigenstates are targeted simultaneously. Accuracies were examined for different sizes $L$, bare states per site $n_s$, the number of states kept in the blocks $m$, and the total number of bosons $N$ and $U$. We found that $n_s = 8$ and $m = 100$ are sufficiently large for $U \in [4, 14]$, whereas $n_s = 32$ and $m = 400$ are necessary for $U < 4$ so that systematic errors due to truncations could be smaller than the symbol size (see below). While systematic studies were made for several properties with $N \in [20, 70]$, novel effects in a crossover regime explicitly show up when $N \geq 50$ at $V_T = 0.01$. In the following, our discussions focus on results for $N = 60$ with $V_T = 0.01$, for which $L = 80$ is long enough to remove the boundary effects.

Let us first discuss the low energy properties. For the homogenous case, it is well-known that the Mott transition from the superfluid phase takes place at $U_c = 3.61 \pm 0.13$ and a gap opens monotonically with respect to $U$ in the Mott insulator phase. Fig. 1 shows gaps $\Delta_{1,2} = E_{1,2} - E_0$ for the two lowest excitations at $V_T = 0.01$ with $E_{0,1,2}$ being the three lowest energies. The phase diagram of the ground state now consists of three parts instead of two for $V_T = 0$. The first part is a weak coupling regime for $U < U_w$ including $U = 0$ with $U_w \approx U_c$. In this regime (see inset), $\Delta_1$ slowly decreases until the emergence of oscillation at $U = U_w$, while $\Delta_2$ behaves similarly except for a sharper change around $U = 0$. Since one has $N = 60$ harmonic oscillators with the center at $x_c$ for $U = 0$, all low-energy properties can also be obtained from numerical exact diagonalization and perturbation calculations for small-$U$. The peaks and dips for sawtooth result from the level crossing. With further increasing of $U$, the ground state becomes degenerate for those small intervals of subpeaks, while $E_2$ can be equal to either $E_1$ or higher excitation energies in the intervals of main peaks. The dips indicate successive quantum transitions in the ground state. One has two kinds of excitations for two sides of each sawtooth (for both main and sub peaks). The left excitation is given by creating one double occupancy from the ground state, while the right one corresponds to the destruction of a double occupancy. Furthermore, the large-$U$ regime, the third part with $U > U_s$, is characterized by a unique ground state and is related to the fixed point of the large-$U$ limit. At this fixed point, $E_0$ is simply determined from the trapping potential and the local density $n_i$, since no double occupancy is allowed and $n_i$ is simply divided into an inner part of $n_i = 1$, an outer part of $n_i = 0$ and an interventional part with $n_i < 1$. One therefore can consider this regime corresponding to the Mott insulator phase of $V_T = 0$. In the large-$U$ regime, two lowest excitations are degenerate. Due to the level crossing at $U = 12.75$, however, one has $\Delta_{1,2} = U - 12.12 + O(1/U^2)$ at first and then a $\Delta_{1,2}(= 0.597)$ almost independent of $U$. The excitations are generated by creating a double occupancy from the ground state for $12.75 \geq U > U_s$ and modifying the interventional part of the configuration of the ground state for $U > 12.75$. In addition, we have checked the low-energy behavior for odd and sufficiently large $N$, e.g. $N = 59$ and found essentially the same features for $U < U_s$ but a two-fold degenerate ground state for $U \geq U_s$. The degeneracy can be understood from the even-odd effect of the number of bosons in the large-$U$ limit.

In the second part, an intermediate regime with $U_w < U < U_s$ where $U_w = 12.12$, $\Delta_{1,2}$ vary smoothly at first and then behave as sawtooth with the emergence of the first subpeak. This behavior might be a consequence of the competition between the confining potential and the interaction. The peaks and dips for sawtooth result from the level crossing. With further increasing of $U$, the ground state becomes degenerate for those small intervals of subpeaks, while $E_2$ can be equal to either $E_1$ or higher excitation energies in the intervals of main peaks. The dips indicate successive quantum transitions in the ground state. One has two kinds of excitations for two sides of each sawtooth (for both main and sub peaks). The left excitation is given by creating one double occupancy from the ground state, while the right one corresponds to the destruction of a double occupancy. Furthermore, the large-$U$ regime, the third part with $U > U_s$, is characterized by a unique ground state and is related to the fixed point of the large-$U$ limit. At this fixed point, $E_0$ is simply determined from the trapping potential and the local density $n_i$, since no double occupancy is allowed and $n_i$ is simply divided into an inner part of $n_i = 1$, an outer part of $n_i = 0$ and an interventional part with $n_i < 1$. One therefore can consider this regime corresponding to the Mott insulator phase of $V_T = 0$. In the large-$U$ regime, two lowest excitations are degenerate. Due to the level crossing at $U = 12.75$, however, one has $\Delta_{1,2} = U - 12.12 + O(1/U^2)$ at first and then a $\Delta_{1,2}(= 0.597)$ almost independent of $U$. The excitations are generated by creating a double occupancy from the ground state for $12.75 \geq U > U_s$ and modifying the interventional part of the configuration of the ground state for $U > 12.75$. In addition, we have checked the low-energy behavior for odd and sufficiently large $N$, e.g. $N = 59$ and found essentially the same features for $U < U_s$ but a two-fold degenerate ground state for $U \geq U_s$. The degeneracy can be understood from the even-odd effect of the number of bosons in the large-$U$ limit.

![FIG. 1](color online). Energy gaps $\Delta_{1,2}$ for the two lowest excitations relative to the ground state. A large-$U$ regime for $U \geq 12.12$. Inset: for $U \in [0, 4]$ at the same scale.

![FIG. 2](color online). The profile of $n_i$ versus $U$ and $i$. A staircase structure develops with increasing $U$ and the upper part with $n_i > 1$ is eventually suppressed into a Mott plateau with $n_i = 1$, i.e. a green interface.

To interpret the above results, we show in Fig. 2 for $U \in [4, 14]$ how the profile of $n_i$ changes from a nearly global bell-shape at $U = 4$ into a complete plateau (green interface) that characterizes a Mott insulator with $n_i = 1$. 

![FIG. 2](color online). The profile of $n_i$ versus $U$ and $i$. A staircase structure develops with increasing $U$ and the upper part with $n_i > 1$ is eventually suppressed into a Mott plateau with $n_i = 1$, i.e. a green interface.
for both $i \in (18, 63)$ and the large-$U$ regime. While the upper part (with red and yellow colors) of the bell-shape with $n_i > 1$ gradually squeezes, a Mott plateau (green) grows from two flanks of $n_i$ horizontally at the height $n_i = 1$ in the intermediate-$U$ regime. We found very surprisingly that the squeezing is discontinuous for sufficiently large $U$ with accompanying staircase structure for $n_i$. Each staircase involves regularly an oscillation with respect to $i$ but has different numbers of peaks. One can clearly see that the last three staircases have one, two and three peaks, respectively. We note that when $U$ is increased, $n_i$ is first reluctant to squeeze by forming a bundle and then suddenly changes into its next bundle with one less peak at a critical value of $U$; The area of the upper part for each $U$ is found precisely equal to the number of bosons involved in the upper part and the area between two-successive bundles is one within 5 digits accuracy. It turns out that each peak essentially reflects the contribution of one extra boson to the central superfluid region. Therefore we can conclude that the superfluid bosons are squeezed one by one into the Mott plateau in the two flanks of $n_i$ when $U$ is increased.

To further elucidate the intrinsic physics for the squeezing process, we analyzed the contributions from different number occupancies to $n_i$ for each site $i$, i.e. $n_i = \sum_\alpha n_i^\alpha$ where $\alpha = s, d, t$, etc. $n_i^s$, $n_i^d$ and $n_i^t$ denote single and double, triple occupancies of bosons at site $i$, respectively. $n_i^\alpha$ can be obtained directly from the eigenvalues of the reduced density matrix $\rho_i$ at $i$. For $U \in [4, 14]$, we found that $n_i^s$ and $n_i^d$ are larger than the rest by two orders of magnitude at least. Figure 3 shows $n_i^s$ and $n_i^d$ only with $U \in [7.6, 14]$ for clearness. One can see that an oscillating structure similar to $n_i$ occurs for both $n_i^s$ and $n_i^d$, but valleys in $n_i^s$ correspond to peaks in $n_i^d$ one by one. This implies the correlation between the single and double occupancies. Moreover, since the quantum fluctuation is not fully eliminated until the size of the Mott plateau $\xi_M$ is sufficiently large, one has $n_i^s = 1 - \delta(\xi_M) < 1$ and $n_i^d = \delta(\xi_M)$ for the large-$U$ regime and $i \in (18, 63)$, although all superfluid bosons in this regime are squeezed such that $n_i = 1$ precisely. For $U \lesssim 12.12$ and the curves with the same number of peaks, we found that the area between $n_i^d$ and $\delta(\xi_M)$ in Fig. 3(a) is twice of the corresponding area in Fig. 3(b) between $1 - \delta(\xi_M)$ and $n_i^s$ such that the area between $n_i$ and the Mott plateau precisely equals to the number of superfluid bosons. This reveals that the superfluid bosons have phase coherence in a “quantized” way one by one when $U$ is increased.

Figure 4 shows, for the intermediate and large-$U$ regimes, the average double occupancy $n_i^d$, the visibility $\mathcal{V}$, and the maximum value $S_{\text{max}}$ and the full-wide half-maximum(FWHM) for the momentum distribution, which were used to study the Mott insulator transition [17]. In the large-$U$ regime, $n_i^d$ and $S_{\text{max}}$ change much slower than $\mathcal{V}$ and FWHM. When $U$ is sufficiently large in the intermediate regime, a series of staircases develop for all four quantities as those shown similarly for $n_i$ in Fig. 2. One can easily see that long and short staircases show up alternatively and correspond to even and odd number of superfluid bosons in the central region of $n_i$, respectively. Comparing this to Fig. 1 one can also see that the shorter staircases correspond to those degenerate ground states with smaller intervals. The longer red and shorter green staircases in Fig. 4 correspond to the red and green curves in Fig. 3 as well as the last main and sub-peaks in Fig. 1. In fact, once the Mott plateau of $n_i$ emerges at $n_i = 1$ in the squeezing process, the number of bosons involved in the intervenient as well as inner parts is even and is no longer changed. It turns out that squeezing one superfluid boson enlarges the size of the Mott plateau by one. This implies that the degeneracy of the ground state, i.e.
the alternating nature, depends crucially on whether the number of superfluid bosons is even or odd. Moreover, when the ground state is non-degenerate, it would evoke larger quantum fluctuation to squeeze a superfluid boson into the Mott plateau since a two-fold degenerate ground state is subsequently generated. Therefore, the alternating nature reflects different quantum fluctuations in the squeezing process and a quantum transition in the ground state occurs at the edge of each staircase.

Finally, we turn to the one-body correlation functions $\rho_{i,j}^{\pm}$ for various $j$ with $i \in [1, 80]$. Black, red, green and blue curves are for $j = i$, 15, 22, and 39, respectively. (a)-(c) and (e) for the even parity ground state, but (d) with the odd-parity.

FIG. 5: (color online). One-body correlation functions $\rho_{i,j}^{\pm}$ for various $j$ with $i \in [1, 80]$. Black, red, green and blue curves are for $j = i$, 15, 22, and 39, respectively. (a)-(c) and (e) for the even parity ground state, but (d) with the odd-parity.

In summary, we have shown that a series of successive quantum transitions exist in the intermediate regime between the superfluid and Mott insulator phases for interacting bosons in one-dimensional optical lattice with a harmonic trapping potential. Those transitions reflect the quantized squeezing process of the interacting bosons into the Mott insulator phase, revealing novel many-body effects resulting from the interplay of the trapping potential with the competition between the kinetic energy and the many-body interaction. These induced effects are relevant for the interpretation of the Mott transition to the trapped atomic systems in all dimensions, in principle, since the trapping potential introduces an independent additional physical parameter, calling for further experimental explorations.

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