Quantized squeezing and even–odd asymmetry of trapped bosons

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We investigate the exact nature of the superfluid–to–Mott–insulator crossover for interacting bosons on an optical lattice in a one–dimensional, harmonic trap by high–precision density–matrix renormalization–group calculations. The results reveal an intermediate regime characterized by a cascade of microscopic steps. These arise as a consequence of individual boson “squeezing” events and display an even–odd alternation dependent on the trap symmetry. We discuss the experimental observation of this behavior, which is generic in an external trapping potential.

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The recent rapid developments in ultra–cold–atom experiments for both bosons and fermions have greatly stimulated the fuller exploration of a number of fundamental properties of strongly correlated systems [1]. One of the most important phenomena to be observed and characterized is the transition from a superfluid to a Mott–insulator phase displayed by interacting bosonic atoms in optical lattices [2]. The Bose–Hubbard model [3] shares a number of the properties of the Hubbard model for correlated electrons, whose properties, including superconductivity and Mott–insulating behavior, have challenged condensed matter physicists for half a century. This model can be realized in one, two, and three dimensions on an optical lattice [4], with the enormous advantage over electronic solids that the ratio between kinetic and interaction parameters of the particles is in principle continuously tunable.

In experiments, a trapping potential is required to confine the atoms. It was shown both theoretically [5] and experimentally [2] [6] [7] that the pure Mott–insulating phase, where the boson distribution is uniform despite the trap profile, is obtained only very at high interaction strengths. Otherwise, a spatial “shell structure” of the local density is found [1] [8] [9], with Mott–insulating and superfluid regions present simultaneously in regions of different trap depth. Extensive studies of this behavior include a demonstrated compression of the superfluid region as the Mott–insulator is approached [10] and quantitative calculations both of the shell structure [11] [12] and of accompanying features in the visibility [13].

Here we show that the nature of the Mott transition in a trapping potential is considerably more complex than recognized previously: “superfluid” bosons are expelled one by one into the Mott–insulating regions with increasing interaction strength. The intermediate regime where this sequence of microscopic quantum transitions takes place is the necessary consequence of the additional energy scale introduced by the trap, and the resulting physics is qualitatively different from the infinite system.

To explore the nature of the states intermediate between the perfect superfluid and the Mott insulator in a trap, we consider the one–dimensional (1D) Bose–Hubbard model with a harmonic trapping potential. This system is realized experimentally for a cloud of interacting bosons loaded in an optical lattice with one dominant recoil energy. The Hamiltonian is expressed [3] [4] as

\[
\hat{H} = -t \sum_{i=1,L} \left( \hat{a}_{i+1}^{\dagger} \hat{a}_{i} + \hat{a}_{i}^{\dagger} \hat{a}_{i+1} \right) + \frac{1}{2} U \sum_{i=1,L} \hat{n}_{i} (\hat{n}_{i} - 1) + V_{T} \sum_{i=1,L} \hat{n}_{i} \left[ (L + 1)/2 \right]^{2},
\]

where the lattice spacing is set to 1 and the on–site interaction \( U \) and (bond–centered) trapping potential \( V_{T} \) are measured in units of the hopping integral \( t \). We apply the density–matrix renormalization–group (DMRG) technique [14], using a specially modified finite–system algorithm optimized for the accuracy of the low–lying energy states. An appropriate sweeping procedure is essential to guarantee convergence in this delicate problem [15]. Sweeping is conducted gradually from the middle to the two ends, convergence is obtained for each sweeping length \( l \in [4, L] \), and the three lowest eigenstates are targeted simultaneously. Extremely high accuracies are required to allocate reliably the symmetries of degenerate states, and these were examined [16] for different system sizes \( L \), numbers \( n \) of bare states per site, and numbers \( m \) of states retained per block, for each total boson number \( N \) and interaction \( U \). Working up to \( n = 32 \) and \( m = 1200 \), we found that \( n = 8 \) and \( m = 100 \) are sufficiently large for \( U \in [4, 14] \) to ensure truncation errors smaller than the symbol sizes in the figures below, while \( n = 32 \) and \( m = 400 \) are necessary for \( U < 4 \).

Systematic studies were performed for systems with \( 20 \leq N \leq 70 \) bosons in a trap with \( V_{T} = 0.01 \), for which \( L = 80 \) is sufficient to remove any boundary effects. The unconventional properties of the intermediate regime begin at \( N = 40 \) and become progressively clearer with increasing \( N \) until a higher Mott plateau is reached. We have performed many calculations to amplify the current results [16], but this parameter and filling regime, shown in Fig. 1, ensures a minimal system reflecting all of the

\[ N = 40, \quad l = 40, \quad m = 400, \quad U = 20, \quad V_{T} = 0.01. \]
FIG. 1: (color online). Results for $V_T = 0.01, t = 1$, and system length $L = 80$ for $N = 30, 40, 50$, and 60 particles. (a) Density profiles $n_i$ as functions of $U$. (b) Energy gaps $\Delta_{1,2}$; inset: $\Delta_{1,2}$ for low $U$. (c) Visibility $\nu$ (left axis) and peak width $w$ (right).

Qualitative physics. We focus only on the ground state and not on the nature of the excitations [16]; however, because $U$–induced changes in the ground state appear as (avoided) level–crossings, it is instructive to consider the lowest three energy levels, $E_{0,1,2}$, represented in Fig. 1 by the gaps $\Delta_{1,2} = E_{1,2} - E_0$. We stress again that this is a finite system, both theoretically and in experiment: we provide numerically exact results for the intrinsic physics of this system, and there are no “finite–size effects” in the conventional sense of approximations to a thermodynamic limit. We also calculate the particle numbers $(n_i^{s,d,t})$ for single, double, and triple occupation, the visibility $\nu$, and the peak height $S_{\text{max}}$ and width $w$ (taken as the full width at half the sum of the maximum and minimum values) of the momentum distribution function. The measurable physical quantities $\nu$ and $w$ illustrate most clearly the effects we consider here.

Figure 1 shows three clear regimes. At low $U$ is the bell–shaped distribution of a “superfluid” (SF) system, which has strong visibility and a trap–related gap above the ground–state condensate. At high $U$ is the flat distribution ($n_i = 1$), despite the energy cost of the trap at the edges, of a pure “Mott insulator” (MI) regime, with falling visibility and gaps of order $t$ to states at the edges. Between these two limits is a complex intermediate phase characterized by oscillating and vanishing energy gaps, step–like changes in the particle distribution and the visibility, and a spatial “shell structure” with MI plateaus around a central SF region. Note that we use the abbreviations SF and MI to refer not to the bulk phases but respectively to the local regions of the distribution shown by the red–yellow curve and by the green plateaus. The almost constant shape of the blue “tails” in $n_i$ at the system edges is dictated not by $U$ but by $V_T$.

For the homogenous Bose–Hubbard model, the Mott transition occurs at $U_c = 3.61 \pm 0.13$ [3]. In a trap, there is little evidence of the energy scale $U_c$, although it corresponds loosely to the onset of oscillations in $\Delta_{1,2}$ and in $n_i$. It is easy to deduce that a pure MI phase is established only when the energy cost $U$ of the last boson in the central SF region exceeds that of placing it at the edge. One effective description of this process is to write $U_{c2} - \alpha(1)t \simeq \frac{1}{4}V_T(N - \delta)^2$, where $\alpha(1) \sim 4$ [10] represents a kinetic–energy contribution due to the last boson and $\delta \sim 6$ [Fig. 2(b)] represents the edge effects at lowest order. Both $\alpha$ and $\delta$ are corrections to a leading quadratic dependence of $U_{c2}$ on $N$, arising directly from the harmonic trapping potential, which makes the width in $U$ of the intermediate regime very significant. This illustrates directly how $V_T$ acts as an additional energy scale, which is responsible for the presence of the additional, intermediate regime. Clearly, if $V_T = 0$ the atoms are no longer trapped, or their density controlled: the trap ($V_T$) is a non–perturbative term in $\hat{H}$ [1], ensuring that any ensemble of trapped atoms is generically in a different class from the homogeneous, infinite system.

As shown in Fig. 1, the width in $U$ of the intermediate regime indeed increases strongly with $N$. The oscillations in $\Delta_{1,2}$ and $n_i$ grow with $U$ until level–crossings and steps appear (we refer to “plateaus” in $i$ and “steps” in $U$). In this cascade of steps, $\Delta_1$ vanishes over short but finite ranges of $U$, indicating the double degeneracy of the ground state when the two MI plateaus contain an odd number of particles. Each level–crossing represents a squeezing process where one particle is ejected from the central SF region and placed on the outer edge of one or other plateau: these processes are quantized. The locations and number of these crossings, which correspond
directly to jumps in $n_i^d$, $\nu$, and $w$ as functions of $U$, are not universal and nor are their spacings identical: the examples in Fig. 1 favor even numbers of particles in the central SF region (“even–odd effect”). We note that such series of discrete, single–particle transitions are present in Monte Carlo simulations performed for a harmonic trap with $n = 1$ and $n = 2$ MI plateaus [13] and in DMRG calculations for a double–well trap [17]; however, neither set of authors appeared to recognize their significance as quantized squeezing, or noticed an even–odd effect.

Additional insight into the squeezing process can be found in Figs. 2(a) and (b), which show the evolution with $U$ of $n_i$ across the intermediate regime for $N = 60$ (right panels of Fig. 1). While $n_i^d$ and higher site occupations are always negligible, $n_i^s$ and $n_i^d$ are perfectly anticorrelated. A key qualitative point must be made here: although $n_i = 1$ in the MI plateaus, this is not due to perfect single–site occupation (because $n_i^s \neq 1$), and the finite constant $n_i^d$ reflects the complete coherence of the many–body wave function mediated by continuous kinetic processes coupling the central SF to the edges through the MI regions. In spite of this system–wide coherence, $n_i$ does not evolve continuously, but instead undergoes 9 abrupt changes across the intermediate regime [Figs. 2(a) and (b)] as $U$ acts to squeeze the initial 9 bosons in the central SF region successively down to zero. The areas represent the exact boson numbers, giving complete quantitative information on the spatial extent and the structure of the central SF part of the wave function, the number of weak maxima for 2, 3, … particles reflecting the boson phase coherence.

Returning to the quantitative information in Fig. 1(b), and to the question of a “phase diagram” for the finite system of trapped bosons, we define the onset $U_{c1}$ of an intermediate phase, which corresponds to the appearance of two true MI plateaus as opposed to flattening shoulders, from the first level–crossing. Proceeding as above, $U_{c1} = \alpha(N_{\text{max}} + 1)t \simeq (N - \delta - N_{\text{max}})^2$, where $N_{\text{max}}$ is the number of bosons accommodated in the central SF region at $U_{c1}$ and $\alpha(N_{\text{max}} + 1)t$ represents the kinetic energy of the squeezed boson. The leading dependence of the width of the intermediate regime is then $U_{c2} - U_{c1} \sim \frac{1}{2}V_T N N_{\text{max}}$, as shown schematically in Fig. 2(c). This type of “canonical phase diagram,” or ‘state diagram’ [11], is appropriate for cold–atom experiments where a fixed number of particles is loaded and the optical lattice tuned adiabatically. Figure 2(c) also shows that no MI can be formed if $N$ is too low ($N < N_m$), while for $N$ sufficiently large, higher plateaus will appear. Although the functional forms and relative positions of the phase boundaries can be changed by altering the trap shape, this is the generic state diagram of any ensemble of bosons whose spatial distribution is contained by a finite external potential.

A further essential qualitative feature of single–boson squeezing is its even–odd asymmetry. Figure 1 shows even boson numbers $N$ in a bond–centered (“even”) trap, where the steps of even boson occupation in the central SF region are wider (more stable) than the odd ones. However, if $N$ is odd, the situation is exactly reversed, and the odd–occupation SF steps are wider [16]. To investigate this effect systematically, we move the trap midpoint continuously from the bond–centered position to a site–centered one (“odd trap”). Again the situation is reversed in the site–centered limit (offset 0.5), with odd steps more stable [Fig. 3(b)] for even $N$. This suggests a very straightforward interpretation: as $U$ is increased, two states, with the squeezed boson at one side of the system or the other, simultaneously become more favorable than the states at the center. This picture is exact in the $t \rightarrow 0$ limit, where it is clear analytically that bosons are squeezed out of the central SF region in pairs, while the effect of a finite kinetic–energy term $t$ is to stabilize a narrow (in $U$) step of the intermediate, symmetry–disfavored boson number. Whether even or odd steps are favored is a simple consequence of the trap symmetry and filling. The confirmation that for spinless bosons there are no special, pairwise correlation effects
in the SF or MI regions is obtained by following the evolution of the asymmetry with the trap offset: specifically, there is no even–odd effect at all for offset 0.25 [Fig. 3(a)], confirming its origin in the trapping potential.

Having understood the physics of quantized squeezing, it is possible to comment on its manifestations in a less minimal context. The same squeezing effect clearly operates with more bosons in the trap, within and between more complex shell structures of higher MI plateaus. We also find an even–odd effect when squeezing bosons from offset 0.02 [Fig. 3(a)], and not only to the system edge (the MI region). This would generate a completely separate mechanism for the tendency of particles to move from SF to MI regimes in groups rather than singly.

We close by discussing how quantized squeezing and even–odd asymmetries would be observed in experiment, restricting our considerations to 1D. Experimental measurements on optical lattices are performed by varying the lattice depth $V_0$ in units of the recoil energy $E_r$. Following the calculations of Ref. [7], we have taken $t/E_r = 1.43(V_0/E_r)^{0.98} \exp[-2.07\sqrt{V_0/E_r}]$, $U/E_r = 0.0386(V_0/E_r)^{0.88}$, and $V_r/E_r = (5.332 + 3.427V_0/E_r) \times 10^{-5}$. Clearly, varying $V_0/E_r$ explores one curve in the 2D space of the parameters $U$ and $V_0$.

In summary, we show that there exists a regime intermediate between the pure superfluid and the Mott–insulator phase for interacting bosons in a one–dimensional optical lattice with a harmonic trapping potential. We have investigated the sequence of microscopic quantum transitions across this regime. These processes reflect the quantized squeezing of bosons into the Mott–insulator region, and occur as discrete events despite the overall coherence of the many–body wave function. The even–odd asymmetry of the squeezing phenomenon is a direct consequence of the trap symmetry. The “phase diagram” of the trapped system is intrinsically, qualitatively different from the infinite system, the intermediate regime being the necessary consequence of the additional energy scale introduced by the trap. The effects revealed by detailed studies of this sort mandate a broader interpretation of the “Mott transition” in cold–atom systems.

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