Mott Domains of Bosons Confined on Optical Lattices

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In the absence of a confining potential, the boson-Hubbard model exhibits a superfluid to Mott insulator quantum phase transition at *commensurate* fillings and strong coupling. We use quantum Monte Carlo simulations to study the ground state of the one-dimensional bosonic Hubbard model in a trap. Some, but not all, aspects of the Mott insulating phase persist. Mott behavior occurs for a continuous range of *incommensurate* fillings, very different from the unconfined case, and the establishment of the Mott phase does not proceed via a traditional quantum phase transition. These results have important implications for interpreting experiments on ultracold atoms on optical lattices.

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A considerable amount of work has been done in the last decade to determine the ground state phase diagram of correlated bosons on a lattice described by the ''boson-Hubbard'' Hamiltonian [1–5]. On-site repulsion can produce a Mott insulating phase at commensurate fillings, with a quantum phase transition to a superfluid as the density is shifted or the interaction strength weakened. Longer range interactions can cause charge density wave, stripe, or even supersolid order [6,7]. Extensions to disordered systems have allowed the detailed study of the interplay of randomness and interactions in quantum systems [8].

Recently, the trapping of atoms on optical lattices has given another experimental realization of these bosonic phases. However, the quadratic confining potential, present in addition to the regular ''lattice'' potential, leads to a number of fundamentally new, and open, issues: (i) Does the confining potential preclude the formation of Mott regions by providing a continuous, unbounded, distribution of local site energies? (ii) If an insulating phase still exists, how is it characterized? (iii) What are the quantitative values of the trap curvature and interaction strength that support Mott phases? These questions are largely unaddressed in the literature.

In this paper we report the first quantum Monte Carlo (QMC) simulation of the one-dimensional boson-Hubbard model in a confining quadratic potential and provide a quantitative map of the state diagram. To our knowledge, the only non-mean-field work on this problem [9] is on very small systems (five particles). We find that the trap changes the physics fundamentally from that found in earlier simulations [2] and subsequent analytic [5] studies. For example, the vanishing of the global compressibility, discussed at length in [1,2] and reported in recent mean-field studies of the boson-Hubbard model in the context of optical lattices [10], but which ignores the confining potential, is absent. Other recent papers [9–13] on bosons in optical traps have likewise emphasized similarities to the physics in the absence of a confining potential, and have used values of the unconfined lattice critical coupling to compare with experimental data.

We find the inhomogeneous potential resulting from the confining trap is a crucial feature in discussing Mott regions at incommensurate fillings [11], and the physics of bosons on optical lattices generally. The Mott insulating regions exist above a threshold interaction strength, even without the commensurate filling required in the nonconfined case. This is a consequence of the inhomogeneous distribution of boson densities which allows extended Mott domains with, for example, one particle per site to coexist with regions of other density and is a unique feature which distinguishes the behavior of the confined model. Similarly, the global compressibility is nonzero for all densities, including commensurate ones. The different regimes of the state diagram can be characterized by the topology of the density and local compressibility profiles.

Therefore, in this context, the (global) density, ρ, defined as the total number of particles divided by the system size, loses its meaning since the particles are not uniformly distributed and the "system size" itself is ill-defined. Adding particles can push bosons deeper into the confining potential at the edges of the system, thus changing the "size."

We review briefly the properties of the ground state of the d-dimensional nonconfined boson-Hubbard model. This model has two phases, a Mott insulator at commensurate fillings and sufficiently strong interactions, as well as a superfluid elsewhere [1,2]. The critical behavior is of two types: mean field for transitions induced by tuning the density and of the $(d + 1)$ dimensional XY universality class when the interaction strength is swept at fixed commensurate filling. One of the key new results of this paper is that this special status of commensurate filling is *lost* in the case of a confining potential since commensuration is well defined only locally.

We study the Hamiltonian

$$H = -t\sum_i(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + V_0\sum_i n_i(n_i - 1) + V_c\sum_i(i - L/2)^2\, n_i, \tag{1}$$

at zero temperature. Here t measures the boson kinetic energy, V_0 the on-site repulsion, V_c the curvature of the quadratic confining potential, and L the number of sites. In the presence of the trap, the value of L should be chosen such that for the given trap curvature, the bosons do not see the edge of the system and therefore do not leak out. Our simulations were done with the world-line quantum Monte Carlo algorithm in the canonical ensemble [2,14]. The chemical potential $\mu = \partial E/\partial N$ is obtained by differentiating numerically the energy with respect to the particle number [15]. In the presence of a confining potential, it is important to measure the local density of bosons, $n_i = \langle a_i^\dagger a_i\rangle$, as well as the local compressibility, $\kappa_i = \partial n_i/\partial \mu_i = \beta[\langle n_i^2\rangle - \langle n_i\rangle^2]$.

Figure 1 shows the evolution of the local boson density with increasing total occupancy of the lattice. At low fillings the density profile is smooth, with an inverted parabolic shape reflecting the confining potential. Above a critical filling of about 30 bosons (for this choice of V_0 and V_c) a plateau with a local filling of one boson per site develops in the density profile which is analogous to the Mott structure of N vs μ in the unconfined model. This plateau indicates the presence of an incompressible, insulating region where κ_i, as defined above, drops to a small but finite value (Fig. 2) which vanishes for $V_0 \to \infty$. Here this behavior of κ_i will be taken as the signal for a Mott region. As the density is increased further, the plateau widens spatially. But when the energy cost of extending the plateau to increasingly large values of the confining potential becomes prohibitive, the occupancy begins to exceed one at the center of the lattice, indicating a breakdown of Mott behavior there, but *not* everywhere.

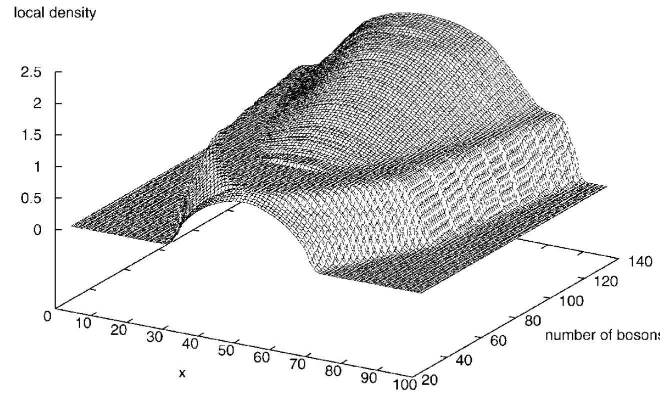

FIG. 1. The evolution of the local density n_i as a function of position x and increasing the total number of bosons. The trap curvature is $V_c = 0.008$, $L = 100$, and the onsite repulsion is $V_0 = 4$. At low fillings the system is in a superfluid phase. Mott insulating behavior appears as the density is increased, but then at yet larger fillings a superfluid begins to form at the center of the insulating region.

Increasing the filling further, for example, $N_b = 116$, eventually produces a second Mott region in the center of the system with a local filling of two bosons per site without destroying totally the first Mott region. Four slices from Fig. 1 are shown in Fig. 2 along with the local compressibilities. It is clear that at higher boson numbers, richer structures where the local compressibility vanishes at several locally commensurate densities can occur. Mean-field work in two dimensions [9] shows a similar coexistence of Mott and superfluid regions.

A central feature of the Mott phase transition of the unconfined boson-Hubbard model is global incompressibility: A charge gap opens up, i.e., the density gets "stuck" at $\rho =$ integer for a range of chemical potentials μ. One might, then, crudely interpret the spatial dependence of the local density in the confined case, Fig. 2, as rather analogous to the chemical potential dependence in the unconfined case [9]. This assumption and the ρ versus μ curve in

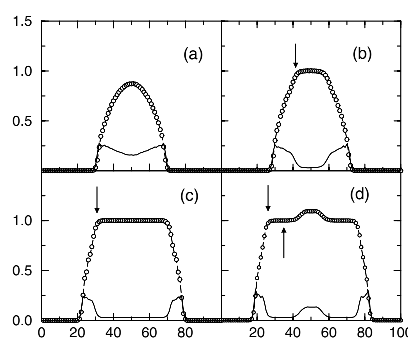

FIG. 2. Cuts across Fig. 1 show the compressibility profile κ_i (solid line) associated with the local density n_i (circles). The fillings are $N_b = 25$ (a), 33 (b), 50 (c), and 60 (d). κ_i is very small when $n_i = 1$. For the arrows see text.

the unconfined case allow us to calculate the site at which a Mott domain is entered or exited. These are shown as arrows in Fig. 2. However, it is vital to emphasize that while the confined system has locally incompressible regions, the global compressibility is *never* zero, which is seen clearly in Fig. 3. The main figure should be contrasted with the nonconfined case (inset).

An important difference in the behavior of the local κ_i is especially evident in one dimension where, in the unconfined case, the global compressibility diverges [2] as the Mott lobe is approached, $\kappa \propto |\rho - 1|^{-1}$ for the first lobe. Here, instead, we find $\kappa_i \propto (n_i - 1)$, as shown in Fig. 4. The origin of these differences is, of course, that the global compressibility, $\kappa = \beta(\langle \sum_{ij} n_i n_j \rangle - \langle n \rangle^2)$, probes density correlations at all length scales. In the unconfined case, contrary to the confined system, the establishment of the Mott phase is a true quantum phase transition: It happens collectively throughout the system and the correlation length diverges. There is, however, an interesting "universality" in the trapped system as a Mott region is approached. That is, the values of κ_i are the same even as the total filling and the on-site repulsion are varied (see Fig. 4). The same behavior is observed for the $n = 2$ locally incompressible phase.

Sets of runs such as those shown in Fig. 1 allow us to determine the state diagram as a function of boson filling and interaction strength for a given trap curvature. This is shown in Fig. 5. Because of the absence of true phase transitions, we have referred to Fig. 5 as a state diagram rather than phase diagram. As the filling is increased at fixed interaction strength, one crosses from a smooth density profile to one which has locally incompressible "Mott" domains, if V_0 is large enough. Further increase in the filling ultimately leads to the formation of regions at the well center where $n_i > 1$. In Fig. 5, region A admits only [16] locally incompressible regions with $n_i = 1$, as in Figs. 2(b) and 2(c). Region B has $n_i > 1$ surrounded by incompressible regions, Fig. 2(d). Region C is where the central part of the system has an $n_i = 2$ incompressible region which, when the boundary of the system is approached, falls off to a shoulder of $n_i = 1$ Mott region before reaching zero density. The $n_i = 1$ and $n_i = 2$ incompressible regions are separated by compressible regions. Region D is where the center of the system is compressible $n_i > 2$, bounded by $n_i = 2$ which in turn is bounded by $n_i = 1$ incompressible regions. Region E has no incompressible regions.

Note that the values of V_0 at which the A and C regions in Fig. 5 are entered are of the same order as those of the first two true Mott lobes in the nonconfined case [2]. This is consistent with the experimental results on three-dimensional optical lattices [11] which appear to be in agreement with the expected value in the nonconfined case. Furthermore, the narrowness of region C could help understand why the experiments [11] have not shown signs of the $n = 2$ Mott region, even though $n_i = 2.5$ in the core of the system.

One of the interesting experimental results [11] is how rapidly coherence is reestablished when V_0 is suddenly reduced from a value large enough to have produced large incompressible regions. It was argued that the characteristic time is of the order of the tunneling (hopping) time between sites [11]. This is entirely consistent with the picture we present here. If, for example, the density profile is as in Fig. 2(c) when V_0 is suddenly reduced to a very small value, the system will evolve to a profile like in 2(a) albeit with higher local density in the center. This is accomplished by particles near the edges hopping towards the center, and is greatly accelerated by the fact that the trap is much lower near the center than near edges. In addition, since there is only one center of nucleation (the geometric center of the system) there is no slowing down due to competition at domain walls where different nucleation zones meet.

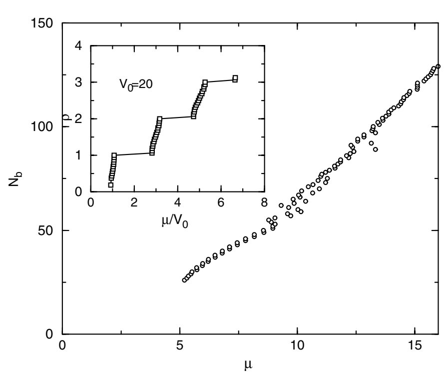

FIG. 3. N_b (number of bosons) as a function of chemical potential, μ for $V_0 = 4.5$. No globally incompressible Mott plateau is observed. Inset shows the unconfined case.

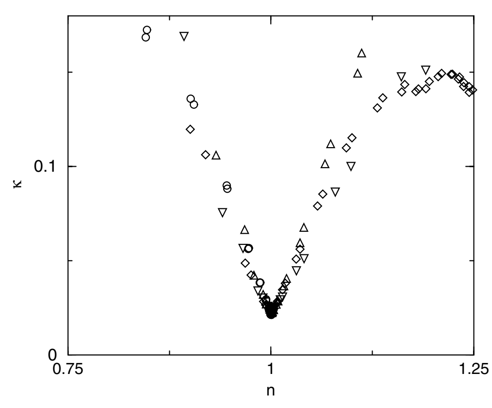

FIG. 4. The local compressibility as a function of local density for $V_0 = 4$, $N_b = 35$ (∘) and $N_b = 80$ (◇) and for $V_0 = 4.5$, $N_b = 90$ (△) and $N_b = 141$ (▽). κ decreases linearly with n as the Mott region, $n = 1$, is approached from below or above. This behavior is dramatically different from the unconfined system where κ diverges.

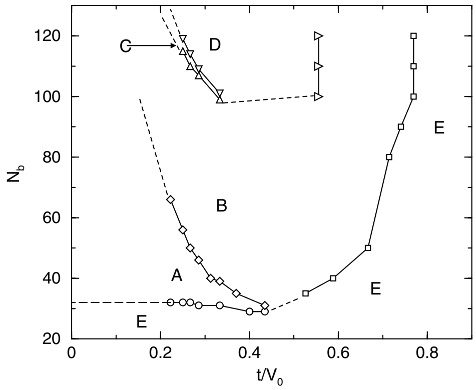

FIG. 5. The state diagram of correlated bosons in a quadratic confining potential. The solid lines are to guide the eye, and the dashed lines are extrapolations. See text for details.

In summary, we have discussed the nature of locally incompressible Mott insulating behavior in a one-dimensional system of interacting bosons in a confining potential at $T = 0$. We conclude that because of the destruction of translation invariance, great care should be taken in drawing on the analogy with the unconfined case at a fundamental level. For one thing, it can support Mott behavior off commensurate fillings. While Mott regions still exist, the critical properties are completely altered: Incompressible regions are established in a very localized way and not at all critically in the usual sense. These localized regions grow or shrink with V_0, but are always in coexistence with other regions, some compressible and some which might be incompressible but at higher local integer filling. In that sense, the formation of these Mott regions is not a true quantum critical phenomenon as it is in the unconfined case.

While we have focused on the new qualitative physics which results from the confining potential, it is important to emphasize that experiments on one and two dimensional trapped systems are currently underway [12,17–19]. For these, our paper should provide specific quantitative predictions for the critical ratios of interaction strength to kinetic energy and trap curvature, as a function of density. We are currently undertaking these comparisons. In addition, in the absence of traps, the phase diagram is qualitatively the same in one and two dimensions [1–3,5]. We expect this to be true in the confined case too. In fact, initial simulation results in two dimensions show this to be true.

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Note added.—A QMC study of the three-dimensional system appeared recently [20] in which the authors also conclude, as we do, that one cannot characterize globally the transitions discussed here. They discuss a signal that can be used experimentally to study the transition.

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