

# Pure Mott phases in confined ultra-cold atomic systems

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We propose a novel scheme for confining atoms to optical lattices by engineering a spatially-inhomogeneous hopping matrix element in the Hubbard-model (HM) description, a situation we term off-diagonal confinement (ODC). We show, via an exact numerical solution of the boson HM with ODC, that this scheme possesses distinct advantages over the conventional method of confining atoms using an additional trapping potential, including incompressible Mott phases at commensurate filling and a phase diagram that is similar to the uniform HM. The experimental implementation of ODC will thus allow a more faithful realization of correlated phases in cold atom experiments.

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In recent years there has been a burgeoning interest in the boson Hubbard (BH) model [1, 2], spurred by the expectation [3] that modern laser cooling and trapping techniques lead to the realization of this model in cold atom experiments. Several experimental groups [4–11] have achieved the BH model with bosonic atoms in optical lattices, observing evidence of the predicted Mott insulating and superfluid phases. Experimental probes include the condensate fraction and momentum distribution [8], noise correlations [9] and RF spectroscopy [7].

The ground state phase diagram for the uniform BH model with chemical potential  $\mu$ , onsite repulsion  $U$ , and hopping parameter  $t$  is well known (Fig. 1), and consists of lobes of incompressible Mott insulating phase (at commensurate fillings) surrounded by a regime of superfluid order, with these states separated by quantum phase transitions [1, 2]. However, present-day cold atom experiments always occur in the nonuniform environment of a smoothly-varying harmonic trap that confines the atoms to the optical lattice, so that the actual Hamiltonian consists of the BH model plus a parabolic single-particle potential. Early theoretical work [12] showed that this kind of diagonal confinement (DC) does not entirely reproduce the physics of the BH model. In particular, the model with DC is characterized by the absence of energy gaps at commensurate fillings, as opposed to the BH model. This results in the absence of true incompressible Mott insulating phases and of a real superfluid to Mott transition in present-day experiments.

The physical origin of the lack of incompressible Mott phases in the BH model with DC [3, 12] can be understood within the local density approximation (LDA). According to the LDA, the harmonic DC potential is treated by replacing  $\mu \rightarrow \mu - \frac{1}{2}m\Omega^2 r^2$  with  $r$  the distance from the center of the lattice,  $\Omega$  the trapping frequency and  $m$  the atom mass. With increasing radius, then, the system traverses the uniform-case phase diagram at fixed  $t$  and a spatially-varying  $\mu$  (vertical arrow on Fig. 1). Then, even if a system is locally in a Mott phase at the center of the trap, it must enter a superfluid phase with

increasing radius (yielding the well-known shell structure [6, 7, 12, 13]), thereby being globally compressible. Recent work has used the LDA to infer the homogeneous

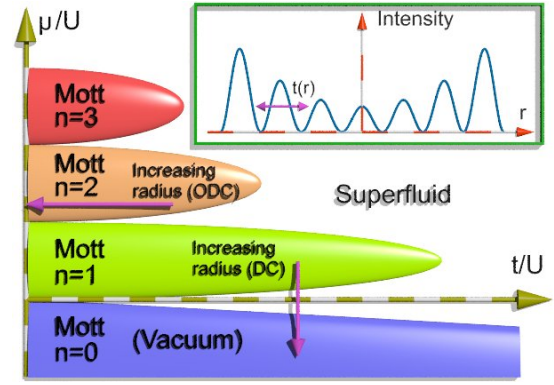


FIG. 1: (Color online) Schematic ground state phase diagram of the uniform boson Hubbard (BH) model [1]. The arrows show two possible sequences of local phases encountered in an atomic system as the radius  $r$  from the center of the lattice increases. Diagonal confinement (DC) is created by a decreasing chemical potential  $\mu$ , leading to a sequence of Mott and superfluid phases. Off-diagonal confinement (ODC) is created by a decreasing hopping parameter  $t$ , and can maintain the whole system in the same Mott lobe. Inset: A decreasing hopping parameter  $t$  can be obtained by increasing the intensity of the optical lattice as one moves away from the center.

BH phase diagram from the DC experimental results [11] and also to place a given DC system on the phase diagram of the uniform BH case [14]. Nevertheless, it is still of great interest to establish truly incompressible Mott phases of bosons in cold atomic gas experiments.

In this Letter, we propose that truly incompressible Mott phases can be achieved via off-diagonal confinement (ODC) of the bosons where the cloud is confined via a spatially varying tunneling matrix element  $t(r)$ , which vanishes at the boundary of the system. This can be realized, for example, by having the optical lattice depth increase with increasing radius, as illustrated in the inset

of Fig. 1. Although a system with ODC is still spatially inhomogeneous, it can exhibit a true gapped and incompressible Mott phase at commensurate fillings. This can be easily understood by extending the above LDA argument to a spatially-varying  $t(r)$  instead of  $\mu(r)$ . Thus, within the LDA, a vanishing  $t(r)$  with increasing  $r$  corresponds to traversing the uniform-case phase diagram at *fixed* chemical potential. In particular, a system that is locally in a Mott phase at the center of the lattice will remain in the same Mott phase for all radii up to the boundary where  $t(r)$  becomes zero.

Thus the ODC setup reproduces important aspects of the BH model, namely the presence of gaps and true Mott phases at commensurate fillings, as we show via an exact numerical calculation for a one-dimensional model. In addition, superfluid phases with ODC are found to lead to condensates (quasicondensates in one dimension) with greater population than the model with DC, and therefore can realize *clean* condensates.

Let us briefly discuss the experimental viability of achieving off-diagonal confinement via a spatially-dependent  $t$ . A uniform periodic lattice of cold atoms yields a tunneling matrix element [15]

$$t \simeq \frac{4}{\sqrt{\pi}} E_r \left( \frac{V_0}{E_r} \right)^{\frac{3}{4}} \exp \left( -2\sqrt{\frac{V_0}{E_r}} \right), \quad (1)$$

with  $E_r$  the recoil energy ( $E_r = \frac{\hbar^2 k^2}{2m}$ ,  $k$  the optical lattice wave vector,  $m$  the atom mass) and  $V_0$  the optical lattice depth. The exponential sensitivity of  $t$  on  $V_0$  implies that even a modest increase in  $V_0$  with increasing radius will yield a rapid suppression of  $t$ , confining the cloud to the optical lattice. Taking parameters from Ref. 4, which has  $E_r \simeq 2.13 \times 10^{-13} J$ , this sensitivity is illustrated by noting that the hopping time  $\tau \sim \hbar/t$  changes by two orders of magnitude as  $V_0/E_r$  is varied (from 0.3ms at  $V_0/E_r = 3$  to 26ms at  $V_0/E_r = 22$ ).

Although conventional optical lattices created with interfering laser beams typically possess a uniform  $t$ , recently the Greiner group has developed a novel holographic method that can produce an arbitrary optical potential using a mask [16]. An optical lattice that produces a spatially-varying  $t$  will also yield a spatially-varying Coulomb repulsion  $U$ . However, examining the expression for this quantity [15]  $U = \sqrt{8/\pi} k a E_r (V_0/E_r)^{3/4}$ , with  $a$  the atom scattering length, we note that  $U$  is only power-law sensitive to  $V_0$ . Therefore, a spatially-varying  $V_0$  will lead to relatively small variations of  $U$  and larger changes in  $t$ . Moreover, variations of  $U$  can be taken into account by generalizing the LDA picture to a varying  $t/U$ , yielding same conclusions. Thus, we expect that such off-diagonal confinement of atoms in an optical lattice will be experimentally realizable in the near future, adding to the rapidly-growing cold-atom toolbox [17].

The above LDA argument suggests that experiments using ODC will achieve a true Mott phase for any

spatially-varying  $t(r)$ . To illustrate this, we consider the following one-dimensional model:

$$\hat{\mathcal{H}} = - \sum_{\langle ij \rangle} t_{ij} (a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \quad (2)$$

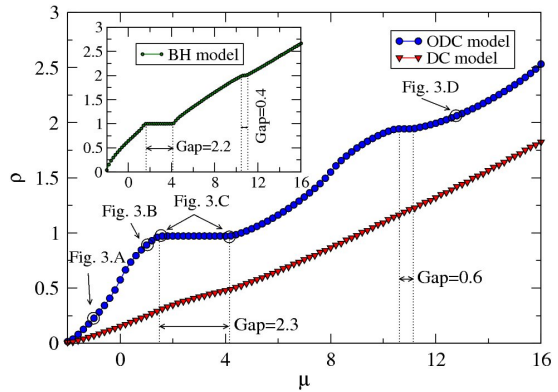


FIG. 2: (Color online) The density as a function of the chemical potential, for  $U = 8$ . The ODC model exhibits Mott gaps at commensurate fillings as in the periodic case (inset). Results for the DC model with a trapping parameter  $W = 0.008$  are shown for comparison.

The sum over  $i$  runs in the range  $[0; L - 1]$ , with  $L$  the number of lattice sites, and the sum over  $\langle ij \rangle$  is restricted to pairs of first neighbors. The bosonic operators  $a_i^\dagger$  and  $a_i$  create and annihilate a particle on site  $i$ , respectively, and  $\hat{n}_i = a_i^\dagger a_i$ . The local hopping parameter  $t_{ij}$  follows an inverted parabola,  $t_{ij} = t(i + j + 1)(2L - i - j - 1)/L^2$ , with a maximum value of  $t$  at the center of the lattice,  $t_{L/2-1, L/2} = t$ , and a vanishing value at the edges ( $t_{-1,0} = t_{L-1,L} = 0$ ). Finally, we choose  $t = 1$  in order to set the energy scale.

We solve the model exactly by means of quantum Monte Carlo simulations, by making use of the Stochastic Green Function (SGF) algorithm [18] with directed updates [19]. The SGF algorithm can be implemented in the canonical ensemble as well as in the grand-canonical ensemble. In the following, we take advantage of this feature. When working in the canonical ensemble, the number of particles  $N$  is chosen and remains strictly constant during the entire simulation. In the grand-canonical ensemble, we add the usual term  $-\mu\hat{N}$  to the Hamiltonian, with  $\hat{N} = \sum_i \hat{n}_i$ , in order to control the mean number of particles  $N = \langle \hat{N} \rangle$  via the chemical potential  $\mu$ . In the following we consider a lattice with  $L = 70$  sites, since this is the typical size currently accessible in one-dimensional optical lattice experiments. We have used increasing values of the inverse temperature  $\beta$ , and found that the ground-state properties are captured with  $\beta = 20$ . All presented results correspond to this inverse temperature. We begin by investigating the behavior of

the density  $\rho = N/L$  as a function of the chemical potential  $\mu$ . Here it is convenient to make use of the grand-canonical ensemble, since the chemical potential is the control parameter. Fig. 2 displays results for  $U = 8$ .

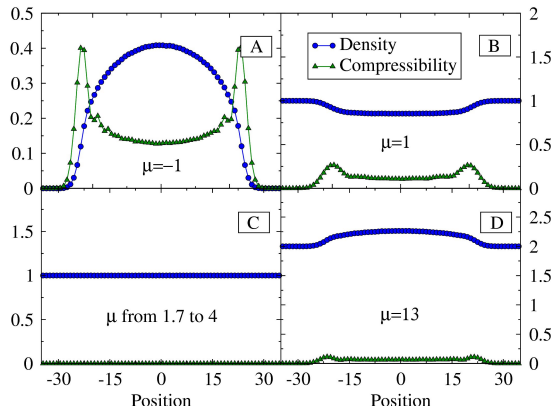


FIG. 3: (Color online) The local density and local compressibility, for  $U = 8$ . A superfluid cloud grows in the center of the lattice, as the number of particles increases (Panel A). Contrary to the DC model, Mott regions in the ODC model form at the edges of the lattice (Panel B), then extend towards the center. At commensurate filling (Panel C), the phase is a pure incompressible Mott insulator. Adding particles above commensurate filling breaks the Mott plateau in the center, which becomes locally superfluid (Panel D).

A comparison between the results in the main panel and the inset in Fig. 2 shows that while the usual model with DC does not display any incompressible phase, the model with ODC has pure Mott gaps at commensurate fillings as in the homogeneous case. For these fillings, the number of particles per site sticks to integer values and is constant over the whole lattice. Note also that the gaps of the ODC model and homogeneous BH model are similar in size. The results for the DC model correspond to a parabolic potential  $W \sum_i (i - L/2)^2 \hat{n}_i$  with  $W = 0.008$ . For this case, the size of the lattice has been increased to  $L = 100$  in order to avoid an overflow of the particles. Note that such an overflow never occurs in the ODC model, since the local hopping parameter vanishes at the edges of the lattice.

Fig. 3 shows typical density profiles and the associated local compressibility, defined as the response of the local number of particles to a change of the chemical potential [20],  $\kappa_i = \frac{\partial \langle \hat{n}_i \rangle}{\partial \mu} = \int_0^\beta [\langle \hat{n}_i(\tau) \hat{N} \rangle - \langle \hat{n}_i(\tau) \rangle \langle \hat{N} \rangle] d\tau$ . For pure Mott phases this quantity vanishes at commensurate fillings for each lattice site  $i$ .

The density profiles in Fig. 3 can be qualitatively understood within the above LDA argument, in which increasing radius corresponds to a decreasing  $t$  and a horizontal path in the homogeneous BH phase diagram of Fig. 1. Thus, Fig. 3A shows a system that is locally superfluid in the center, and enters the vacuum as the

radius increases and the ratio  $t/U$  decreases. For greater  $\mu$ , Fig. 3B corresponds to a path beginning in the superfluid phase and crossing into the  $n = 1$  Mott phase of Fig. 1, therefore the system is still globally compressible with a local Mott phase at the edge. The incompressible Mott phase in Fig. 3C corresponds to a LDA path that remains entirely inside one Mott lobe. Fig. 3D at higher  $\mu$  is qualitatively similar to Fig. 3B, but with the inner superfluid having a higher local density than the Mott region at the edges. Finally, all density profiles corresponding to the  $\mu$  values explored in Fig. 2 are represented on Fig. 4. The figure clearly shows the Mott plateaux at  $\rho = 1$  and  $\rho = 2$  extending over the whole lattice.

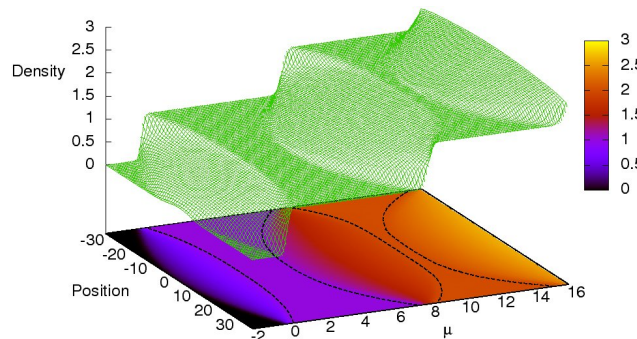


FIG. 4: (Color online) The density as a function of the position and the chemical potential for  $U = 8$ . The Mott plateaux at  $\rho = 1$  and  $\rho = 2$  appear clearly, and extend over the whole lattice.

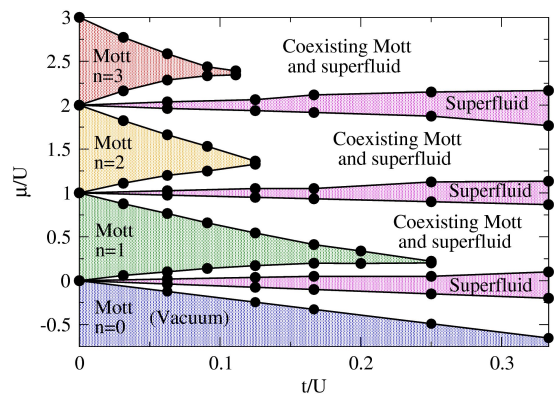


FIG. 5: (Color online) The ground state phase diagram of the ODC model given by Eq. (2), showing lobes of incompressible pure Mott phase (like Fig. 3C), and regions of compressible superfluid and compressible coexisting Mott and superfluid phases (like Figs. 3A, 3B, and 3D).

Next, we work in the canonical ensemble at fixed densities and scan the values of the onsite repulsion parameter  $U$  for which the system exhibits the Mott insulating state. In the canonical ensemble the ground state chemical potential is not a control parameter, but instead it is computed as  $\mu(N) = E(N+1) - E(N)$ . Fig. 5 shows the



phase diagram which exhibits pure Mott lobes similar to those of the homogeneous BH model [2], which again are not present in the DC model [12]. In addition, new lobes where the phase is purely superfluid arise as the onsite interaction decreases. Another particularity of the ODC model is that coexistence of Mott and superfluid can occur at any value of the onsite repulsion  $U$ . This mixed state is absent in the uniform BH model; and in the DC model there is a critical value of  $U$  [21] below which the system is purely superfluid.

Finally, we make connection with an experimental probe by plotting in Fig. 6 the maximum intensity  $I_{max}$  of the interference pattern (the population of the quasi-condensate) as a function of the chemical potential. The visibility  $\mathcal{V} = (I_{max} - I_{min}) / (I_{max} + I_{min})$  is also shown. The variations in the visibility are stronger with ODC than with DC, since in the former case we are in the presence of a true superfluid-to-Mott transition. The maximum intensity curve also reveals another interesting feature of the ODC model: condensates have greater population than the DC model. Thus, the experimental realization of the ODC model should improve the quality of condensates.

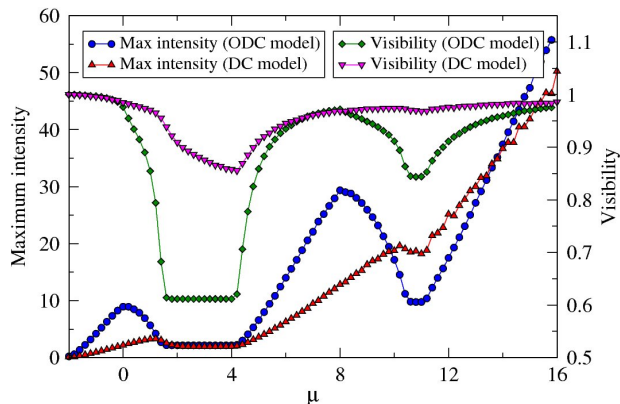


FIG. 6: (Color online) The maximum intensity of the interference pattern and the visibility as functions of the chemical potential, for  $U = 8$ .

In this Letter, we proposed a novel scheme for confining atoms on optical lattices based on off-diagonal confinement, in which the Bose-Hubbard tunneling matrix element is engineered to vanish at the system boundary. We show by using an exact quantum Monte Carlo method that our model reproduces important aspects of the boson Hubbard model. In particular, truly incompressible bosonic Mott phases occur at commensurate fillings and strong interactions, an important requirement for quantum-computing [17]. Indeed, optical lattices provide intrinsically scalable and well-defined sets of qubits. These qubits must be initialized in a "zero" state, which corresponds to having one particle per site. This is precisely achieved by having the system in a pure Mott phase. Additionally the establishment of a global

Mott phase will pave the way to further experimental simulations of the Mott-superfluid transition, a problem of broad interest due to its connections to condensed-matter systems such as the high-temperature superconductors [22]. In addition, our simulations show that the model leads to highly populated condensates, which are of great interest in the production of coherent matter waves.

To achieve the ODC, it may be easiest to start with a conventional DC cloud (a system that has already been taken to low temperatures) and adiabatically apply the ODC optical potential. We have studied the entropy of the DC and ODC phases in a hardcore-boson model at finite temperatures, finding, for comparable system size, a comparable entropy in the ODC and DC states, implying that a low temperature can be maintained upon adiabatically moving from DC to ODC. Additionally, one may ask how equilibrium is established with ODC given that the local hopping time  $\tau \sim \hbar/t$  is spatially varying; rapid equilibration may be stymied if much of the system possesses a large value of  $\tau$ . To address this it may be necessary to engineer ODC to have  $V_0$  increase rapidly over a few lattice sites near the edge. Given the above-mentioned rapid variation of  $\tau$  with  $V_0$ , this should be feasible.

The flexibility of the techniques used in present-day experiments allows the realization of our model, and should open new perspectives on the physics of Mott phases. Future work will utilize the Stochastic Green Function (SGF) algorithm [18, 19] to compute other experimentally relevant quantities such as the momentum distribution [8], noise correlations [9] and RF spectroscopies [7]. Finally, we note that our model can also be easily generalized to fermionic systems where we expect a similarly rich behavior.

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