Bose-Hubbard model with local two- and three-body interaction under off-diagonal confinement

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Abstract. We calculate the density profiles of a system of bosons with off-diagonal confinement and local interaction between two or three particles, using the density matrix renormalization group method. We found different ground-states: Mott insulator, superfluid and diverse mixed states. We observe that the Mott insulator lobes are surrounded by Mott insulator-superfluid coexistence state regardless the kind of the local interaction. The area of the Mott insulator lobes decreases for the two-body interactions and remain the same for three-body interactions.

1. Introduction
The experiments realized with boson system about phase transitions have opened novel theoretical studies for proposing deeper insights in the Bose-Hubbard model. In 2002, Greiner et al.[1] observed a phase transition from superfluid to Mott Insulator. Initially each atom is spread out over the entire lattice, however when the hopping parameter or the density changes, the atoms can be localized at individual lattice sites leading to the Mott insulator phase. The above experimental observations were interpreted using the Bose-Hubbard model which describes a system of bosons in a lattice, where the bosons interact under a two-body term. The phase diagram and the main features of this model have been studied widely [2, 3, 4].

Recently Willet al. [5] highlighted the importance of considering more than two-body interaction by an experimental observation of the local wave-function. With an interferometric technique, they measured the absolute energies of atoms at a lattice site. The results demonstrated the presence of ultracold bosonic-system multi-body interaction in a three-dimensional optical lattice. Recently, a modified Bose-Hubbard model (with local interaction terms between two and three bodies) was studied by B. L. Chen et al. [6] and K. Zhou et al. [7] with the mean-field aproximation. Silva-Valencia and Souza [8, 9] used the density matrix renormalization group method to determine the phase diagram of the Bose-Hubbard model with two- and three-body interactions, finding that the Mott insulator lobes increases with the density and the three-body interaction.

When atoms are confined in optical lattices they undergo a harmonic potential, which leads to a Mott insulator state without gap i.e. this state is compressible. With the aim of finding true Mott insulator states in experiments, Rousseau et al. [10] proposed the off-diagonal confinement (ODC), which leads to an inhomogeneous hopping parameter. Using quantum Monte Carlo,
Figure 1. The density profile and local compressibility of bosons under ODC potential and two-body interaction. Here $t = 0.05$.

Figure 2. Phase diagram of bosons under ODC potential and two-body interaction. The lattice size of the system is $L = 80$.

This new confinement method allows to obtain incompressible Mott insulator states and a novel Mott-superfluid coexistence phase.

This paper is focused in the study of a one-dimensional system with off-diagonal confinement considering two- or three-body interaction, using the canonical ensemble and the density matrix renormalization group method to find the ground-state and his properties.

The present work is organized as follows: in Section 2, we explain the Hamiltonian models. In section 3 we show the results such as one-dimensional density profiles with two- or three-body interaction and the ODC phase diagrams. Finally, in Section 4, we summarize our results.

2. Hamiltonian models

The Hamiltonian of the Bose-Hubbard model that describes a system of bosons under ODC potential and two-body interaction is given by

$$H_1 = - \sum_{\langle ij \rangle} t_{ij} (b_i^\dagger b_j + b_j^\dagger b_i) + \frac{U}{2} \sum_i n_i(n_i - 1),$$

(1)

where $b_i^\dagger (b_i)$ creates (annihilates) a boson on site $i$ and $n_i = b_i^\dagger b_i$ is the local density operator. The sum in the above Hamiltonian runs in the range $[0; L - 1]$, with $L$ representing the lattice size, and the symbol $\langle ij \rangle$ restricts the interactions to the nearest neighbors. The two-body interaction between the bosons is given by the second term of the above Hamiltonian, and his strength is $U = 1$.

The first term in the Hamiltonian (Eq. 1) represents the kinetic energy, where the hopping parameter $t_{ij}$ is given by $t_{ij} = t((i + j + 1)/(2L - i - j - 1))/L^2$, which changes like as an inverted parabola, i.e., there is a maximum value $t$ in the lattice center and a null value in both ends of the lattice. This non-constant hopping parameter is due to the ODC confinement.

When we consider the three-body interaction between the bosons, the Hamiltonian of the systems is

$$H_2 = - \sum_{\langle ij \rangle} t_{ij} (b_i^\dagger b_j + b_j^\dagger b_i) + \frac{W}{6} \sum_i n_i(n_i - 1)(n_i - 2),$$

(2)

where the strength of the three-body interaction is $W = 1$. 

The ground-state above Hamiltonians is studied using the density matrix renormalization group (DMRG) [11], we consider 200 states and obtain an error of $10^{-8}$.

The chemical potential to add a particle to the system of size $L$ is given by $\mu(L) = E(N+1,L) - E(N,L)$, where $E(N,L)$ is the ground-state energy of a system of lattice size $L$, with $N$ particles.

3. Results

The density profiles of a system of bosons that interact under a two-body term are shown in Fig. 1 for a maximum hopping parameter $t = 0.05$. Considering that the real systems of bosons confined in optical lattices are finite, we consider lattice of $L = 80$ sites [1]. In Fig. 1(a), we show a typical profile for low density, for example $N = 5$. ODC potential generates a charge redistribution where empty sites in both ends of the lattice and a superfluid phase in the center are obtained. So, we can establish a coexistence phase between superfluid and band insulator. The insulator regions can be confirm with the local compressibility, which is given by $\kappa_i = <(n_i)^2> - (<n_i>)^2$, and we note that the local compressibility in the band insulator sites is zero because the particle number fluctuations are insignificant.

In Fig. 1(b), a superfluid state appears with $N = 40$ particles, where the local density and the local compressibility vary in the lattice. A Mott insulator state characterized by a null local compressibility appears in Fig. 1(c), with $N = 80$ particles, therefore, for integer density and two-body interaction a truly Mott insulator is obtained. In Fig. 1(d), with $N = 90$ particles the coexistence phase between the superfluid phase and the Mott insulator phase is presented, in this figure the local compressibility in the lattice ends is zero and the local density in the extremes of the lattice shows one particle for site.

The phase diagram of a system of bosons under the ODC potential and two-body interaction term is shown in Fig. 2. We observe the already-known Mott insulator lobes and the superfluid regions, however a new Mott insulator-superfluid coexistence regions surrounding the Mott insulator lobes appear. Also, we found that the area of the Mott insulator and superfluid phases are smaller than in the harmonic potential case (diagonal confinement).

In Fig. 3, we show the density profiles for the Bose-Hubbard model with ODC potential as well as the interaction between three bodies (Eq. 2). Again, the coexistence between superfluid and band insulator regions appear for low densities when we consider $N = 20$ bosons in a lattice of $L = 80$ sites, and a maximum hopping parameter $t = 0.05$ (see Fig. 3(a)).

A superfluid profile is presented in Fig. 3(b), the local compressibility is nonzero for each lattice site except at both ends. Also there is not a Mott insulator for $N = 80$ contrary to the two-body interaction profiles, because the system with one particle for site and three-body interaction do not generate a insulator region.

With $N = 100$, there is another superfluid profile, where the lattice ends are not empty and the compressibility is nonzero, this is presented in Fig. 3(c). In Fig. 3(d), for $N = 160$ a truly Mott insulator phase appears characterized for a local compressibility equal to zero.

In Fig. 3(e), with $N = 170$ we show the coexistence between Mott insulator and superfluid. Equally, in Fig. 3(f), for $N = 220$ there is a coexistence phase but this profile has a minimum value in the superfluid cloud.

The phase diagram of the system of bosons interacting with a three-body term under a ODC potential is shown in Fig. 4. We note that the Mott insulator lobes are surrounded by coexistence states alike than the two-body case, however the area of the Mott lobes remain the same, this is due to strong localization generates by the three-body interaction term. Also, we observe that the Mott lobes area increases with the density, and the superfluid regions of the phase diagram are smaller than in the homogeneous lattice.
Figure 3. The density profile and local compressibility of bosons under ODC potential and three-body interaction. Here $t = 0.05$.

4. Conclusions
In this paper we have studied the novel scheme for confining atoms in lattices based on off-diagonal confinement, for which the hopping parameter $t$ is maximum in the lattice center and vanish at the lattice extremes. This confinement permits us to obtain truly Mott phases, which are observed when we calculate the local density and local compressibility for system with interaction between two or three bodies by DMRG.

The ODC potential generates different ground-state configurations, such as: truly Mott insulator, superfluid and states where coexist superfluid regions with Mott insulator ones.

We obtained that the area of the Mott insulator lobes decreases due to the ODC potential for the two-body interaction, whereas remain the same for the three-body interaction.

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Figure 4. Phase diagram of bosons under ODC potential and three-body interaction. The lattice size of the system is $L = 80$. 