Effect of dominant three-body interaction in two-dimensional square lattice

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Abstract. The effect of dominant three-body interaction to hard-core boson Hubbard model is studied on a two-dimensional square lattice. In terms of quantum Monte Carlo method, it is shown explicitly a $\rho = 2/3$ solid phase with coexistence of charge-density-wave and bond orders appears due to the presence of the dominant three-body interaction. For strong three-body interaction, the $\rho = 2/3$ solid phase appears between superfluid phases and shrinks as decreasing the strength of the three-body interaction, forming a lobe structure in the phase diagram. For weak three-body interactions, superfluid phase exists for the whole range of hard-core densities except the full filled case, where the system is a Mott insulator.

1. Introduction
Phenomena in condensed matter physics are usually dominated by two-body interactions, such as Coulomb force. Interactions between more than two particles are small in most cases because more-body interactions only provide small corrections. Nevertheless, developments in theoretical condensed matter physics showed that exotic quantum phases are often identified as ground state of Hamiltonians with three or more body interactions. However it is hard to achieve dominating multi-body interactions experimentally. Recently, a study suggested that strong three-body interactions can be obtained by using polar molecules driven by microwave fields[1]. If the polar molecules are loaded into an optical lattice, the physics can be described by boson Hubbard model[2, 3], with dominant three-body interactions. Inspired by this, boson Hubbard model with dominant three-body interactions has been studied in both one dimension and two dimensions using quantum Monte Carlo (QMC) and other ways[2, 3]. In one dimension, superfluid and $\rho = 2/3$ solid phase with coexistence of charge density wave (CDW) and bond order wave (BOW) orders are found[2]. In two-dimensional square lattice, a study including all types of three-body terms existing in two dimensions shows a sequence of solid and supersolid phase[3].

However, in this paper, we just introduce one special three-body interaction (TBI) (three hard-core bosons arranged one by one in one line) to the two-dimensional (2D) hard-core boson Hubbard model on a square lattice and study the phases due to its presence. This study may be helpful to understand the interplay among all kinds of three-body interactions existing in two dimensions. By employing QMC method[4, 5], we derive the phase diagram of the system and found the existence of the superfluid (SF) state, the $\rho = 2/3$ solid phase with both CDW and BOW orders and the Mott insulating state.
2. The model and method

The 2D hard-core boson Hubbard model on a square lattice with the dominant TBI can be expressed as

\[ H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i \hat{n}_i + W \sum_{i\bar{\eta}} \hat{n}_{i-\bar{\eta}} \hat{n}_{i+\bar{\eta}}, \]  

(1)

where \( \langle ij \rangle \) indicates the sum over the nearest neighbor sites and and \( \hat{n} = \hat{x}(\hat{y}) \); The operator \( a_i^\dagger \) (\( a_i \)) creates (destroys) a hard-core boson on site \( i \); \( \hat{n}_i = a_i^\dagger a_i \) is the hard-core boson number operator; \( \mu \) is the chemical potential and therefore to controls the filling number of the system; The hopping \( t \) describes the coherent hopping between nearest neighbor sites, and the last term is the TBI with strength \( W \). In the hard-core limit, the Hubbard constant \( U \to \infty \). In this case, each site can be occupied by 0 or 1 hard-core boson. Since hard-core bosons are restricted in this Hilbert subspace, therefore the hard-core operators \( a_i^\dagger \) and \( a_i \) obey commutation relations \([a_i, a_j^\dagger] = 0\) at sites \( i \neq j \), while they satisfy anti-commutation relations \([a_i^\dagger, a_j] = 1\) on sole site \( i \).

In the following discussions, QMC simulations based on the stochastic series expansion method with directed loop updates are carried out[4]. In order to characterize different phases, we study the static structure factor \( S_{CDW}(Q) \), bond order structure factor \( S_{BOW}(Q) \) at wave vector \( Q \) and superfluid density \( \rho_s \), which are expressed as:

\[ \rho_s = \frac{\langle W^2 \rangle}{2\beta H}, \]

(2)

\[ S_{CDW}(Q) = \frac{1}{N^2} \sum_{j,l} e^{iQ(j-l)} \langle n_j n_l \rangle, \]

(3)

\[ S_{BOW}(Q) = \frac{1}{N^2} \sum_{j,l} e^{iQ(j-l)} \langle K_j K_l \rangle, \]

(4)

where \( W \) is the winding number of the bosonic world lines and the bond operators \( K_l = b_{l+\bar{\eta}}^\dagger b_{l+\bar{\eta}} + b_{l^\dagger}^\dagger b_{l+\bar{\eta}} \).

3. The numerical results

We derive the phase diagram of Hamiltonian (1) and the results are shown in Fig.1. For \( \mu < -zt \), the system is empty and for \( \mu > 6W + zt \), it is fully occupied by one boson per site. At large values of \( t/W \sim 0.58 \), the bosons form a superfluid (SF) with off-diagonal long-range order, characterized by a finite SF density. For smaller values of \( t/W \), the system exhibits a solid phase of density \( \rho = 2/3 \). The solid phase is incompressible, giving rise to the characteristic lobe structure in the \( \mu - W \) plane. Its largest extend is set by the point \((t/W, \mu/W) \sim (0.58, 4)\). In the lobe, the density of the system is \( \rho = 2/3 \) and the system has both zero SF density and zero compressibility, indicating that it is a \( \rho = 2/3 \) solid. At the same time, this solid phase is characterized by both nonzero \( S_{CDW} \) and nonzero \( S_{BOW} \). So CDW and BOW orders coexist in this solid phase. The CDW order can be understood in the zero-hopping limit \( t = 0 \), when the ground state is sixfold degenerate, and exhibits CDW order with \( S_{CDW} = \frac{\mu^2}{4} = 1/9 \). Due to the presence of this \( \rho = 2/3 \) CDW order, the symmetry of hopping to the left (up) or hopping to the right (down) is broken, which causes the hopping correlations. Thus the system exhibits a BOW order simultaneously.
Figure 1. The ground state phase diagram of hard-core boson Hubbard model with dominant TBI in the $\mu - W$ plane.

4. Conclusions
In conclusion, we study the effect of dominant three-body interaction to hard-core boson Hubbard model on a two-dimensional square lattice using QMC method. We show explicitly a $\rho = 2/3$ solid phase with coexistence of charge-density-wave and bond orders appears due to the presence of the dominant three-body interaction. For strong three-body interaction, the $\rho = 2/3$ solid phase appears between superfluid phases and shrinks as decreasing the strength of the three-body interaction, forming a lobe structure in the phase diagram. For weak three-body interactions, superfluid phase exists for the whole range of hard-core densities except the full filled case, where the system is a Mott insulator. Our these results are closely related to the relevant experiments.

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