Entanglement entropy, fidelity and the phase transition of one-dimensional hard-core bosonic system with three-body interactions

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We study the one-dimensional hard-core Bose-Hubbard model with three-body interactions. In previous work [1], the two-thirds filling solid with both bond-wave order (BOW) and charge-density wave order (CDW) is found and it undergoes a second order phase transition to the superfluid phase. However, in recent work [2], we found the BOW not independent with CDW order. Thus, by utilizing the density matrix renormalization group, we make use of both entanglement entropy and fidelity susceptibility to detect the phase transition. In two-thirds filling, the extreme point of the entanglement entropy also indicates the superfluid phase transition point. However, the pairwise entanglement entropy drop quickly after additional critical point, such disentangled behaviour demonstrates another melting point to the CDW phase. Thus, a novel intermediate phase between CDW phase and superfluid phase is found. At last, we analyzed the half filling case with entanglement entropy.

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I. INTRODUCTION

Quantum phase transition is a very important phenomenon in condensed matter physics, and it happens in low temperature by tuning the parameter in Hamiltonian. A typical example is the transition from Luttinger liquid to CDW phase, which occurs when the repulsive interaction is twice the hopping in the one-dimensional spinless fermion model. In the real materials, quantum phase transitions usually result from the dominant two-body interactions, because relatively small multi-body interactions can only provide tiny corrections. On the other hand, the cold atom in the optical lattice give us a great platform to realize the three body interactions in both lattice and free space. It is shown that the three-body interactions can be dominated, meanwhile the two-particle interaction can be independently controlled and even switched off by driving microscopic fields. The system with leading multi-body interactions can induces many exotic phenomenons, such as supersolid phase, the first order Mott insulator phase transition and several kinds of solid phases in different geometric lattices. In the work [2], BOW order parameter is demonstrated also not zero in the CDW solid phase, so the CDW+BOW phase in one dimensional chain needs to be further studied.

Thanks to the quantum information theory, the quantum phase transition can be also detected by using “the entanglement witnesses as observables” and even the spin liquid phase which has no order parameter can also be touched. Furthermore, the ground-state entanglement entropy (EE) and fidelity have been used to qualify quantum phase transitions in strong correlated systems. In order to figure out the quantum phase transition in the one dimensional bosonic system with three-body interactions, it is better to consider these two “entanglement witnesses” again.

In this paper, we make use of the ground-state EE and fidelity to analyze the quantum phase transitions in one-dimensional hard-core bosons model with three-body interactions. The paper is organized as following. The model and its properties in weak and strong interactions limitation is discussed in Sec. II. The algorithm and the quantum information observables we used are described in Sec. III. The results of EE and the fidelity at two-thirds filling are presented in Sec IV. At last, we consider EE calculation at half filling in Sec V.

II. MODEL

The Hamiltonian we considered is one-dimensional hard-core Bose-Hubbard model with three-body interactions

$$\mathcal{H} = -t \sum_i (b_i^\dagger b_{i+1} + h.c.) + W \sum_i n_{i-1} n_i n_{i+1}$$

where $b_i^\dagger (b_i)$ is creation (annihilation) operator of hard-core boson at site $i$, $t$ is the hopping interaction chosen as unit of energy, and only the leading three-body interactions with strength $W$ is considered.

When hopping processes are switched off, only three-body interactions need to be considered. Besides the
saturated phase, only two-thirds filling is incompressible. Meanwhile, it breaks the translational symmetry and the ground state is $|\psi\rangle = \prod_{\text{mod } (1,3) \neq 0} b_{l}|0\rangle$. On the other hand, the Luttinger superfluid phase exists in the weak coupling limit $W \ll t$, so the quantum phase transition should happen in the intermediate region. B. Capogrosso-Sansone et al. found the second order phase transition from the solid phase to the superfluid phase at $W/t = 2.8 \pm 0.15$ and the solid exhibits both CDW and BOW orders. However, the order parameter of BOW they used is demonstrated not suitable, because the local fluctuation of the particles in the CDW solid can also induce the non-zero BOW order parameter. In other words, both order parameters are not indecently. To figure out the quantum phase transition, we reconsider it with quantum information witnesses $EE$ and $\delta \lambda$. According to Ref. [8], in the spin half XXZ model, the block EE can be chosen as a measurement of the bipartite entanglement, and it is realted to detect quantum phase transitions. Taking a fidelity.

\[ F(\lambda, \delta \lambda) = \text{Tr}[\sqrt{\rho_0^{1/2}(\lambda)\rho_0(\lambda + \delta \lambda)\rho_0^{1/2}(\lambda)}], \]

where $\delta \lambda$ is a small deviation. For a pure state $\rho_0 = |\psi_0\rangle \langle \psi_0|$, Eq. (4) can be rewritten as $F(\lambda, \delta \lambda) = |\langle \psi_0(\lambda)|\psi_0(\lambda + \delta \lambda)\rangle|$ which represents the overlap of the wavefunction at two adjacent quantum parameter points, and $F(\lambda, \delta \lambda)$ reaches its maximum value $F_{\text{max}} = 1$ at $\delta = 0$. Expanding $|\psi_0(\lambda + \delta \lambda)\rangle$ to first order, we got

\[ |\psi_0(\lambda + \delta \lambda)\rangle = |\psi_0(\lambda)\rangle + \delta \lambda \sum_{n \neq 0} \frac{H_n |\psi_n(\lambda)\rangle}{E_0(\lambda) - E_n(\lambda)} \]

where $H_{n0} = \langle \psi_n(\lambda)|H_I|\psi_n(\lambda)\rangle$, and the eigenstates $|\psi_n(\lambda)\rangle$ satisfy $H(\lambda)|\psi_n(\lambda)\rangle = E_n|\psi_n(\lambda)\rangle$. Therefore, we have

\[ F^2(\lambda + \delta \lambda) = 1 - \delta \lambda^2 \sum_{n \neq 0} \frac{|\langle \psi_0(\lambda)|H_I|\psi_0(\lambda)\rangle|^2}{|E_0(\lambda) - E_n(\lambda)|^2} \]

From results above, the average fidelity susceptibility \[20\] can be calculated by

\[ \chi(\lambda, \delta \lambda) = \lim_{\delta \lambda \to 0} \frac{-2nF(\lambda, \delta \lambda)}{L\delta \lambda^2}. \]

Different from the EE, the divergence of fidelity susceptibility can directly point out the critical point. The related phase transition is exactly convincing [30].

In order to calculate both observables, the ground state is necessary. However, the exact solution of the model with three body interactions is difficult to get even in one dimensional system. Although the small size system can be achieved with exact diagonalization (ED), the thermodynamical properties need large scale numerical simulations. Thanks to the density-matrix renormalization-group (DMRG) \[31\] method, the ground state of the one dimensional system can be calculated with very high accuracy. Recently, even the two dimensional frustrated system can be touched beyond the sizes of ED method [14, 20]. We implement GPU speeding up Matlab code for the finite-size DMRG with double precision. The maximum total number of density matrix eigenstates held in system block is $m = 400$ in the basis truncation procedure, and it makes sure the truncation error is smaller than $10^{-7}$ for system sizes up to $L = 200$. With such high performance calculation, we can precisely analyze the quantum phase transition with both EE and fidelity.

### III. ALGORITHM AND MEASUREMENTS

The EE can be chosen as a measurement of the bipartite entanglement, and it is realted to detect quantum phase transition [29]. The EE is defined as follows. Assuming $|g.s.\rangle$ is the ground state which can be divided into two subsystems $A$ and $B$, and it is often useful to get the von Neumann entropy associated with larger subsystem. One convenient choice of subsystem $A$ is composed from the first site to the $L$th site and the subsystem $B$ is the rest sites of the system. The reduced density matrix of part $l$ can be obtained by taking the partial trace over system $L - l$, which is given by

\[ \rho_l = Tr_{L-l}(|g.s.\rangle \langle g.s.|). \]

Then, the bipartite entanglement between parts $l$ and $L - l$ can be measured via the block EE as

\[ S_l = -Tr(\rho_l \log_2 \rho_l). \]

Another option is to take two nearest neighbor or next nearest neighbor sites $(i,j)$ as subsystem $A$ and other sites as $B$. And such entanglement can be named as pairwise EE $S_{i,j}$. According to Ref. [29], in the spin half XXZ model, the block EE is more efficient than the pairwise EE to detect the phase transitions.

Another concept from quantum information theory, ground-state fidelity, can also be applied to capture the existence of the quantum phase transitions. Taking a general Hamiltonian $H(\lambda) = H_0 + \lambda H_I$ as an example, where $H_0$ is the main part, $H_I$ is the driving part and the quantum parameter $\lambda$ denotes its strength. If $\rho_0(\lambda)$ represents a state of the system, the ground-state fidelity between $\rho_0(\lambda)$ and $\rho_0(\lambda + \delta \lambda)$ can be defined as

\[ F(\lambda, \delta \lambda) = \text{Tr}[\sqrt{\rho_0^{1/2}(\lambda)\rho_0(\lambda + \delta \lambda)\rho_0^{1/2}(\lambda)}], \]

### IV. TWO-THIRDS FILLING

As discussed in Sec. II, the system is CDW phase in the strong coupling limit, and superfluid phase in the weak case. To figure out the quantum phase transition between them, at first, we considered the pairwise EE. Because the open boundary can introduce the edge effects in the fractional filling [34, 35], we adopted the periodical boundary condition for the simulation.
In the superfluid phase, the off-diagonal correlation is strong and long range, in other words, each site is highly entangled with the others. In contrast, the particles are localized in the CDW phase, and only their tiny local vibrations due to quantum fluctuation contribute small short range entanglement. These properties are also reflected by nearest neighbor (NN) pairwise EE $S_{i,i+1}$ shown in Fig. 1. It slowly increases during enhancing the three-body interactions $W$ from zero, and represents the NN sites are strongly entangled. However, after the critical point $W_c$, NN pairwise EE decreases rapidly to apparent small value which indicates the system enters into the CDW phase. Different from weak interactions case, the EE in the CDW phase is strongly size affected, the slope of the curve attends to be vertical for large size. Such kink of the EE hints a novel phase transition to the CDW phase. Different from weak interactions, the EE in the CDW phase is strongly size affected, and drop to low value after the critical point $W_c$. It also supports the superfluid and CDW phase in two limits.

Although the BOW structure factor introduced in Ref. [1] is not sufficient for distinguishing BOW and CDW phase, it can reflect the nonuniform correlations in the intermediate region. Thus, to find critical point of superfluid phase transition, we consider the next nearest neighbor (NNN) pairwise EE $S_{i,i+2}$ in different sizes shown in Fig. 2. Similar to the NN pairwise EE, the NNN pairwise EE also has a high value in the weak interactions region and drop to low value after the critical point $W_c$. It also supports the superfluid and CDW phase in two limits.

However, it doesn’t increase monotonically with $W$ as $S_{i,i+1}$ and has an extreme point at $W_{c2} = 3.35$. In the superfluid phase, both EE should have the same monotonicity, so the different behavior after $W_{c2}$ indicates the nonuniform of the system. However, the extreme points of pairwise EE are not the sufficient condition for the critical points.

After the Holstein-Primakoff transformation $b_i^\dagger \rightarrow S_i^+$, $b_i \rightarrow S_i^-$ and $n_i \rightarrow S_i^Z + 1/2$, the bosonic Hamiltonian (1) is mapped into spin-1/2 XXZ model with NNN and three-spin interactions

$$H = -t \sum_i (S_i^+ S_{i+1}^- + h.c.) + W \sum_i S_i^Z S_{i+1}^Z + \frac{3W}{4} \sum_i S_i^Z + \frac{W}{2} \sum_i S_i^Z S_{i+2}^Z + W \sum_i S_i^Z S_{i+1}^Z S_{i+2}^Z.$$  \hspace{1cm} (8)

Considering the critical point of superfluid phase transition in the XXZ model can be found with the extreme point of the block EE [29], we also investigate the block EE between two half subsystems shown in Fig. 3. Same as the XXZ model, the extreme point $W_{c2} = 3.5 \pm 0.1$ of block EE is also stable with increasing sizes. The left side of extreme point shows logarithm divergence with chain size $L$, and the right side drop quickly. Such behaviors are also similar to the superfluid phase transition in the spin half XXZ chain [29], so we argue that the superfluid phase undergoes the Kosterlitz-Thouless phase transition and its critical point may also exist at the extreme point of the block EE. We notice that the extreme point $W_{c2}$ is different from QMC result, and it may be due to the temperature effect or finite size scaling of the QMC simulations.

From the both NN pairwise EE and the block EE, we can see some clues of the superfluid phase transition found in Ref. [1]. Meanwhile, the sharp drop of both pairwise EEs seems indicate additional phase transition. In
2.5
4.5
5
0.06
4
0.04
0.02
5
4.5
4.5
3.5
4
3.5
5.5
FIG. 3. (Color online) The block EE between two half subsystems is plotted as a function of the three-body interactions for different system sizes.

order to figure out the phase transition to the CDW solid, we also considered the ground-state fidelity susceptibility with system size $L$ up to 96 and $\lambda = 0.01$. The ground-state fidelity susceptibility $\chi$ is plotted as a function of the interaction $W$ for different sizes in Fig. 4 with dimensionless units. Single peak of fidelity susceptibility is found in each size, and its value increases while the system size increases. To be more clear, we also plotted the maximal value of fidelity susceptibility in Fig. 4(b). The logarithm of maximum fidelity susceptibilities is treated as a function of the system size, and logarithmically divergent with $L$. The finite size scaling of fidelity susceptibility shows a power-law divergence at criticality, and the peak’s location moves to high $W$ up to a particular value as the system size increases.

Fidelity measures the similarity between two states, meanwhile quantum phase transitions are intuitively accompanied by an abrupt change in the structure of the ground-state wave function. This primary observation motivates researchers to use the fidelity to predict quantum phase transitions. According to the analysis of Ref. [36], a divergence in the fidelity susceptibility implies a quantum phase transition, but the converse is not true. Thus, the logarithmical divergence here concludes the phase transition. Moreover, because its divergence is power-law type, the phase transition should be second-order [38]. In order to get the critical point in the thermodynamic limit, scaling of the extreme point locations of $\chi$ as the system length increases becomes necessary. We find that the changes of the maximal points can also be fitted by the formula $W \sim W_c + aL^b$, where $a$ and $b$ are fitting parameters. We plot the location of the maximum fidelity susceptibility as a function of $L^b$ and show the numerical fit in Fig. 2(c). We obtain the critical point $W_c = 4.692$, $a = -19.51$, $b = -0.8306$ which is much near to the CDW melting point NN pairwise EE predicted. Considering phase transition detection is much convincing by using fidelity susceptibility, we conclude that the intermediate phase undergoes a second order phase transition to the CDW phase at $W_c = 4.692$.

Although we don’t know what the intermediate phase is, we can still discuss the excitation in the CDW phase. Because three adjacent sites are rarely empty, as shown in Fig. 5(a), we can define new occupation number of $i$th site as $n_i = (n_{i-1} + n_i + n_{i+1}) - 1$. By using such mapping, the CDW solid is mapped into the filing one Mott insulator. From the boundary, we can find the edge state with hole. It can freely move and decrease the CDW order, so the periodical boundary condition is also necessary. When one particle move to nearest neighbour site, for the new mapping configuration, it is equivalent to particle-hole excitation with long range hopping process which is shown in Fig. 5(b). Such excitation costs energy $W$, so in the new frame, it can be treat as onsite repulsion term $Wn_i(n_i - 1)$ of the Bose-Hubbard model. It is interesting that such excited quasi-particle can hop away from quasi-hole without costing additional energy. As shown in Fig. 5(c), if the system size is very large, when the kinetic energy $-4t$ is larger than the three body interactions $W$, the quasi-particle and quasi-hole prefer to separate with each other in a long distance. Considering the three-body interactions can also induce the effective repulsion, the model in new frame is similar to the extended Bose-Hubbard model in one dimensional system [38]. Thus, we think the intermediate phase may be related to the Haldane insulator and need more future works.
V. HALF FILLING

For the case of filling $n = 1/2$, there is no quantum phase transition in the system. We do not have to investigate the fidelity, while the investigation of EE is also interesting. For simplify, the open boundary condition is considered here. At half filling, the Hamiltonian at $W = 0$ can be transformed to spin XX model. For the open boundary condition, the block EE oscillates with odd subsystems and even subsystems. In order to prevent oscillation, we only choose the even subsystems block EE. Here we choose the subsystem $l = 2n(n = 1, 2, 3 \cdots$ and $l \leq L/2$), and see the entanglement is critical or non-critical. Our EE result at fixed density $n = 1/2$ is shown in Fig.4 for different three-body interactions $W$. The EE is plotted as a function of $l$ with $L = 200$. When the subsystem is fixed, the EE decreases with $W$ and increases when the subsystem $l$ is large. It confirms that there is no quantum phase transition.

For gapless system, the EE treated as a function of the subsystem’s size is logarithmically divergent with $l$ and increases when the subsystem $l$ is large. The extreme points of them indicates the related transition. The slopes of lines, which are corresponding to the central charge of the corresponding conformal field theory. The parameter $\log_2 g$ is boundary entropy and $S_0$ is a non-universal number. When $W = 0$, the EE can be fitted by Eq.9. We can obtain the central charge $c \approx 1.05$ at $W = 0$. It is a little larger than 1, because of finite sizes effect. When $W \neq 0$, the EE can also be fitted by Eq.9. The slopes of lines, which are corresponding to the central charge $c$, change slightly and they are shown in inset of Fig.4. For the antiferromagnetical anisotropic Heisenberg XXZ model, the entanglement is critical (non-critical) when $|\Delta| \leq 1$ ($\Delta > 1$), and it demonstrates the phase transition point between critical and non-critical entanglement region at $\Delta = 1$. Considering all the data show the critical behavior, we conclude that the system is in gapless SF phase all the time, no matter how large the three-body interaction is.

VI. CONCLUSION AND DISCUSSION

We reconsidered the one-dimensional hard-core Bose-Hubbard model with three-body interactions by using the DMRG methods. Different from the previous works [1], we found additional intermediate phase between the superfluid and CDW phase at two-thirds filling. From the NN and NNN pairwise EE, we found both of them increase monotonically in the superfluid region but different in the intermediate phase. In addition, both of them drop quickly when $W$ enters into the CDW phase and the slope becomes larger in the longer system length. Meanwhile, we also studied the block EE, and they reflect the Kosterlitz-Thouless phase transition of the superfluid phase. The extreme points of them indicates the related critical point.

Because the EE is not sufficient condition for the phase transition, we also considered the fidelity. And we found the convincing critical point $W_c = 4.692$ from the intermediate phase to the CDW phase with finite size scaling of the fidelity susceptibility. Combining with the previous QMC results [1] and the EE, we conclude the region $3.5 < W_c < 4.692$ is in the novel intermediate phase . With the new mapping process, we analyze the excitation in the CDW phase, and we argue that the phase transition may be induced with quasi-particle-hole excitations. Basing on the its similarity to the extended Bose-Hubbard system, we think the intermediate phase may be related to the Haldane insulator. The related possible topological excitation needs to be considered in the future work. At last, we consider the half filling case, we investigated the effects of interactions on EE and also
the scaling of the EE. Both results demonstrate that the system is always superfluid.

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