Entanglement in a hardcore-boson Hubbard model

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I. INTRODUCTION

Quantum entanglement is an important property which plays an essential role in the quantum information processing [1, 2, 3]. There are different types of entanglement, such as bipartite, multipartite, block [3], and localizable entanglement, etc [5]. The relative entropy of entanglement [6] and the entanglement of formation [7] can be used for qubits. Arbitrary bipartite entanglement can be assessed by the ”negativity” [8]. In recent years, the entanglement in Heisenberg models of finite systems of spins has been investigated [9, 10, 11, 12, 13, 14, 15, 16, 17]. The anisotropy effect [9, 10, 11] and the thermal energy [18, 19, 20] have all been studied in Heisenberg models. The entanglement in solids can also be witnessed by the magnetization [18] and the thermal energy [19, 20, 21]. In solids, there is a characteristic temperature below which a thermal entangled state can be obtained. The effects of quantum entanglement have been detected in the experimental situation [22]. Some attention has been drawn to the entanglement in the models of infinite spin systems [23, 24]. Owing to the quantum nonlocal correlations, the connection of the entanglement and quantum criticality in spin systems has been discussed [25, 26, 27, 28, 29, 30, 31, 32, 33, 34]. The quantum criticality can be shown by the entanglement of the ground state [3]. Next to Heisenberg models, boson Hubbard models have been extensively used to study the metal-insulator transition [35]. The Hubbard chain of hardcore bosons is one of the simplest models which can embody such quantum criticality. It is of interest to investigate the entanglement in the hardcore boson Hubbard chain.

In this paper, the entanglement of a hardcore boson Hubbard chain is studied for the ground and thermal states. In Sec. II, the global entanglement measure of the ground state is analytically expressed by the magnetization. The critical properties of the transition between the Mott-insulating phase and the superfluid phase are shown by the derivative of the global entanglement at ground state. In Sec. III, the ”negativity” of any two sites in the chain is derived. The multipartite entanglement at finite temperature is derived. The effects of the number of lattice sites, the temperature, and the chemical potential are investigated. A discussion concludes the paper.

II. GLOBAL ENTANGLEMENT OF GROUND STATE

Recently, the quantum entanglement of strongly correlated spin systems has been extensively studied. One of the interesting focuses was the relation of quantum phase transitions and entanglement in the ground state. As is well known, the phenomenon of quantum phase transitions describes the global properties of the ground state. Therefore, the measurement of global quantum entanglement is relevant to the investigation of the quantum phase transition. For a typical case, the spin version of the one-dimensional boson Hubbard is expressed by

$$H = -w \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i n_{ai} + U \sum_i n_{ai}(n_{ai} - 1)$$

(1)

where $a_i^\dagger$ and $a_i$ are the creation and annihilation operator for bosons on the site $i$ of the lattice, $n_{ai} = a_i^\dagger a_i$ is the number operator. The parameter $w > 0$ allows hopping of bosons from one site to another, $\mu$ represents the chemical potential of the bosons, and $U$ denotes the possible repulsive interaction among bosons on each site. For simplicity, only the nearest-neighbor pairs $\langle ij \rangle$ are considered. The off-site and long-range repulsive interactions are neglected. If the repulsion is very strong, when $U \to \infty$, there is only one boson at each site. The model is reduced to the simplest one of a hardcore boson Hubbard chain, which can also be written as a magnetic model of $S = \frac{1}{2}$ spin with pairwise interaction. The relation $\sigma_i^z = 1 - 2a_i^\dagger a_i$ is satisfied. In this following, the hardcore boson Hubbard chain is studied. It is known that this model is equivalent to the spin-1/2 Heisenberg XX

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chain with the ferromagnetic interaction $-w/2$ and the external magnetic field $\mu$. Through the Jordan-Wigner and Fourier transformations, the Hamiltonian $H$ can be exactly expressed by

$$H = - \sum_k \epsilon_k c_k^\dagger c_k$$

where $\epsilon_k = -2w \cos \frac{2\pi k}{L} - \mu$, $L$ is the number of sites on the lattice, and $c_k^\dagger, c_k$ are the Fourier-transformed fermionic operators.

To show the relation of entanglement and quantum criticality, the global entanglement $E$ of the ground state can be introduced by [36, 37].

$$E = 2[1 - \frac{1}{L} \sum_j \text{tr}(\rho_j^2)]$$

where $\text{tr}(\rho_j^2)$ is the trace of the reduced density matrix $\rho_i$ on the $i$th site of the ground state. Here, the eigenstates of $\sigma_z^i$ are assumed to be $\{|0\rangle_i, |1\rangle_i\}$. The reduced density matrix is given by $\rho_i = \frac{1}{M} \sum_j \text{tr}(\rho_j \sigma_z^i)$. Therefore, the global entanglement $E$ of the ground state can be just obtained by

$$E = 1 - M^2$$

For the values of $|\mu| \leq 2w$, there is partial occupation of sites at the ground state and $M = \frac{2}{\pi} \cos^{-1} \frac{\mu}{2w} - 1$. When $|\mu| \geq 2w$, $|M| = 1$. The global entanglement of the ground state is plotted as functions of the hopping coefficient $w$ and the potential $\mu$ in Fig. 1(a) when the number of sites is $L = 10^4$. It is shown that the global entanglement $E$ exists at the ground state if the potential satisfies $|\mu| \leq 2w$. The values of $E$ are decreasing in $|\mu|$ and then drop to zero when $|\mu| = 2w$. When $\mu \to 0$, it is the maximally entangled ground state which is exactly the Greenberger-Horne-Zeilinger state of the form $\langle \psi \rangle_g = \frac{1}{\sqrt{2}}(|010\cdots1 + |101\cdots0\rangle)$. The values $\mu \leq -2w$ or $\mu \geq 2w$, the ground state is an unentangled pure state $|00\cdots0\rangle$ or $|11\cdots1\rangle$. According to [33], there are two different kinds of phases namely the Mott-insulating phase and the superfluid one. It is found that the transitions between them occur under the condition $\mu = \pm 2w$. The global entanglement always exists in the superfluid phase while there is no entanglement in the Mott-insulating phase. To clearly demonstrate the phenomenon of a quantum phase transition in the ground state, the derivative of the global entanglement $E'_\mu$ is obtained

$$E'_\mu = \frac{\partial E}{\partial \mu} = \frac{4}{\pi^2 \sqrt{4w^2 - \mu^2}} [2 \cos^{-1} \frac{\mu}{2w} - \pi], \quad |\mu| \leq 2w.$$

When the potential $\mu \to 2w_-$, $\frac{\partial E}{\partial \mu} \to -\infty$ which reveals the divergence of $\frac{\partial E}{\partial \mu}$. The quantum criticality is depicted in Fig. 1(b) when the hopping coefficient is chosen to be $w = 1$. If $\mu \to 2w_+$, the derivative $\frac{\partial E}{\partial \mu} = 0$ for the global entanglement $E = 0$. It is found that the quantum criticality in the hardcore boson Hubbard chain can be shown by the global entanglement at the ground state.

### III. Entanglement at Finite Temperature

The thermal equilibrium state is $\rho(T) = e^{-H/kT}/Z$, where $Z$ is the partition function at finite temperature $T$ and $k$ is the Boltzmann constant. For convenience, both the Boltzmann constant $k$ and the Planck constant $\hbar$ are assumed to be one. Because the Hubbard chain of hardcore bosons is equivalent to the spin-1/2 Heisenberg XX chain, the reduced density matrix $\rho_{ij}$ on any two sites $i$ and $j$ can be expressed by the correlation function $K^{\alpha\beta}_{ij} = \text{tr}(\rho_i \sigma^\alpha_i \sigma^\beta_j)$. In the Hilbert space of $\{|00\rangle_{ij}, |01\rangle_{ij}, |10\rangle_{ij}, |11\rangle_{ij}\}$, the expression for $\rho_{ij}$ can be obtained

$$\rho_{ij} = \begin{pmatrix} u & 0 & 0 & 0 \\ 0 & w & t & 0 \\ 0 & t & w & 0 \\ 0 & 0 & 0 & v \end{pmatrix}$$

where $u = \frac{1}{4}(K^{xx}_{ij} + 2M + 1)$, $v = \frac{1}{4}(K^{xx}_{ij} - 2M + 1)$, $w = \frac{1}{4}(1 - K^{xx}_{ij})$, and $t = \frac{1}{4}K^{xx}_{ij}$. The analytical calculations of correlation functions $K^{\alpha\beta}_{ij}$ and the magnetization $M$ are straightforward given. For the number of sites $L$, the magnetization is given by $M = -\frac{1}{2} \sum_{L=1}^{L} \text{tanh}(\epsilon_q/2T)$. The two-site correlations can be by

$$K_{ij}^{xx} = K_{ij}^{yy} = \begin{pmatrix} G_1 & G_0 & \cdots & G_{r+2} \\ G_2 & G_1 & \cdots & G_{r+3} \\ \vdots & \vdots & \ddots & \vdots \\ G_r & G_{r-1} & \cdots & G_1 \end{pmatrix}$$

$$K_{ij}^{zz} = 4M^2 - G_r G_{-r}$$

where the parameter $r=|j-i|$ is the separation distance between two sites, and the item $G_r = G_{-r} = \frac{1}{2} \sum_{q=1}^{L} \cos(2\pi qr/L) \text{tanh}(\epsilon_q/2T)$.

The thermal entanglement in the chain can be investigated by the negativity $N$. Based on the separability principle, the negativity $N$ can be used to quantify the bipartite entanglement between two sites [8]. The negativity $N$ is introduced by

$$N(\rho) = 2|\sum_i \lambda_i|$$

where $\lambda_i$ is the $i$th negative eigenvalue of $\rho^T$ which is the partial transpose of the mixed state $\rho$. From the separability of quantum states, the partial transpose matrix $\rho^T$ has nonnegative eigenvalues if the states are unentangled and the value $N(\rho) = 0$. In the Hubbard model of hardcore bosons, the negativity of the two-site entangled state is given by

$$N(\rho_{ij}) = |u + v - \sqrt{(u-v)^2 + 4t^2}|$$
Thus, the entanglement on any two sites can be calculated numerically through Eqs. (7)-(9). The negativity $N$ is plotted as a function of site number $L$ in Fig. 2(a) when the temperature is $T = 0.5$, the hopping coefficient $w = 1$, and the potential $\mu = 0.2$. It is found that the pairwise entanglement always exists whatever the number $L$ of sites is. There is no thermal entanglement on two sites when the separation distance is $r > 2$. The value of $N$ is rapidly decreasing in $L$, and then reaches a constant value at $L = 16$. This result illustrates that the thermal entanglement can be detected in real solids of a very large number of particles.

The multipartite entanglement $E_L$ for the thermal states of systems with an even number of sites $L$ can be introduced \cite{DiVincenzo10}:

$$E_L(\rho) = \max \left\{ 0, \nu_0 - \sum_{j=1}^{2L-1} \nu_j \right\}$$

(10)

where $\{\nu_j\}_{j=0}^{2^n-1}$ is the spectrum of the operator $\sqrt{\rho U \rho U^{-1}}$ in decreasing order, $U$ is an anti-unitary time reversal operator and can be written as $U = \prod_{j=1}^n (-i\sigma_j^y)|\tau, \tau$ is the complex conjugate operator. The multipartite entanglement $E_L$ is plotted in Fig. 2(b). In Fig. 2(b), the value of $E_L$ is decreased with the increase of the number of sites $L$. The multipartite entanglement $E_L$ vanishes at $L = 10$. However, the bipartite entanglement still exists in this case.

It is also very interesting to study the effects of the temperature $T$ and the chemical potential $\mu$ on the thermal entanglement. By the analytical expression for the bipartite entanglement in Eq. \cite{DiVincenzo10}, the negativity $N$ is plotted as a function of $T$ and $\mu$ in Fig. 3(a) for $w = 1$ and $L = 10^4$. When the temperature $T$ and the chemical potential $|\mu|$ increase, the negativity $N$ decreases. It is found that the values of the negativity $N$ are symmetric about the chemical potential $\mu$. When $\mu \rightarrow 0$, the value of $N$ is maximal. For a definite chemical potential, the bipartite entanglement disappears at a certain temperature $T_c$. It is clear that the values of $T_c$ can be increased by decreasing the chemical potential $|\mu|$. It is seen that the entanglement can be detected at low temperatures in solids. The multipartite entanglement $E_L$ for the thermal state of $L = 6$ is plotted in Fig. 3(b) when $w = 1$. It is shown that the values of $E_L$ are also symmetric about the chemical potential $\mu$ and decreased with the increase of $|\mu|$. The ground state for $|\mu| < 0.5$ is just the maximally entangled GHZ state \[ \sqrt{2}(|010\cdots1\rangle + |101\cdots0\rangle) \]. The values of $E_L$ are declined with the temperatures $T$ and vanishes at about $T = 0.6$.

IV. DISCUSSION

The entanglement in a hardcore boson Hubbard chain at ground and thermal equilibrium states is investigated. The global entanglement at ground state is analytically expressed by the magnetization. When the potential $\mu \rightarrow 0$, the maximally entangled Greenberger-Horne-Zeilinger state can be obtained. The quantum criticality is revealed by the divergence of the derivative of the global entanglement at ground state. In the parameter plane of Mott-insulator and superfluidity phases, it is found that the entanglement exists in the SF phase while there is no entanglement in the MI phase. The bipartite entanglement between any two sites is deduced by the negativity. For a very large number of sites $L$, the pairwise entanglement can always exist. When the number $L$ increases, the negativity decreases rapidly and then reaches a constant value at a certain number of site. While the multipartite entanglement will decrease to zero with increasing $L$. The thermal entanglement vanishes at a certain temperature and is decreased with the increase of the potential $\mu$. It is shown that the entanglement can be detected at low temperature in real solids of a large number of sites.

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**Figure Captions**

**Fig. 1**
(a) The global entanglement $E$ of the ground state is plotted as a function of the hopping coefficient $w$ and the potential $\mu$. The number of sites is $L = 10^4$; (b) The derivative $\frac{\partial E}{\partial \mu}$ is plotted to show the quantum criticality of the ground state.

**Fig. 2**
The thermal entanglement is plotted as a function of the number of sites when $w = 1$, $\mu = 0.2$, and $T = 0.5$. (a) The pairwise entanglement of the negativity $N$; (b) The multipartite entanglement $E_L$.

**Fig. 3**
The thermal entanglement is plotted as a function of the potential $\mu$ and the temperature $T$ when the hopping coefficient is $w = 1$. (a) The pairwise entanglement for $L = 10^4$; (b) The multipartite entanglement $E_L$ for $L = 6$. 
Fig. 1
Fig. 2
Fig. 3