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Quantum Monte Carlo study of hard-core bosons in Creutz ladder with zero flux*

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The quantum phase of hard-core bosons in Creutz ladder with zero flux is studied. For a specific regime of the parameters ($t_x = t_p, t_y < 0$), the exact ground-state is found analytically, which is a dimerized insulator with one electron bound in each rung of the ladder. For the case $t_x, t_y, t_p > 0$, the system is exactly studied using quantum Monte Carlo (QMC) method without a sign problem. It is found that the system is a Mott insulator for small t_p and a quantum phase transition to a superfluid phase is driven by increasing t_p. The critical t_p^c is determined precisely by a scaling analysis. Since it is possible that the Creutz ladder is realized experimentally, the theoretical results are interesting to the cold-atom experiments.

Keywords: quantum Monte Carlo method, Creutz ladder, Mott insulator

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1. Introduction

Creutz model is a cross-linked ladder threaded by a flux, in which Creutz shows that edge states emerge at open boundaries.[1,2] While Creutz's study is in the context of lattice gauge theory, the model can be thought as a one-dimensional (1D) topological insulator, which belongs to AIII class and is characterized by an integer.[3] The Creutz ladder is closely related to two-dimensional Bernevig–Hughes–Zhang model describing two-dimensional topological insulator HgTe quantum well and it can be obtained through a dimensional reduction from the latter.[4–8] Based on the Creutz ladder, many studies have been carried out, such as the effects of interaction and disorder in the topological phase. For specific parameters, Creutz ladder has flat bands, in which fermions and bosons exhibit exotic quantum phases.[11–13] With induced s-wave superconductivity in the Creutz ladder, a transition from fractionally charged solitons to Majorana bound states is found.[14] The Creutz ladder may be realized in cold atoms and their concrete implementations have been proposed.[15,16]

Besides the Creutz ladder, its variational versions have also attracted increasing interests, one of which is the ladder without next-nearest-neighbor interchain hopping.[17,18] It is found that free-fermions and hard-core bosons in such a ladder exhibit different physics. One of them is that the charge gap exists as long as the transverse hopping $t_y \neq 0$ for hard-core bosons, while a large enough t_y is needed to open a charge gap for fermions. It is also shown that the Meissner currents and a vortex phase emerge in the presence of a uniform magnetic field.[19,20]

Fermions and bosons on a ladder subjected to magnetic fields have been the topic of current theoretical and experimental works. It is noted that the studies of Creutz ladder mainly focus on fermions and the behaviors of bosons in Creutz ladder are largely unexplored. In this work, the quantum phase of hard-core bosons in Creutz ladder with zero flux is studied. For a specific regime of the parameters, we analytically obtain the ground-state, which is a dimerized insulator with one electron bound in each rung of the ladder. Then we apply quantum Monte Carlo (QMC) method to study a parameters' regime without a sign problem.[21,22,25–29] We find that the system is a Mott insulator for small next-nearest-neighbor interchain hopping t_p and a quantum phase transition to a superfluid phase is driven by increasing t_p. By performing a scaling analysis, the critical t_p^c is precisely determined. Since it is possible that the Creutz ladder is realized experimentally, the theoretical results are interesting to the cold-atom experiments.

2. Results

2.1. Creutz ladder

The Creutz ladder is described by the Hamiltonian

$$\begin{aligned}\hat{H} = & -\sum_i [t_x e^{-i\phi} \hat{c}^\dagger_{1,i} \hat{c}_{1,i+1} + t_x e^{i\phi} \hat{c}^\dagger_{2,i} \hat{c}_{2,i+1} \\ & + t_p \hat{c}^\dagger_{1,i} \hat{c}_{2,i+1} + t_p \hat{c}^\dagger_{2,i} \hat{c}_{1,i+1} + t_y \hat{c}^\dagger_{1,i} \hat{c}_{2,i} + \text{H.c.}] \\ & - \mu \sum_{l,i} n_{l,i}, \end{aligned} \tag{1}$$

where $\hat{c}^\dagger_{l,i}$ ($\hat{c}_{l,i}$) is the creation (annihilation) operator of fermion on the i-th site with $l = 1, 2$ labeling the legs of the ladder; t_x, t_y, and t_p are the longitudinal, transverse, and next-nearest-neighbor interchain hopping amplitudes respectively, and t_x is set to 1 as the energy scale; 2ϕ is a mag-

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netic flux threading each plaquette; $n_{l,i} = c^{\dagger}_{l,i}c_{l,i}$ is the number operator; and μ is the chemical potential. In the momentum space, the Hamiltonian is given by $\mathcal{H}(k) = -(h_0 I + h_x\sigma_x + h_z\sigma_z)$, where $h_0 = 2t_x\cos\phi\cos k$, $h_x = t_y + 2t_p\cos k$, $h_z = 2t_x\sin\phi\sin k$; σ_x and σ_z are Pauli matrices; and I is the identity matrix. Its energy spectrum is obtained directly as $E_{\pm}(k) = -h_0 \pm \sqrt{h_x^2 + h_z^2}$. The system is gapped except the cases when $\sin\phi = 0$ and $|t_y| \leq 2$ or $|t_y| = \pm 2$. The topological property of the insulators can be characterized by the Berry phase, which is defined as[23,24]

$$\gamma = \mathrm{i}\oint \langle\varphi(k)|\frac{\mathrm{d}}{\mathrm{d}k}|\varphi(k)\rangle, \tag{2}$$

with $\varphi(k)$ the eigenfunction of the occupied states. For $|t_y| < 2$, the Berry phase $\gamma = \pi$ and the insulator is topological nontrivial, while the insulators with $|t_y| > 2$ are trivial with $\gamma = 0$.

Then we load hard-core bosons into the Creutz ladder. The Hamiltonian of such system has the same form as the one in Eq. (1) except that the creation (annihilation) operator of fermion $\hat{c}^{\dagger}_i(\hat{c}_i)$ is replaced by the corresponding ones of hard-core bosons $\hat{b}^{\dagger}_i(\hat{b}_i)$. The hard-core boson operators obey commutation relationship $[\hat{b}_i, \hat{b}^{\dagger}_j] = 0$ for $i \neq j$, but anticommutation one $\{\hat{b}_i, \hat{b}^{\dagger}_i\} = 1$ on the sole site. This makes the hard-core bosons exhibit different physical properties from the fermions. We first compare the ground-state energies of bosons and fermions with the same form of the Hamiltonian. As shown in Fig. 1, hard-core bosons usually have a lower ground-state energy than fermions. However if the hopping is frustrated due to the presence of the magnetic flux, hard-core bosons can have a higher ground-state energy. The momentum distributions of hard-core bosons and fermions are also different. For noninteracting fermions, each momentum eigenstate below the Fermi energy are filled and $n_{\mathrm{f}}(k) = 1$ for $k < k_{\mathrm{F}}$, whereas hard-core bosons tend to condense near the bottom of the band and the momentum distribution exhibits a peak near the corresponding momentum.

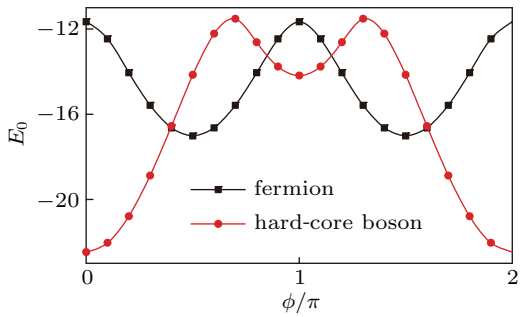


Fig. 1. (color online) The ground-state energies of fermions and hard-core bosons in Creutz ladder as a function of the flux ϕ.

In the remainder of the paper, we study the quantum phases of hard-core bosons in the Creutz ladder. We focus on the case with zero flux, i.e., $\phi = 0$, for which the quantum phases can be exactly studied using QMC without a sign problem.

2.2. Quantum phases of hard-core bosons in Creutz ladder with zero flux

2.2.1. Exact ground state for the case $t_x = t_p$, $t_y < 0$

The Hamiltonian has a fully dimerized eigenstate $|\psi\rangle = |0\rangle_1 \otimes |0\rangle_2 \ldots \otimes |0\rangle_L$ at half filling, with

$$|0\rangle_i = \frac{1}{\sqrt{2}}(|0,1\rangle - |1,0\rangle), \tag{3}$$

where $i = 1, \ldots, L$ labels the rung of the ladder and $|n_1, n_2\rangle$ is product state with $n_1(n_2) = 0, 1$ the hard-core boson numbers on the sites of the rung. To show that $|\psi\rangle$ is an eigenstate, we define two local operators on each rung

$$\begin{aligned} \alpha^{\dagger}_i &= \hat{b}^{\dagger}_{1,i} + \hat{b}^{\dagger}_{2,i}, \\ \beta^{\dagger}_i &= \hat{b}^{\dagger}_{1,i} - \hat{b}^{\dagger}_{2,i}. \end{aligned} \tag{4}$$

It is noted that $\alpha^{\dagger}_i|\psi\rangle = \alpha_i|\psi\rangle = 0$. In terms of the rung operators, the Hamiltonian can be written as

$$\begin{aligned} \hat{H} = -\sum_i^L \Big[& t_y(\alpha^{\dagger}_i\alpha_i - 1) \\ & + \left(\frac{t_x + t_p}{2}\alpha^{\dagger}_i\alpha_{i+1} + \frac{t_x - t_p}{2}\beta^{\dagger}_i\beta_{i+1} + \mathrm{H.c.}\right)\Big]. \end{aligned} \tag{5}$$

If $t_x = t_p$, the last term vanishes and $|\psi\rangle$ is the eigenstate of $\hat{H}$ with the eigenenergy $E = Lt_y$. So when t_y is negative, the above eigenstate may be the ground state with the energy per rung $-|t_y|$. We also show the exact diagonalization (ED) result in Fig. 2. From a critical t_y, the energy from ED is exactly $-|t_y|$, thus the dimerized eigenstate described in Eq. (3) is the ground state.

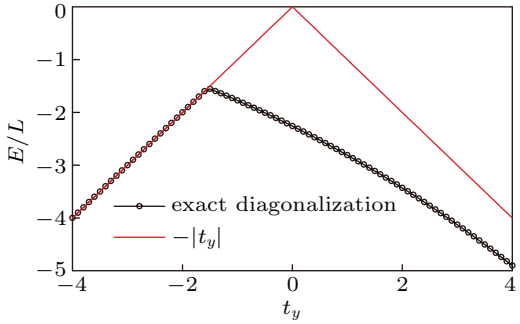


Fig. 2. (color online) The energy per rung of the ground state as a function of t_y. The hopping amplitudes $t_x = t_p = 1$.

2.2.2. QMC study of the case $t_y > 0$

When the parameters t_x, t_y, and t_p in Eq. (1) are all positive, the Hamiltonian can be exactly studied using QMC with SSE algorithm. The SSE method calculates the mean density of particles by

$$\rho = n/L, \tag{6}$$

where n labels the total particle number of the system and L is the system size. The corresponding superfluid density is thus given by[18]

$$\rho_{\mathrm{SF}} = \frac{\langle W^2 \rangle}{2td\beta L^{d-2}}, \tag{7}$$

where β is the inverse temperature, W is the winding number of the particle world lines, and d is the dimensionality.

We first study the case without next-nearest-neighbor interchain hopping t_p to confirm our methodology. The results are demonstrated in Fig. 3. A plateau with vanishing superfluid density in the ρ–μ curve is clearly visible at half-filling for $t_y = 2$, implying the existence of a charge gap and that the system is in a Mott insulating state. However for $t_y = 1$ the ρ–μ curve becomes almost continuous and it is hard to determine whether the plateau exists. In fact the plateau shows its presence through the sharp decrease of the superfluid density. A further scaling analysis shows that the plateau exists down to $t_y = 0$. These results are consistent with the previous work, thus our QMC simulations are reliable.

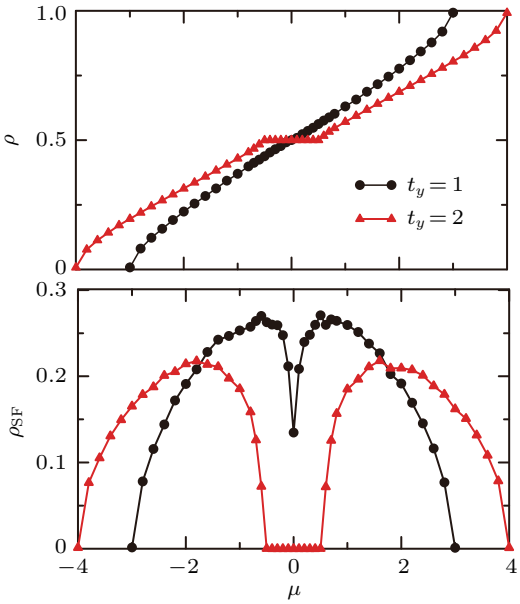


Fig. 3. (color online) QMC results for the particle density ρ and the superfluid density ρ_{SF} as a function of the chemical potential μ without next-nearest-neighbor inter-chain hoppings. The size of the ladder is 2×64.

In the following we explore whether the Mott insulator still exists after the next-nearest-neighbor interchain hopping t_p are included. The average density ρ at different t_p are calculated, shown in Fig. 4. It has been known that at $t_p = 0$ the system is a Mott insulator with a finite charge gap. As t_p is included and increased, the plateau representing the size of the gap gets narrower. At around $t_p = 0.6$, the plateau is not visible in the ρ–μ curve. A key issue is whether a critical value t_p^{c} exists, beyond which the system becomes gapless superfluid phase. To address this question, we perform scaling analysis of the superfluid density. A superfluid phase is characterized by the persistence of nonzero ρ_{SF} as the lattice size increases.

To perform the scaling analysis, the superfluid densities are calculated on lattices with different sizes. The length of the chain L is taken from 16 up to 256. The inverse of the temperature $\beta = 4L$ is low enough to ensure the ground state. For a Mott insulating state, the superfluid density as a function of the lattice size L is expected as $\rho_{\mathrm{SF}} \sim \mathrm{e}^{-L/\xi}$. As shown in Fig. 5, the above formula fits the data well. A further check

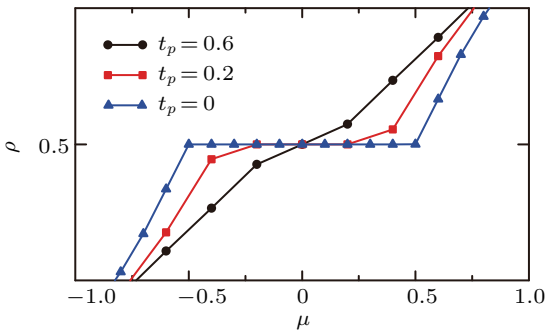


Fig. 4. (color online) The density ρ as a function of μ obtained on 2×64 Creutz ladder with zero flux for $t_y = 2$ and $t_p = 0$, 0.2, 0.6. The plateaux get narrower when t_p is increased.

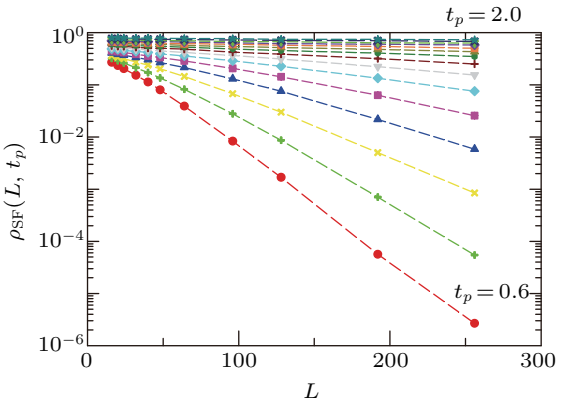


Fig. 5. (color online) The superfluid density versus the length of the ladder L for various values of t_p with $t_y = 2$. t_p varies from 0.6 to 2.0 with the interval 0.1.

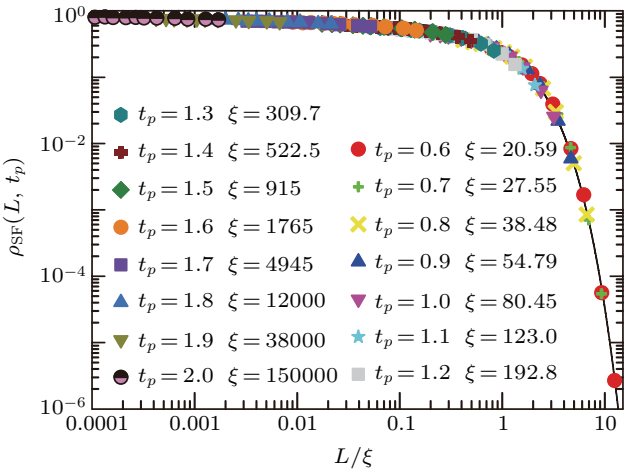


Fig. 6. (color online) Collapse the data in Fig. 5 by rescaling the x-axis $L \to L/\xi$.

of the wellness is to collapse the data, i.e., those in Fig. 5 are analyzed by rescaling the x-axis $L \to L/\xi$ (see Fig. 6). Then the correlation length ξ can be extracted. If a critical point t_p^c exists, the correlation length should be divergent at the critical point.

We plot ξ curve versus t_p in Fig. 7. It is obvious that ξ increases exponentially with t_p. The function form $\xi = \xi_0 e^{a/(t_p - t_p^c)}$ is used to fit the data. The fitting process gives $t_p^c = 3.001$. Thus the correlation length diverges here and the superfluid density is finite in the thermodynamic limit. The Mott insulating state is driven to a gapless superfluid phase by a finite next-nearest-neighbor interchain hopping. We also analyze the cases with other t_y using the same method. For $t_y = 1$, the scaling analysis yields the critical value $t_p^c = 0.9761$.

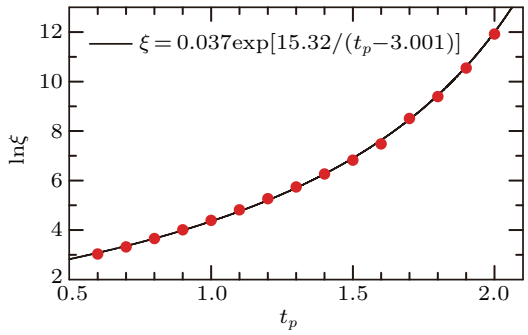


Fig. 7. (color online) The correlation length ξ versus next-nearest-neighbor interchain hopping t_p. The function form $\xi = \xi_0 \exp[a/(t_p - t_p^c)]$ is used to fit the points.

3. Conclusion

The quantum phase of hard-core bosons in Creutz ladder with zero flux is studied. For a specific regime of the parameters ($t_x = t_p$, $t_y < 0$), the exact ground-state is found analytically, which is a dimerized insulator with one electron bound in each rung of the ladder. For the case $t_x, t_y, t_p > 0$, the system is exactly studied using QMC method without a sign problem. It is found that the system is a Mott insulator for small t_p and a quantum phase transition to a superfluid phase is driven by increasing t_p. The critical t_p^c is determined precisely by a scaling analysis. Since it is possible that the Creutz ladder is realized experimentally, the theoretical results are interesting to the cold-atom experiments.

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