Interacting electrons on Moebius strip with disorder

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Abstract. Since the discovery of NbSe3 Möbius strip in 2002, topological shape materials have attracted attention from various fields. Focus has been put mostly on their electronic property with the expectation of possible application to a new device. However the electronic property is not fully understood yet. In particular the roles of electron interactions and impurities and their interplay are not quite clear and need to be understood for full clarification of the electronic property and for practical application. In the present study we numerically investigated a Möbius strip using a simple model Hamiltonian and studied the effect of interactions and impurities on electronic transport property. We found that electron interaction in transverse direction had a strong influence to charge ordering under a certain condition. Localization effect of impurity potentials is also discussed.

1. Introduction

Ring geometry is a simple example of finite low-dimensional systems. Electrons in a ring form persistent current with a flux penetrating in the ring. Issues of persistent current have been discussed especially with emphasis on the roles of electron-electron interactions and impurities. The width or finite cross section of the ring wire is another element to examine to explain experimental results. With a long strip with a finite width, we could make a ring geometry by imposing a periodic boundary condition in the longitudinal direction. But if we impose a twisted boundary condition, we have a Möbius strip.

Persistent current in a Möbius strip was already studied by Refs.[1, 2], which focused on interactions between electrons or on electron scattering from impurities. In this article we studied another interaction effect, formation and destruction of Mott insulator, on a Möbius strip. The formation of Mott insulating state on an ordinary ring with no topological twist in the boundary condition is expected when electron-electron interactions are sufficiently strong and electron number density satisfies a certain condition of commensurability with the lattice sites. However on a Möbius strip, we found that interactions in transverse direction played a crucial role in stabilizing the electron density order in longitudinal direction. To eliminate subtle approximation issues, we performed quantum Monte Carlo simulation of spinless fermions on a Möbius strip with electron-electron interactions and impurity potentials. The paper is organized as follows. In Sec. 2 we introduce the Hamiltonian that we used in the simulations and show the details of the parameters that we employed. In Sec. 3 we present the result of the numerical calculation and Sec. 4 is devoted to conclusions.
2. Model

We started from the simplest model of Möbius strip, imposing a twisted boundary condition to a two-leg ladder system as shown in Fig. 1. Before going to our model Hamiltonian, let us first point out the fact that the parity of the number of electrons plays an important role in the formation of Mott insulator in the absence of the random potential. Figures 2 and 3 show typical electron configuration (with only two electrons shown) in a Mott insulator with an odd and even number of electrons, respectively. These two types of configurations would be stable if there is no interaction in transverse direction. The configuration in Fig. 3 becomes unstable, however, as the transverse direction interaction gets stronger, while the interaction stabilizes the electron configuration in Fig. 2.

Now we show the Hamiltonian that we employed in the quantum Monte Carlo simulation. To focus on the role of interactions and impurity potentials, we neglected transverse hopping of electrons and spin degree of freedom and the Hamiltonian is therefore given by:

$$H = -t \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + V \sum_i n_i n_{i+1} + V' \sum_i n_i n_{i+L/2} + \sum_i \epsilon_i n_i,$$

(1)

where $t$ presents hopping energy in the longitudinal direction, $V$ and $V'$ denote the electron-electron interaction in the longitudinal and transverse directions respectively, and $\epsilon$ is random site energy representing the impurity potential. The probability distribution of the random site energy is assumed to be uniform in the range from $\epsilon = -\Delta$ to $\Delta$. The total number of the lattice sites is set to be an even number $L$ and the interaction term of $V'$ is therefore expressed by the interaction between electrons on the site $i$ and on the site $i + L/2$. Using this Hamiltonian, we measured current-current correlation function

$$C(\tau) = \langle j(\tau) j(0) \rangle$$

(2)

where $\tau$ is imaginary time in the path integral formalism and $j = i \sum_i (c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i)$ is current operator. We are particularly interested in the zero frequency limit of the Fourier transform of the correlation function, for the following reason[4].

Persistent current is generated when a flux $\phi$ is applied to penetrate a ring (Möbius ladder in our case), and is given by

$$I(\phi) = \frac{\partial F}{\partial \phi} = -\frac{2\pi i}{\beta \phi_0} < W >,$$

(3)

where $\beta$ is inverse temperature, $\phi_0$ is flux quanta and $W$ is winding number. From the Fourier expansion form of $I(\phi)$

$$I(\phi) = \sum_n \sin \frac{2\pi n \phi}{\phi_0},$$

(4)
we obtain
\[ \frac{2\pi i}{\phi_0} < W^2 > |_{\phi=0} = \beta i \sum_n I_n n. \]  
(5)

If we neglect higher harmonics \( I_2, I_3, \cdots \), which would be allowed at least in the presence of random potential, we get
\[ I_1 = \frac{2\pi}{\beta \phi_0} < W^2 > |_{\phi=0}, \]  
(6)

where the fluctuation of the winding number \( < W^2 > \) is given by the zero frequency limit of the Fourier transform of the correlation function \( C \).

In the following result we set \( < n_i > = 0.5 \) (half filling) and \( t = 1 \) as energy unit, and fixed \( V = 10 \).

3. Result
We here show only the simulation result of the current-current correlation functions of half-filled band electrons with and without random potential. The number of the electrons was chosen to be even, so that the electron configuration in Fig. 3 is realized when the transverse interaction and random potential are both absent. Turning on the transverse interaction and the random potential changes the electronic state. Figure 4 shows the correlation function vs. frequency for 6 electrons on 12 sites under different strength of the random potential. Remember that the first harmonics of the persistent current \( I_1 \) is proportional to the correlation function at zero frequency, and characterizes electronic transport. In Fig. 4, \( I_1 \) is zero even in the absence of the random potential (indicated by the symbol “+”), suggesting that the transverse interaction \( V' = 2.0 \) is too weak to destroy the Mott insulator which is formed by the longitudinal interaction \( V = 10.0 \). In this case the Möbius ladder behaves like an ordinary one-dimensional ring system, and the application of the random potential drives the system into Anderson insulator. In fact the correlation function in Fig. 4 is always zero at zero frequency, indicating that the system remains insulating in the presence of the random potential. The finite frequency part of the correlation function is first enhanced by the application of the random potential and decreases as the strength of the random potential \( \Delta \) becomes larger.

Figure 5 shows, on the other hand, that moderately strong electron-electron interaction in the transverse direction, \( V' = 10 \), destroys the Mott insulator when \( \Delta = 0 \) (indicated by "+" in the figure) and drives the system into a metal with finite \( I_1 \). As the strength of the random
potential increases, the zero frequency part as well as finite frequency part of the correlation function gradually decrease, and electron localization develops. However, with weak disorder, the localization length is still larger than the system size and the system stays in metallic phase with finite $I_1$. When the random potential exceeds a critical value (around $\Delta = 5$), the system is completely localized and becomes an Anderson insulator with $I_1 = 0$.

Comparing Figs. 4 and 5, we notice that the transverse interaction $V'$ could destabilize the Mott insulator and change the system to a metal, making the zero-frequency part of the current-current correlation function finite, but it also suppresses the finite-frequency part of the correlation function. So the transverse interaction not only plays a crucial role in the formation (or destruction) of Mott insulator but also has a certain effect on dynamical property of the system.

4. Conclusions

Structural shape is one of major characteristics of an electron system, especially if it is topologically nontrivial. Systems of topologically nontrivial shape have been studied, not extensively though, mostly from theoretical viewpoints, until a Möbius strip of single crystal was developed experimentally[3]. In this article we picked up the simplest model of Möbius strip, i.e. ladder system with twisted boundary condition, and studied numerically the role of electron-electron interactions and random potentials performing quantum Monte Carlo simulations. To see the most drastic feature, we focused on the stability and instability of Mott insulator in terms of the longitudinal and transverse interactions and on the interplay between the interactions and random potentials.

Unlike ordinary ladders with periodic boundary condition, Mott insulator of half-filled band electrons on the Möbius ladder, formed by the electron-electron interactions in the longitudinal direction, can be destabilized by the interactions in the transverse direction when the number of the electrons is even. Let us consider this problem in a different manner. Note that the Möbius ladder with the twisted boundary condition can be constructed by twisting and folding a single large ring, where $V$ is the interaction between electrons on neighboring sites and $V'$ between electrons on the opposite sides of the ring diameter. So there are short range interaction $V$ and long range one $V'$ acting on the ring. It can be easily imagined that they work sometimes collaboratively and sometimes competitively in forming a Mott insulator, depending on the number of the electrons in the ring, and that the long range interaction $V'$ has strong influences on the transport of the electrons along the ring.

Since we did not include electron hopping in the transverse direction in our Möbius ladder, coherent motion of the electrons which might be characteristic to topologically nontrivial systems was outside the scope of our study. Work is in progress in this prospect.

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