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Hole localization in strongly correlated and disordered systems: DMRG studies for 1-D and 3-leg ladder random Hubbard models

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ABSTRACT

We study one-dimensional and 3-leg ladder repulsive Hubbard models with random potential by using the density-matrix renormalization group method. When holes are slightly doped to the half-filling, the local Mott phase called "Mott plateau" and the local dip structure in density profile called "hole localized valley" are well-separately observable in strong on-site repulsive U/t and strong randomness for both models. We suggest that these separated structures qualitatively capture locally inhomogeneous characters seen in heavily under-doped High-T_c superconductors.

1. Introduction

Metal–Insulator transition observable in transition metal oxides and the others has been a major focus of research in solid state physics. Electronic states drastically change close to the transition, and emergent phases show very rich varieties depending on crystalline structures and other factors. For example, High-T_c superconductors are weakly coupled layered materials, and their superconductivity emerges close to antiferromagnetic insulator by doping hole career.

Generally, careers, i.e., electrons or holes simply localize in the insulating phase. There are two well-known reasons for the localization. The first one is randomness, which is inevitable in solid states, and the Anderson transition [1] is its consequence. The second one is Coulomb repulsion, which causes the Mott transition and creates rich strongly correlated phases close to the transition.

Recently, an interplay between the randomness and the Coulomb repulsion has attracted much attentions of condensed matter physicists [2]. The reason is that their competition or cooperation may give rise to non-trivial phases, which are much beyond our theoretical expectation. In fact, there is an argument that randomness has an important role on mysterious features observed in under-doped High-T_c superconductors.

As a model system capturing the interplay, the random Hubbard model has been intensively examined. However, the main theoretical target has been limited to the half-filling and the quarter filling, and the doped cases have been never explored. This is because the doped system is too difficult to solve for not only theoretical treatments but also numerical simulations. Namely, any theoretical studies may fail to predict the ground state in the model due to difficulties.

Very recently, we have suggested that the difficulty is broken by employing the density-matrix renormalization group (DMRG) method [3,4]. In this paper, we study the one-dimensional (1-D) random Hubbard model by using DMRG method and also examine 3-leg ladder random Hubbard model by using directly extended DMRG method [5], which was developed by three authors of this paper (S. Yamada, M. Okumura, and M. Machida). We note that our focus of interest is a slightly doped region very close to the half-filling, which is deeply related to complicated phenomena seen in heavily underdoped High-T_c superconductors.

2. 1-D random Hubbard model

In this section, we treat the 1-D random Hubbard model and focus on the slightly doped regime to the half filling.

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2.1. Model and parameters

The 1-D random Hubbard model is given by

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i\sigma}c_{j\sigma} + \sum_{i,\sigma}\epsilon_i n_{i,\sigma} + \sum_i U n_{i\uparrow}n_{i\downarrow} \quad (1)$$

where t is the amplitude for hopping between the nearest neighbor lattice sites, U is the on-site repulsion, ϵ_i is local amplitude of the disorder, $c_{i\sigma}(c^{\dagger}_{i\sigma})$ is the annihilation-(creation-)operator with spin index σ, $n_{i,\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ is the local density operator, and $\langle i,j\rangle$ refers to nearest neighbors i and j. In this paper, we choose a continuous probability distribution for $\epsilon_i : \mathscr{P}(\epsilon_i) = \theta(W/2 - |\epsilon_i|)/W$, where $\theta(x)$ is the step function and the parameter W is a measure of the disorder strength.

In the following, we examine 1-D chain system whose length $L = 50$ and the filling is in a slightly underdoped range as $\bar{n} = 0.96$ and 0.88, where $\bar{n} = \sum_{i=1}^{L}(n_{i,\uparrow} + n_{i,\downarrow})/L$. In the presently used DMRG, the number of states kept, m is 100 for all calculations.

In this paper, we present local density profiles of the particles, which are quite difficult for theoretical techniques to obtain.

2.2. Density profile with $U/t = 20$ in 2 hole case

In this subsection, we consider $\bar{n} = 0.96$ case, i.e., 2 hole doped system. The interaction strength is fixed to be $U/t = 20$, and the randomness magnitude parameter varies as $W/t = 0, 2, 12$, and 30. In Fig. 1, we show typical density distributions of electrons with the random potential whose shape is depicted on the bottom of the figure. When $W/t = 0$, i.e., the randomness turns off, the observed density profile is smooth, keeping the values of the density lower than unit except for the both edges. On the other hand, when weak randomness ($W/t = 2$) turns on, one finds "Mott plateaus" in a wide range. In addition, one can find two valleys whose centers locate at $i = 5$ and $i = 41$. Here, we note that the number of doped holes equals to the number of the valleys. This indicates that a doped hole tends to localize at a valley. When stronger randomness ($W/t = 12$) is given, it is found that the Mott plateaus become flatter (wider) and the hole valleys consequently deeper. These behaviors in the density profiles are non-trivial because the increase of the randomness magnitude is expected to usually make the profile more random. In this case, the randomness promotes the organization [2]. However, when the randomness is larger than the interaction strength ($W/t > U/t$), it is found that the Mott plateau is destroyed and the density profile is governed by the shape of random potential.

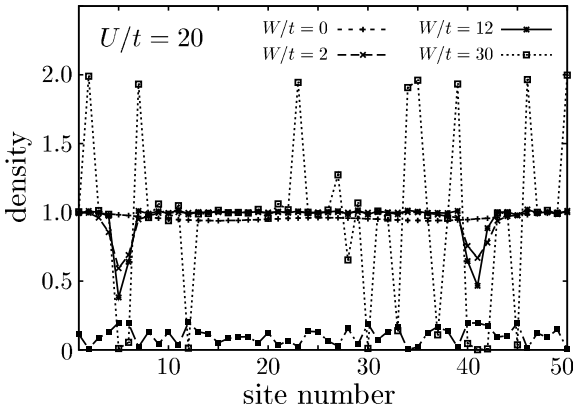

Fig. 1. Density profiles of electrons with varying randomness strength $W/t = 0, 2, 12$, and 30 and the fixed interaction strength $U/t = 20$. The number of holes is 2 ($\bar{n} = 0.96$). The horizontal and the vertical axes represent the site number and the density, respectively. The shape of the random potential (arbitrary unit) is also shown on the bottom of the figure.

2.3. Characterization of density profiles

In the previous subsection, we have found the localized behaviors of doped holes from the randomness dependence of the density profile under a fixed U/t. To characterize how the localization depends on the interaction strength and the randomness, we introduce the following function:

$$M(U,W) = \left\langle \sum_{i=1}^{L} \exp\left[\frac{-(n_{i,U,W;\epsilon} - 1)^2}{2\Delta^2}\right]/nL \right\rangle_{\epsilon}, \quad (2)$$

where $n_{i,U,W;\epsilon} = n_{i,\uparrow} + n_{i,\downarrow}$, and $\langle\cdot\rangle_{\epsilon}$ is the arithmetical average for realizations of the random potential. We use $\Delta = 0.05$ and take the average of 10 realizations of random potential in this paper. Here, let us discuss the meaning of the function. The function approaches a unit ($M(U,W) \to 1$) when almost all sites are occupied by the Mott plateau. This means that a doped hole localizes on a site i.e., $n_i = 0$ in a site and $n_i = 1$ in the other sites. Fig. 2 presents $M(U,W)$ in $\bar{n} = 0.96$ (2 holes) case. The range of U/t and W/t is from 0 to 30, and the step value is 2 for U and W axes. In the figure, one finds that there is a boundary line, i.e., just on the $W = U$ line, where the color gradation drastically changes. This indicates that the Mott plateaus rapidly grow and the holes simultaneously localize with increasing U/t (along $W/t = const.$) closes to the line.

Let us explain more details of the diagram. Firstly, it is found that the value of $M(U,W)$ slightly increases when the value of W varies from the bottom ($W = 0$) toward the boundary line along a fixed U line. This represents a tendency that the density profile in the Mott plateau becomes flatter with increasing the random potential magnitude, which is found in Fig. 1. Next, when the value of (U,W) reaches the boundary line, the total length of the Mott plateaus becomes the longest. Finally, when the value (U,W) passes over the boundary line, the value of $M(U,W)$ rapidly drops. The final behavior reflects the randomization in the density profile caused by the strong random potential as seen in Fig. 1. When one sees Fig. 2 along the boundary line ($W = U$), again, one finds that the value of $M(U,W)$ around the line becomes larger as U and W increases. This behavior indicates that the strong interaction prevails against the random potential and makes the size of the Mott plateaus longer to lower the total energy of the system.

2.4. Density profiles in 6 hole case

In the previous two subsections, we have shown the typical density profiles and the $U - W$ dependence of the total length of

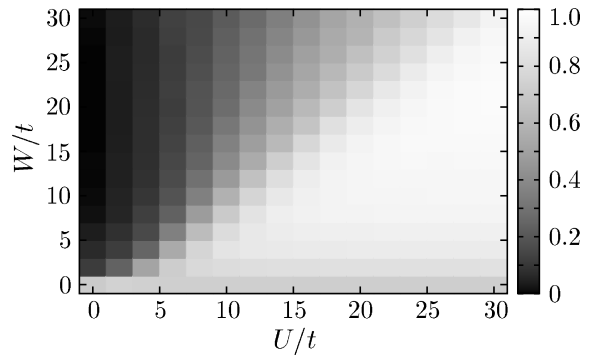

Fig. 2. A contour plot of the value of $M(U,W)$ in $\bar{n} = 0.96$ (2 holes) case. The horizontal and the vertical axes represent the coupling strength and the randomness strength, respectively, both of which are normalized by the hopping constant t; U/t and W/t.