

Hole Localization in the One-Dimensional Doped Anderson-Hubbard Model

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We study an interplay of disorder and correlation in the one-dimensional hole-doped Hubbard-model with disorder (Anderson-Hubbard model) by using the density-matrix renormalization group method. Concentrating on the doped-hole-density profile, we find in a large U/t regime that the clean system exhibits a simple fluidlike behavior whereas finite disorders create locally Mott regions which expand their area with increasing the disorder strength contrary to the conventional sense. We propose that such an anomalous Mott phase formation assisted by disorder is easily observable in atomic Fermi gases by setting up the box-shape trap.

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Recently, atomic Fermi gas loaded on an optical lattice (FGOL) has attracted a lot of attention, since FGOL is expected to be an excellent testbed to resolve controversial issues in condensed matter physics [1]. One of the advantages of FGOL is a tunability of the interaction between two atoms associated with the Feshbach resonance [2], which opens up a pathway to systematically study not only BCS-BEC crossover but also strongly correlated behaviors. Another advantage is the flexibility in making playgrounds such as the periodical lattice, which provides various stages including disorder effects for many-body interacting systems [1].

Among a huge number of proposals on FGOL, one of the unique challenges is a study of interplay between randomness and strong correlation [1]. This is one of the most difficult but important problems in real solids because high- T_c superconductor is a typical reality. In high- T_c superconductors, their common mother phase is the Mott insulator showing antiferromagnetism [3]. The carrier is doped by chemical substitution, which inevitably brings a random potential. However, the disorder effects in strongly correlated systems have been too complicated issues to study theoretically and experimentally in condensed matters. Thus, its interplay has remained as an unsolved issue. On the other hand, FGOL is a very good experimental reality in systematically examining such a complex issue due to the wide tunability and flexibility.

In this Letter, we study the doped Mott insulator with disorder in a form of the Anderson-Hubbard model [see Eq. (1) below], and predict experimental results on FGOL by means of the density-matrix renormalization group (DMRG) method [4,5]. Consequently, we find that the disorder does not destroy the Mott insulator but help the growth of the Mott phase domains contrary to our naive expectation. Such a nontrivial feature is kept and amplified until the disorder amplitude fully exceeds over the repulsive interaction strength.

So far, the harmonic trapped FGOL has been considered in theoretical studies. For instance, Gao *et al.* have reported

their DMRG calculation results for the 1D Anderson-Hubbard model [6,7] with the harmonic trap potential [8]. However, the harmonic trap induces spatially inhomogeneous filling which is different from usual situations in solid state matters. On the other hand, the box trap with disorder provides almost equivalent stages. Thus, our target reality is one-dimensional (1D) FGOL confined in a box-shaped trap with lattice including randomness. In its experimental setup, see Ref. [9] for the box-shape trap and Ref. [1] for the random potential.

The Hamiltonian of the 1D Anderson-Hubbard model is given by

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

where $\langle i, j \rangle$ refers to the nearest neighbors i and $j = i \pm 1$, t is the hopping parameter between the nearest neighbor lattice sites, U is the on-site repulsion, $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) is the annihilation (creation) operator with spin index $\sigma = \uparrow, \downarrow$, $n_{i,\sigma} (\equiv c_{i\sigma}^\dagger c_{i\sigma})$ is the site density operator, and the random on-site potential ϵ_i is chosen by a box probability distribution $\mathcal{P}(\epsilon_i) = \theta(W/2 - |\epsilon_i|)/W$, where $\theta(x)$ is the step function and the parameter W controls the disorder strength. In all DMRG calculations, we employ the open boundary condition for the box-shape trap, and focus on the site density of fermions as $n_i = n_{i\uparrow} + n_{i\downarrow}$.

The 1D Anderson-Hubbard model has been intensively investigated in the context of the transition between the Anderson and Mott insulators [10–12]. To our knowledge, however, this model has not been fully studied in a range of slight to under doping. Although the model may look simple, the interplay among the disorder, the interaction, and the doped holes requires more accurate and more systematic studies. This Letter provides the first systematic results of doped-hole profiles under a full accuracy.

In order to calculate the ground state of the Hamiltonian (1), we use the DMRG method [4,5]. The validity of our DMRG results was verified by results of the exact diago-

nalization in a case of ($8 \uparrow, 8 \downarrow$) with 18 sites ($L = 18$) at $U/t = W/t = 30$. Both the results give a good agreement. The size dependence in terms of doped-hole profiles is checked for $L = 50, 100, 150$, and 200 , which reveal that $L = 50$ is enough to characterize hole profiles. In the following, we present results of 1D system with the length $L = 50$ in three fillings, $\bar{n} = \sum_{i=1}^L n_i/L = 0.96, 0.88$, and 0.52 . In the use of DMRG, the number of states kept m is set maximum 256 for several cases, and $m = 100$ is confirmed to be enough to obtain convergent results because the largest deviation of the local density between them is below 10^{-4} .

First, let us show DMRG results of density profiles when 2 holes (\uparrow, \downarrow) are doped and the filling $\bar{n} = 0.96$. Figures 1(a)–1(d) display typical profiles obtained by varying W in a fixed $U/t = 30$ under a certain random configuration as depicted at the bottom. In the clean limit ($W = 0$), one finds a fluidlike density profile as Fig. 1(a), which belongs to the Tomonaga-Luttinger liquid with open boundary conditions. With switching on W , flat density regions whose site density equals to a unit emerge with two clear dips as Fig. 1(b). The locations of the dips do not shift by choice of the boundary condition, i.e., open or periodic boundary condition. We also confirm the fact by using the exact diagonalization in $L = 18$ sites. Here, we name the flat density region and the dip “Mott plateau” and “hole valley”, respectively. We note that the number of observed

hole valleys equals to that of doped holes. This implies that holes tend not to collect but to localize separately. Furthermore, one finds from Figs. 1(b) and 1(c) that the edges of the Mott plateaus become sharper and the hole valleys become deeper as the randomness strength W increases from $W/t = 2$ to 18 [see also Figs. 3(b) and 3(c) for another doping case]. This clearly indicates that the randomness *assists* the formation of Mott plateaus rather than breaking the structure. This is quite nontrivial because disorder is usually believed to break flat homogeneous distribution. Since the clean system exhibits Tomonaga-Luttinger liquid except for the half-filling, these results clearly illustrate that the randomness is essential for the local development of the Mott state, where the strong interaction and the randomness cooperatively form the Mott plateaus with localizing the doped holes. This is suggestive for the fact that the insulator phase in high- T_c superconductors survives tiny doping.

When the randomness W increases and approaches $W \sim U$, the Mott plateaus are disturbed partly by disorder [see Fig. 1(d)]. By further increase of W above U , the Mott plateau with localized holes breaks down. Figures 1(e)–1(h) show typical density profiles in a weaker interaction $U/t = 10$. Similar to Figs. 1(b) and 1(c), the structure of the Mott plateau with localized holes is seen for $W < U$, as Figs. 1(f) and 1(g). The structure is, however, completely destroyed by the strong random potential $W > U$ as seen in Fig. 1(h). Under the strong randomness, the local density takes values close to 2 (the double occupation) at several sites, and the Mott plateaus are too small to be identified as a region.

The W dependent density profiles seen in Fig. 1 suggest that there is an optimum W (U) for a fixed U (W) in making the Mott plateaus as wide as possible and the hole valleys as sharp as possible. To evaluate an optimum set of parameters (U, W), we introduce a function $M(U, W)$ in the two variable space to characterize the extent of the Mott plateau in the total density profile, which is defined by a summation of “closeness” of the local density to unit expressed as

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

where $n_i(\epsilon, U, W) \equiv n_{i,\uparrow} + n_{i,\downarrow}$ means the local site density under a realization of the random potential at a certain set of U, W and a local potential ϵ , and $\langle \cdot \rangle_{\epsilon}$ is the algebraic average for multiple random realizations. Δ characterizes the peak width of the function, for which we fix $\Delta = 0.05$. We note that the factor $1/(\bar{n}L)$ is the normalization constant which is adjusted to make $M(U, W) \simeq 1$ when the extent of the Mott plateaus is the maximum, e.g., $M(U, W) \simeq 1$ when $n_i = 0$ at two lattice points and $n_i = 1$ at other 48 lattice points if two holes are doped in $L = 50$.

Figure 2 shows a contour plot of $M(U, W)$ obtained by the arithmetical average over ten realizations of random

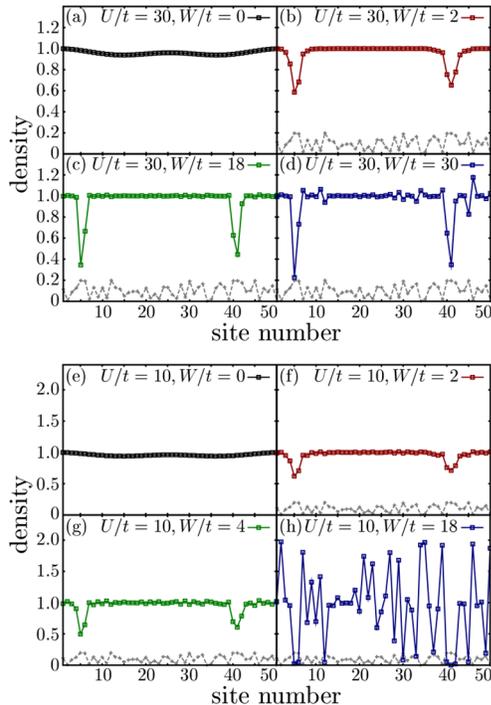


FIG. 1 (color online). The randomness W dependent density profiles $n(i)$ for 2-holes doped case ($\bar{n} = 0.96$) at two fixed interaction strengths, (a)–(d) for $U/t = 30$, and (e)–(h) for $U/t = 10$, under a random potential depicted in the bottom of each figure in arbitrary unit (gray dashed line).

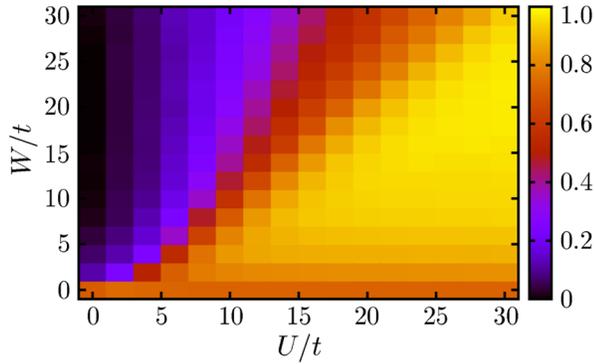


FIG. 2 (color online). A contour plot of $M(U, W)$ in 2 holes doped case ($\bar{n} = 0.96$) as a function of U/t and V/t . Arithmetic average over ten realizations of random potentials is taken. The step values are 2 for both U/t and W/t axes.

potentials for $\bar{n} = 0.96$ (2 holes doped) case. Along a fixed W/t line, one finds that the value of $M(U, W)$ increases monotonically with increasing U/t . This is consistent with what one sees in Fig. 1; i.e., the width of the Mott plateaus in the $U/t = 30$ case [Fig. 1(c)] is wider than that in $U/t = 10$ case [Fig. 1(h)] on the same randomness strength $W/t = 18$. On the other hand, along a fixed U line, the value of $M(U, W)$ initially increases with increasing W , reaches the maximum values close to $W + 2t \sim U/2$ line, and then decreases after crossing the maximum value. Thus, one finds in the slightly doped case that holes are confined as compactly as possible when W is about a half of U so that the width of the hole valley is almost a unit lattice constant. It indicates that doped holes almost lose their quantum delocalizing character.

Here, we turn our attention to the cases in which more holes are doped. Figures 3(a)–3(d) show the total density distributions of fermions in $\bar{n} = 0.88$ (6 holes) case with $U/t = 20$, where we can confirm almost the same behaviors as $\bar{n} = 0.96$ (2 holes) case. Namely, the introduction of disorder results in the formation of both the Mott plateaus and hole valleys, and further increase of W makes the Mott plateaus wider and hole valleys deeper [compare Fig. 3(b) ($W/t = 2$) with (c) ($W/t = 14$)]. One also finds that the number of valleys is exactly the same as that of doped holes at $W/t = 2$ case while the number becomes smaller than that of doped holes at $W/t = 14$ and $W/t = 20$. The tendency to create the Mott plateau still remains even for far away from the half-filling. Figures 3(e)–3(h) show the density profile for $\bar{n} = 0.52$ (24 holes, i.e., close to the quarter filling) at $U/t = 10$. Although the number of valleys is no longer the same as that of doped holes in all cases ($W/t = 2, 12$, and 20) and the number of fermions is not enough to simply form the Mott plateau at this filling, the maximum density is nearly a unit [see Figs. 3(g) and 3(h)]. This suggests even in such a high doping level that both the interaction and randomness cooperatively work.

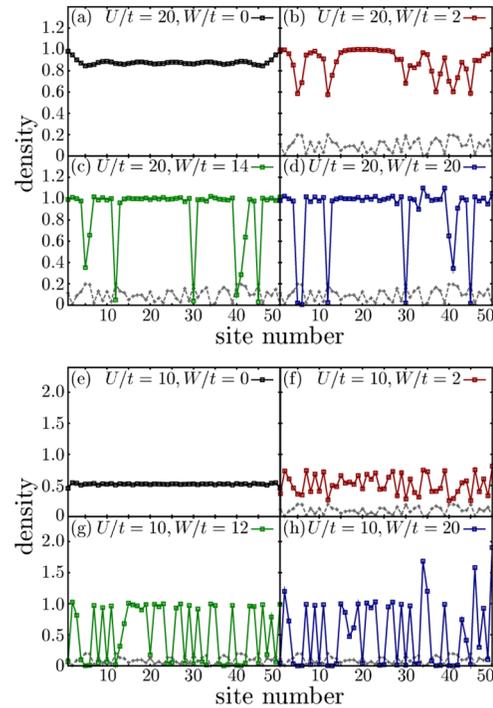


FIG. 3 (color online). The randomness W dependent density profiles $n(i)$ of (a)–(d) 6 ($\bar{n} = 0.88$) and (e)–(h) 24 ($\bar{n} = 0.52$) holes doped cases under a random potential shown in the bottom of each figure in arbitrary unit (gray dashed line).

Figures 4(a) and 4(b) show contour plots of $M(U, W)$ for $\bar{n} = 0.88$ (6 holes) and $\bar{n} = 0.52$ (24 holes) cases, respectively. These essentially show the same tendency as $\bar{n} = 0.96$ (2 holes) case. The value of $M(U, W)$ increases with

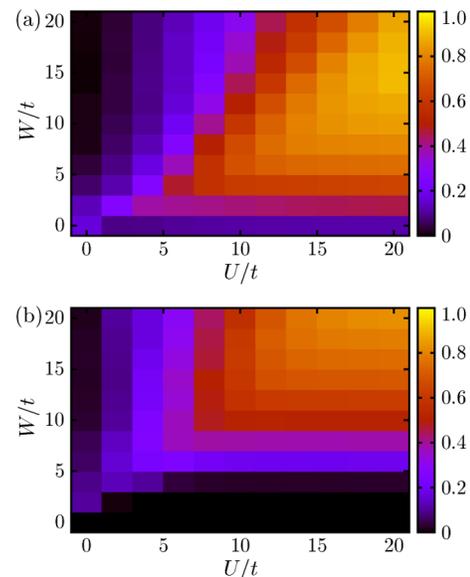


FIG. 4 (color online). Contour plots of the value of $M(U, W)$ in (a) $\bar{n} = 0.88$ (6 holes) and (b) $\bar{n} = 0.52$ (24 holes) cases with the arithmetic average of ten realizations of random potentials. The step value for both U/t and W/t is 2.

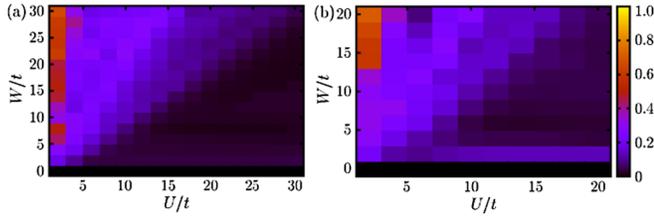


FIG. 5 (color online). Contour plots of $D(U, W)$ in (a) 2 holes doped case ($\bar{n} = 0.96$) and (b) 6 holes doped case ($\bar{n} = 0.88$) as a function of U/t and W/t . Arithmetic average over ten realizations of random potentials is taken. The step values are 2 for both U/t and W/t axes.

increasing U/t at a fixed W/t , and the optimum value of $M(U, W)$ exists for a fixed U/t . On the other hand, one finds in more details that the maximum of $M(U, W)$ shifts to $W + 2t > U/2$ side with increasing the number of doped holes. This is because, in high hole-density cases, the random potential magnitude required to push the local density up to the unit becomes larger. In addition, high hole-density causes the reduction of the maximum value of $M(U, W)$, because it suppresses the correlation effect and works unfavorably in forming the Mott plateaus.

We also examine fluctuations of $M(U, W)$ on different randomness by evaluating the standard deviation per average $D(U, W) = \sqrt{\langle (M_\epsilon(U, W)/M(U, W) - 1)^2 \rangle_\epsilon}$, where $M_\epsilon(U, W) = \sum_{i=1}^L \exp(-[n_i(\epsilon, U, W) - 1]^2/2\Delta^2)/(\bar{n}L)$. As expected, one finds in Fig. 5(a) (2 holes doped case) that $D(U, W)$ becomes relatively small when $M(U, W)$ shows large values, and vice versa. This clearly demonstrates that the formation of Mott plateaus does not depend on the realization of random potential and $M(U, W)$ is a good measure to know it. We also obtain almost the same behavior of $D(U, W)$ in the 24 holes case as shown in Fig. 5(b).

In conclusion, we calculated the density profiles of fermions in the 1D Anderson-Hubbard model by varying interaction strengths, random potential amplitudes, and fillings below the half-filling by means of DMRG. We found a clear signature that the presence of disorder assists the local formation of the Mott state in the weak disorder region whereas the Mott phase is destroyed by strong disorder. As a characterization of the width of the Mott phase, we calculated the function $M(U, W)$ from the density profiles, and found that the increase of the doping rate shifts the maximum of $M(U, W)$ from $W + 2t = U/2$ line to $W + 2t > U/2$ side. These nontrivial behaviors of doped holes like the present DMRG works can be systematically examined by FGOL with the box trap. The experimental confirmation will give a crucial contribution to studies for doped Mott insulators.

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