Numerical study of disorder effects on the three-dimensional Hubbard model

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Combined effects of interactions and disorder are investigated using a finite temperature quantum Monte Carlo technique for the three-dimensional Hubbard model with random potentials of a finite range. Temperature dependence of the charge compressibility shows that the Mott gap collapses beyond a finite disorder strength. This is a quantum phase transition from an incompressible phase to a compressible phase driven by disorder. We calculate the antiferromagnetic structure factor in the presence of disorder as well. Strong antiferromagnetic correlation, which is characteristic of the Mott insulator, is destroyed by a finite amount of disorder.

I. INTRODUCTION

As well as the repulsive interaction between electrons, the influence of disorder is essential in many electronic systems. Although either of these two effects causes a metal-insulator transition, the physical characters are quite different. The repulsive interaction tends to suppress the double occupancy of electrons. On the other hand, in random potentials, electrons can favor doubly occupied states if the random potential is sufficiently low at the site. Therefore, the interaction and disorder may have opposite effects on the charge degree of freedom. In the insulator due to the interaction (Mott insulator), the charge fluctuation is strongly suppressed and a finite charge gap opens, while the insulating phase due to disorder (Anderson insulator) does not necessarily have a charge gap. Another difference between these two insulators is the existence of magnetic correlation. Since the repulsive interaction induces local magnetic moments, the Mott insulator has a strong antiferromagnetic correlation. On the other hand, the Anderson insulator does not necessarily enhance magnetic correlation. Therefore one may expect that the interaction and disorder compete in both charge and spin degree of freedom. Especially, it is important to investigate to what extent the stability of the Mott insulator remains in the presence of disorder.

The Hubbard model with disorder is one of the simplest models that include these two effects. In one and two dimensions, the transition from the Mott to the Anderson insulator is confirmed by various methods \cite{1} - \cite{9}. Also the dynamical mean field theory \cite{10} is applied to the infinite dimensional Hubbard model and consistent results are obtained \cite{10}. On the other hand, there is no work beyond the mean field approximation in three-dimensional case \cite{12}. Therefore approximation-free results can be useful to understand the three-dimensional strongly correlated system with disorder.

In the present paper, we study the three-dimensional Hubbard model with random potentials using a finite temperature quantum Monte Carlo (QMC) method. The rest of this paper is organized as follows. In Sec.II, we introduce the three-dimensional disordered Hubbard model and describe physical observables. In Sec.III, we discuss the effects of disorder on the charge compressibility and the magnetic structure factor.

II. MODEL AND METHOD

The Hamiltonian of the disordered Hubbard model is given by

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle \sigma} (\hat{c}_i^\sigma \hat{c}_j^\sigma + \hat{c}_j^\sigma \hat{c}_i^\sigma) + U \sum_i \hat{n}_i^\uparrow \hat{n}_i^\downarrow + \sum_{i\sigma} w_i \hat{n}_i^\sigma, \]

where \( t \) is the nearest neighbor hopping amplitude, \( \langle i, j \rangle \) is a nearest-neighbor link, \( U \) is the on-site interaction and \( \{ w_i \} \) are random potentials chosen from a flat distribution in the interval \([-W,W]\). The system is on the cubic lattice in three dimensions and we use the periodic boundary condition. We treat the system in a grand canonical ensemble with the chemical potential \( \mu \). The grand canonical method is suitable to study the charge degree of freedom because the charge fluctuation is taken into account statistically \cite{13}. In this treatment, we make the system half-filled by setting \( \mu = U/2 \). In the absence of disorder with sufficiently large \( U \), the ground state is an antiferromagnetic insulator where the charge fluctuation is strongly suppressed.

In order to obtain approximation-free results, we employ a finite temperature determinantal Quantum Monte Carlo method \cite{14}, \cite{15}. We also use the matrix-decomposition technique to remove numerical instabilities at low temperatures \cite{16}. The simulations are performed in the half-filled sector (\( \mu = U/2 \)) for lattices with sizes up to \( N = 6 \times 6 \times 6 \) with \( U/t = 6 \). We choose a Trotter time slice size \( \Delta \tau \simeq 0.15/t \). We have checked that the systematic error due to the Suzuki-Trotter decomposition is almost independent of temperatures and does not change the qualitative feature. For each realization of disorder, we have typically run 2000 Monte Carlo sweeps for measurements after 500 sweeps in the warming up run. For all the observables, we average over 24 realizations of disorder and the errors are estimated.
by the variance among realizations of disorder. Since the system does not have a particle-hole symmetry in each realization of disorder, the negative-sign problem occurs. For example, the value of average sign is $\sim 0.1$ for $N = 4 \times 4 \times 4$ and $W/t = 1$ at temperature $T/t = 0.1$. Although it is not so severe as a doped case, a simulation at a very low temperature with strong disorder is difficult.

The physical observables we have calculated are the compressibility $\kappa$ and the magnetic structure factor $S(q)$ defined as

$$\kappa = \frac{1}{N} \frac{\partial N_e}{\partial \mu} = \frac{\beta}{N} \left( \langle \hat{N}_e^2 \rangle - \langle \hat{N}_e \rangle^2 \right),$$

$$S(q) = \frac{1}{N} \sum_{i,j} e^{i q (r_i - r_j)} (\langle \hat{n}_{i\uparrow} \hat{n}_{j\downarrow} \rangle - \langle \hat{n}_{i\downarrow} \hat{n}_{j\uparrow} \rangle),$$

where $N$ is the number of sites, $N_e$ is the number of electrons and $\beta$ is an inverse temperature. The charge compressibility $\kappa$ measures the charge fluctuation. If the system has a finite charge gap, the compressibility shows thermally-activated behavior in a low temperature region and vanishes at $T = 0$. On the other hand, the system without a charge gap has a finite compressibility at $T = 0$ due to the existence of low-lying excitations. The magnetic structure factor $S(q)$ at $q = (\pi, \pi, \pi)$ diverges in a low temperature region when the system has an antiferromagnetic (quasi-) long-range order.

### III. RESULTS AND DISCUSSION

Figure 1 shows the temperature dependence of the charge compressibility for several different strength of disorder. Average over 24 realizations of disorder is performed. Without disorder, the temperature dependence of the compressibility $\kappa$ shows thermally-activated behavior reflecting the existence of a finite charge gap. The compressibility $\kappa$ at $T = 0$ is zero within the numerical accuracy for the pure system. It indicates that the ground state of the pure Hubbard model in three dimension is in an incompressible phase. In the presence of disorder, the compressibility is enhanced. For weak disorder, although enhanced, the compressibility still shows thermally-activated behavior and the value at $T = 0$ seems to be zero. On the other hand, there is no tendency to decrease in $\kappa$ for $W > W_c$ ($W_c \sim U/2$) down to the lowest temperature we studied. It means that the critical disorder strength to destroy the Mott gap, $W_c$, is of the order of the Mott gap since the system is in the strong coupling region ($U/t = 6$). Although we cannot exclude the possibility of vanishing $\kappa$ at $T = 0$, what we have shown here is the best data within the numerical restriction. The results imply that sufficiently strong disorder destroys the Mott gap which is of the order of the interaction in the strong coupling region. In the presence of disorder, when we discuss the physics locally, making one doubly occupied site gains an potential energy $2W$ at the maximum, while it costs a Coulomb energy $U$.

Therefore one may expect that the Mott gap collapses at $W > W_c$ ($W_c \sim U/2$) regardless of dimensionality in the strong coupling region. In other words, since charge properties of the Mott insulators in the strong coupling region is determined locally, the effect of disorder would be also local and independent of dimensionality. Indeed, the Mott gap collapses at $W_c \sim U/2$ in one, two and infinite dimensions in the strong coupling region. It is in contrast to the quantum nature of the long-range properties of the correlation functions which have a drastic difference in the dimensionality. (e.g. Luttinger liquid in one dimension). The transition we observed is a disorder-driven quantum phase transition from an incompressible (gapped) to a compressible (gapless) phase. However, it does not necessarily mean an insulator-metal transition. The compressibility takes a finite value in both a metallic phase and an insulating phase due to disorder (Anderson insulator). It is possible that the competition between the interaction and disorder leads to a metallic phase especially in the three-dimensional system. However, to distinguish these two phase, one needs simulations for a sufficiently large system, which we cannot perform because of the negative-sign problem.

Figure 2 shows the temperature dependence of the antiferromagnetic structure factor $S(\pi, \pi, \pi)$. Since the ground state has an antiferromagnetic long-range order, the $S(\pi, \pi, \pi)$ shows diverging behavior toward the Néel temperature in the absence of disorder. For weak disorder, the structure factor is slightly suppressed, but diverging behavior is still observed down to the temperature we studied. This means that the ground state still has an antiferromagnetic long-range order. When sufficiently strong disorder is included, the temperature dependence of the $S(\pi, \pi, \pi)$ changes qualitatively. The diverging behavior of $S(\pi, \pi, \pi)$ disappears. This indicates that the long-range antiferromagnetic correlation is also destroyed by a finite amount of disorder. Umke et al. argue that weak disorder stabilizes antiferromagnetic order for $U > U_c$, where $U_c$ is the interaction for which the Néel temperature takes a maximum value. [6], [11]. Since the strength of the interactions we studied is $U \approx U_c$, [6], we did not observe it.

In summary, the three-dimensional Hubbard model with random potential of a finite range has been studied numerically using a finite temperature quantum Monte Carlo method. The temperature dependence of the charge compressibility suggests that sufficiently strong disorder closes the Mott gap. The transition from an incompressible phase to a compressible phase occurs at a finite strength of disorder. The disorder also destroys an antiferromagnetic long-range order which is characteristic of the Mott insulator. As in the case of the Mott gap, the antiferromagnetic correlation is robust against weak disorder. These features are common in one, two and infinite dimensional systems.
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**FIG. 1.** Temperature dependence of the charge compressibility $\kappa$, where $U/t = 6$, a) $L = 4 \times 4 \times 4$ and b) $L = 6 \times 6 \times 6$. Without disorder, $\kappa$ shows thermally-activated behavior and decreases toward $T = 0$, indicating the existence of a charge gap. For weak disorder, $\kappa$ still shows thermally-activated behavior. On the other hand, for strong disorder, $\kappa$ does not decrease down to the temperature we studied. It is a disorder-driven transition from an incompressible phase to a compressible phase.

**FIG. 2.** The antiferromagnetic structure factor as a function of temperature ($T/t$), where $U/t = 6$, a) $L = 4 \times 4 \times 4$ and b) $L = 6 \times 6 \times 6$. For weak disorder, the antiferromagnetic structure factor shows diverging behavior down to the temperature we studied. On the other hand, for strong disorder, the divergence behavior is not observed. This indicates that sufficiently strong disorder destroys the long-range antiferromagnetic correlation which is characteristic of the Mott insulator.
Fig. 1

(a) and (b) show graph comparisons for different values of $W/t$. The x-axis represents $T/t$, and the y-axis represents $\kappa$. Each graph includes symbols for $W/t = 0.0, 0.5, 1.0, 2.0, 3.0$. The points are connected by lines to illustrate trends as $T/t$ increases.
