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2000 J. Phys.: Condens. Matter 12 9317

(http://iopscience.iop.org/0953-8984/12/44/312)

J. Phys.: Condens. Matter **12** (2000) 9317–9322. Printed in the UK PII: S0953-8984(00)14767-8

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

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Received 16 June 2000, in final form 18 September 2000

Abstract. The 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 finite range. The temperature dependence of the charge compressibility shows that the Mott gap seems to collapse 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 the presence of a finite amount of disorder.

1. Introduction

Like the repulsive interaction between electrons, the influence of disorder is crucial in many electronic systems. Although both of these effects lead to metal–insulator transition, the physical characters of the resulting transitions are quite different. The repulsive interaction tends to suppress the double occupancy of electrons. On the other hand, in random potentials, electrons can favour 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 as regards the existence of a 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 have an enhanced magnetic correlation. Therefore one may expect the interaction and disorder to compete as regards both charge and spin degrees of freedom. In particular, it is important to investigate how stable the Mott insulator is against disorder. Indeed, many of the correlated electron systems such as the prototype Mott insulators, heavy-electron systems and the parent compounds of high-T_c superconductors are intrinsically disordered, in particular upon doping. The effects of disorder on these systems have been studied in many experiments [1].

The Hubbard model with disorder is one of the simplest models that includes these two effects. In one and two dimensions, the transition from the Mott to the Anderson insulator is confirmed by various methods [2–10]. Also the dynamical mean-field theory [11] has been applied to the infinite-dimensional Hubbard model and consistent results obtained [12]. On

0953-8984/00/449317+06$30.00

the other hand, there has been no work beyond the mean-field approximation in the three-dimensional case [13]. Therefore approximation-free results can be useful for understanding the three-dimensional strongly correlated system with disorder. This is one of the motivations of our study.

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 section 2, we introduce the three-dimensional disordered Hubbard model and describe the physical observables. In section 3, we discuss the effects of disorder on the charge compressibility and the magnetic structure factor.

2. Model and method

The Hamiltonian of the disordered Hubbard model is given by

$$\mathcal{H} = -t \sum_{\langle i,j\rangle\sigma} (\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}) + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_{i\sigma} w_i \hat{n}_{i\sigma} \tag{1}$$

where t is the nearest-neighbour hopping amplitude, $\langle i,\ j\rangle$ is a nearest-neighbour 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 μ. The grand canonical method is suitable for studying the charge degree of freedom because the charge fluctuation is taken into account statistically [14]. In this treatment, we make the system half-filled on average 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 [15, 16]. We also use the matrix-decomposition technique to remove numerical instabilities at low temperatures [17]. The simulations are performed in the half-filled sector ($\mu = U/2$) for lattices with sizes up to $N = 6 \times 6 \times 6$. We take the strength of the interaction $U/t = 6$ so that the Néel temperature takes around its maximum value [18]. (If the interaction is too small, we must perform simulations for larger systems in order to detect the small charge gap, which is expensive as regards computer time. On the other hand, for large U, calculations are difficult due to the negative-sign problem.) 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 temperature and does not change any qualitative features. For each realization of disorder, we have typically run 2000 Monte Carlo sweeps for measurements after 500 sweeps in the warm-up run. For all the observables, we average over 24 realizations of disorder and the errors are estimated as the variance among the realizations of disorder. Since the system does not have particle–hole symmetry in each realization of disorder, the negative-sign problem occurs; for example, the value of the 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 in a doped case, a simulation at a very low temperature with strong disorder is difficult.

The physical observables that we have calculated are the compressibility κ and the magnetic structure factor $S(\boldsymbol{q})$ defined as

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

$$S(\boldsymbol{q}) = \frac{1}{N}\sum_{i,j} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)} \langle (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow})\rangle \tag{3}$$

where N is the number of sites, N_e is the number of electrons and β is an inverse temperature. The charge compressibility κ measures the charge fluctuation. If the system has a finite charge gap, the compressibility shows thermally activated behaviour 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 charge excitations. The magnetic structure factor $S(\boldsymbol{q})$ at $\boldsymbol{q} = (\pi, \pi, \pi)$ diverges in a low-temperature region when the system has an antiferromagnetic long-range order.

3. Results and discussion

Figure 1 shows the temperature dependence of the charge compressibility for several different strengths of disorder. Averaging over 24 realizations of disorder is performed. Without disorder, the temperature dependence of the compressibility κ shows thermally activated behaviour reflecting the existence of a finite charge gap. The compressibility κ at $T = 0$ is zero within the numerical accuracy for the pure system. This indicates that the ground state of the pure Hubbard model in three dimensions is in an incompressible phase. In the

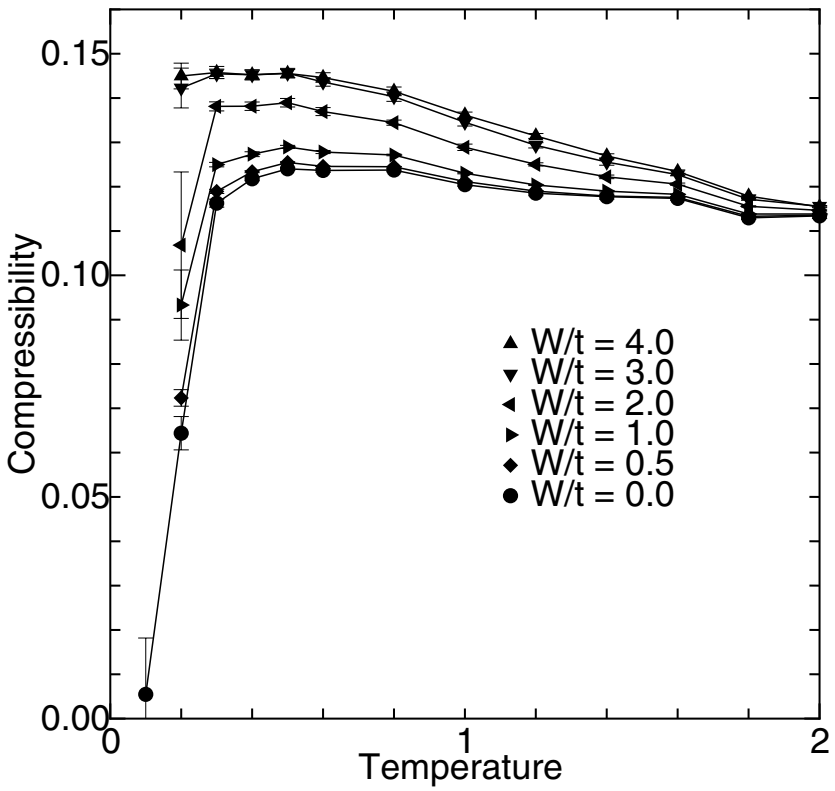

Figure 1. The temperature dependence of the charge compressibility κ, where $U/t = 6$ and $L = 6 \times 6 \times 6$. Without disorder, κ shows thermally activated behaviour and decreases toward $T = 0$, indicating the existence of a charge gap. For weak disorder, κ still decreases toward $T = 0$. On the other hand, for strong disorder, κ does not show thermally activated behaviour down to the lowest temperature that we studied. This is a disorder-driven transition from an incompressible phase to a compressible phase.

presence of disorder, the compressibility is enhanced. For weak disorder, although enhanced, the compressibility still shows thermally activated behaviour and the value at $T = 0$ seems to be zero. On the other hand, κ does not show thermally activated behaviour for $W > W_c$ ($W_c \sim U/2$) down to the lowest temperature that we studied. This means that the critical disorder strength required 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 κ at $T = 0$ for strong disorder, what we have given here are the best data within the numerical restriction. If the strength of disorder is so strong that the interaction can be negligible ($W/U \gg 1$), the system is essentially the Anderson insulator and there must be no charge gap. This implies that sufficiently strong disorder destroys the Mott gap, which is of the order of the interaction in the strong-coupling region. Our results support the discussion here. In the presence of disorder, when we discuss the physics locally, making one doubly occupied site provides a potential energy $2W$ at the maximum, while it costs a Coulomb energy U. Therefore one may expect the Mott gap to collapse at $W > W_c$ ($W_c \sim U/2$) regardless of the dimensionality in the strong-coupling region. In other words, since charge properties of the Mott insulators in the strong-coupling region seem to be determined locally [11, 12], the effect of disorder would also be local and independent of the dimensionality. Indeed, the

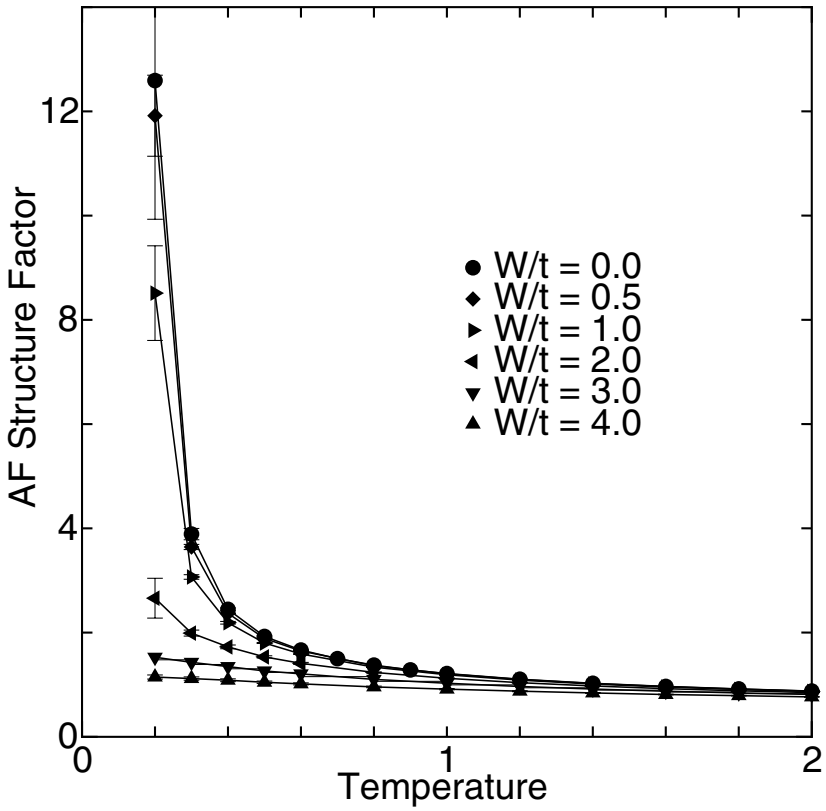

Figure 2. The antiferromagnetic structure factor as a function of temperature (T/t), where $U/t = 6$ and $L = 6 \times 6 \times 6$. For weak disorder, the antiferromagnetic structure factor shows diverging behaviour down to the lowest temperature that we studied. On the other hand, for strong disorder,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

Mott gap collapses at $W_c \sim U/2$ in one [7], two [8] and infinite [19] dimensions in the strong-coupling region. This is in contrast to the quantum nature of the long-range properties of the correlation functions which have a drastic difference in dimensionality (e.g. the Luttinger liquid in one dimension). The transition that we observed is a disorder-driven quantum phase transition from an incompressible (gapped) to a compressible (gapless) phase. However, this does not necessarily imply an insulator–metal transition. The compressibility takes a finite value in both the metallic phase and the insulating phase due to disorder (Anderson insulator). To distinguish these two phases, one needs simulations for a sufficiently large system, which we cannot perform because of the negative-sign problem. (In principle, it could be an interesting problem.)

Figure 2 shows the temperature dependence of the antiferromagnetic structure factor $S(\pi, \pi, \pi)$. Since the ground state has antiferromagnetic long-range order, $S(\pi, \pi, \pi)$ shows diverging behaviour toward the Néel temperature in the absence of disorder. For weak disorder, the structure factor is slightly suppressed, but diverging behaviour is still observed down to the lowest temperature that we studied. This means that the ground state still has antiferromagnetic long-range order. When sufficiently strong disorder is included, the temperature dependence of $S(\pi, \pi, \pi)$ changes qualitatively. Then the diverging behaviour of $S(\pi, \pi, \pi)$ disappears. This indicates that the long-range antiferromagnetic correlation is also destroyed by a finite amount of disorder. Ulmke *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 [8, 12]. Since the strength of the interactions that we studied is $U \simeq U_c$ [18], we did not observe it.

In summary, the three-dimensional Hubbard model with a random potential of 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 the 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 in the three-dimensional case are common in one-, two- and infinite-dimensional systems.

Acknowledgments

We are grateful to Y Morita, N Kawakami, S Fujimoto, P J H Denteneer, R S Römer and J-i Kishine for helpful correspondence. YH is supported in part by a Grant-in-Aid from the Ministry of Education, Science and Culture of Japan. The computation in this work was done using the facilities of the Supercomputer Centre, ISSP, University of Tokyo.

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