Collapse of the charge gap in random Mott insulators

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Effects of randomness on interacting fermionic systems in one dimension are investigated by quantum Monte Carlo techniques. At first, interacting spinless fermions are studied whose ground state shows charge ordering. Quantum phase transition due to randomness is observed associated with the collapse of the charge ordering. We also treat random Hubbard model focusing on the Mott gap. Although the randomness closes the Mott gap and low-lying states are created, which is observed in the charge compressibility, no (quasi-)Fermi-surface singularity is formed. It implies localized nature of the low-lying states. [S0163-1829(98)00748-6]

Effects of Coulomb interaction and randomness in fermionic systems have been studied separately for a long time. Their combined effects, however, remain unsolved especially in the strong-coupling regime. The strong Coulomb interaction can cause the Mott transition and lead the metallic system to the Mott insulator. Also, the randomness can make the electrons localized, which is the Anderson localization. Although both are metal-insulator transitions, the physical characters are quite different. For example, in the Mott insulator, the ground state has a finite charge gap due to the Coulomb interaction. On the other hand, the insulator due to the Anderson localization does not necessarily have a charge gap. Therefore, the competition between the Coulomb interaction and the randomness is interesting from a theoretical point of view[1–4] and it may shed new light on some real materials. In this paper, we systematically investigate one-dimensional fermionic systems with both Coulomb interaction and randomness by quantum Monte Carlo (QMC) techniques.[5–7] Although the conventional wisdom is that there is no quantum-phase transition driven by randomness in one and two dimensions,[8] we confirmed the existence of quantum-phase transitions due to combined effect of Coulomb interaction and randomness. In this paper, at first, we focus on the charge-density-wave (CDW) ordering in interacting spinless fermions with randomness. Next, in order to understand low-lying excitations of the random Mott insulator, we study the charge compressibility of the random Hubbard model in the half-filled sector. Also, the one-particle Green's function is investigated to discuss nature of the low-lying excitations.

Random spinless fermions

To begin with, we focus on CDW structure factor $\mathcal{O}_{\mathrm{CDW}}$ of interacting spinless fermions with randomness in one dimension. The Hamiltonian is given by

$$\mathcal{H}_{sf}=\mathcal{H}_v+\mathcal{H}_w, \tag{1}$$

$$\mathcal{H}_v=-t\sum_{\langle i,j\rangle}(c_i^\dagger c_j+c_j^\dagger c_i)+V\sum_{\langle i,j\rangle} n_i n_j, \tag{2}$$

$$\mathcal{H}_w=\sum_i w_i n_i, \tag{3}$$

where $c_i^\dagger$ (c_i) creates (annihilates) a spinless fermion at the ith site, $n_i=c_i^\dagger c_i$ and $\langle i,j\rangle$ is a nearest-neighbor link. $\mathcal{H}_w$ denotes site randomness where w_i's are chosen from W or $-W$ at random. We set $t=1$ as an energy unit and use open boundary conditions.[9] In the following, the system is set to be half-filled, i.e., $N_e=L/2$, where N_e is number of the electrons and L is the system size. The pure system without randomness is one of the typical examples that show quantum-critical phenomena. When the interaction is weak ($0\leqslant V/t\leqslant 2$), the system is metallic and it belongs to a universality class of the Tomonaga-Luttinger liquid. A metal-insulator transition accompanied with a charge ordering occurs at $V/t=2$. For strong interaction ($V/t>2$), the charge degree of freedom becomes frozen and the energy gap opens. We focus on the charge-ordered phase ($V/t>2$) where the charge gap is finite due to the nearest-neighbor interaction, and study the effect of randomness.

In order to study the charge ordering when the randomness is included, we calculate the CDW structure factor with momentum π defined by

$$\mathcal{O}_{\mathrm{CDW}}(T)=\frac{1}{N_{\mathcal{B}}}\sum_{i,j\in\mathcal{B}}(-1)^{|i-j|}\langle(n_i-1/2)(n_j-1/2)\rangle, \tag{4}$$

where $\mathcal{B}$ is set to be a subset of the lattice to avoid a boundary effect, $\mathcal{B}=[L/4,3L/4]$ and $N_{\mathcal{B}}$ is number of sites in $\mathcal{B}$. Without randomness, $\mathcal{O}_{\mathrm{CDW}}$ is strongly enhanced and diverging toward zero temperature, which corresponds to charge ordering in the ground state due to Coulomb interaction ($V/t>2$). On the other hand, when sufficiently strong randomness is included, the charge ordering is expected to collapse and the diverging behavior of $\mathcal{O}_{\mathrm{CDW}}$ to vanish. In order to obtain the $\mathcal{O}_{\mathrm{CDW}}$ for each realization of randomness, world-line QMC method is employed.[5] In Fig. 1, temperature dependence of the $\mathcal{O}_{\mathrm{CDW}}$ is shown for several strength of randomness where simulations are performed in the half-filled sector with typical system size $L=128$ and $V/t=3$. Without randomness, since the charge ordering occurs at zero temperature, the structure factor shows diverging behavior toward zero temperature. For weak randomness, the structure factor still has similar behavior down to the temperature we studied. It means (quasi-)long-range order in the ground state or long localization length beyond the available

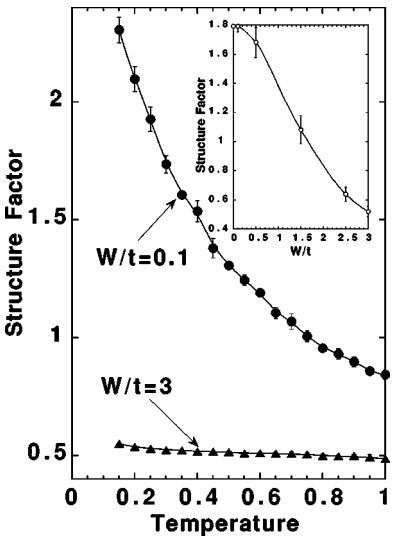

FIG. 1. The CDW structure factor as a function of temperature (T/t) for a particular realization of randomness ($L=128$ and $V/t=3$). For weak randomness ($W/t=0.1$), the structure factor shows diverging behavior down to the temperature we studied. On the other hand, for strong randomness ($W/t=3$), the divergence vanishes. The inset shows how the structure factor at $T/t=0.2$ depends on the strength of randomness (W/t), where $L=64$, $V/t=3$, and average over 30–40 realizations of randomness is performed. The line is a guide for the eyes.

system size. On the other hand, when sufficiently strong randomness is included, the temperature dependence of the $\mathcal{O}_{\mathrm{CDW}}$ shows qualitatively different behavior. The rapid enhancement at low temperature vanishes. It implies that the charge ordering completely fades out due to randomness. In order to investigate the detailed nature of the transition, we study how the structure factor depends on the randomness at $T=0.2t$. As shown in the inset of Fig. 1, sudden decrease of $\mathcal{O}_{\mathrm{CDW}}$ at finite strength of randomness is observed. It implies that the collapse of the charge gap occurs at finite strength of randomness, which is the order of the charge gap, although we can not exclude a possibility that the transition is the Kosterlitz-Thouless (KT) type at infinitesimally weak randomness.

Random Hubbard model

Next, in order to study effect of randomness on the Mott insulator, let us consider the half-filled sector of one-dimensional random Hubbard model. The Hamiltonian is given by

$$\mathcal{H}=\mathcal{H}_u+\mathcal{H}_w, \tag{5}$$

$$\mathcal{H}_u=-t\sum_{\langle i,j\rangle\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma}+c^{\dagger}_{j\sigma}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{6}$$

$$\mathcal{H}_w=\sum_{i\sigma} w_i n_{i\sigma}, \tag{7}$$

where t is the nearest-neighbor hopping amplitude and U is the on-site Coulomb interaction. $\mathcal{H}_w$ denotes random potentials and w_i's are taken from the interval $[-w,w]$ at random. We treat the system in a grand canonical ensemble with the chemical potential μ. The boundary condition is periodic. In the absence of randomness, an infinitesimal interaction U causes a charge gap (Mott gap) E_g at half filling ($\mu=U/2$). The charge gap E_g is exponentially small in the weak-coupling region ($U/t\ll 1$) and linear in U in the strong-coupling region ($U/t\gg 1$), for example, estimated $E_g\simeq 1.3t$ for $U/t=4$.[10] Here we shall discuss effects of randomness on the Mott insulator (see also Ref. 11).

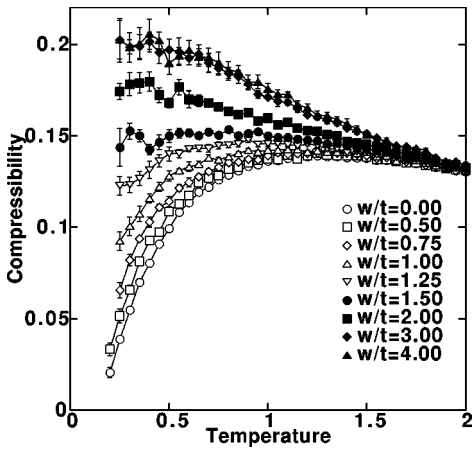

FIG. 2. Temperature dependence of the charge compressibility κ for a particular realization of randomness ($L=36$ and $U/t=4$). Without randomness, κ shows thermally activated behavior and decreases toward zero at low temperature indicating the existence of a charge gap. With weak randomness, $w<w_c$ ($w_c/t\sim 1.5$), κ still shows thermally activated behavior. On the other hand, for strong randomness, $w>w_c$, κ does not decrease down to the temperature we studied.

To obtain approximation-free results, we use the finite-temperature auxiliary-field QMC method.[6,7] Since we use the grand canonical ensemble, there is a finite-charge fluctuation that is crucial for the knowledge of low-lying excitations. Although the random potential breaks the particle-hole symmetry for each realization of randomness, a half-filling condition is recovered after averaging over different realizations of randomness. Our simulations are performed with the system size $L=36$ at $U/t=4$. Severe finite-size effect due to energy discretization is observed in the low-temperature region (lower than $T\sim 0.2t$ for $L=36$) and the data for that region are not shown. Moreover, since the particle-hole symmetry is broken for each realization of randomness, a negative-sign problem occurs in general. However, in the parameter region we investigated, it is not serious and the data are obtained with sufficient accuracy. To investigate the change of low-lying excitations due to randomness, we calculate the charge compressibility κ defined by

$$\kappa(T)=\frac{1}{L}\frac{\partial N_e}{\partial\mu}=\frac{\beta}{L}(\langle\hat{N}_e{}^2\rangle-\langle\hat{N}_e\rangle^2). \tag{8}$$

It measures fluctuation in the charge sector and shows thermally activated behavior when the system has a finite charge gap. On the other hand, in the absence of the charge gap, the charge compressibility is expected to be finite due to the low-lying excitations. For example, in the noninteracting case, $\kappa(T=0)$ is equal to the density of states at the Fermi energy. Figure 2 shows temperature dependence of the

charge compressibility κ for different strength of randomness. Although a snapshot for a particular realization of randomness is shown in Fig. 2, the simulations for other realizations were also performed and we confirmed that the global feature does not depend on each realization. Without randomness, κ decreases toward zero and shows thermally activated behavior as the temperature is lowered indicating the existence of a charge gap. This is a typical feature of the Mott insulator. As randomness is turned on, the enhancement in κ is observed for all temperature. For weak randomness, $w/t \lesssim 1.5$, although κ is enhanced, it still seems to show a thermally activated behavior as in the pure case. On the other hand, with strong randomness $w/t \gtrsim 1.5$, there is no tendency for κ to decrease down to the lowest temperature we studied and it seems that κ is finite at $T=0$. It suggests the collapse of the charge gap. These behaviors imply that sufficiently strong randomness, which is the order of the charge gap, takes the system away from the Mott insulator.[3,4] This is a quantum-phase transition of the Mott insulator driven by randomness. Although it has been confirmed that low-lying excitations are created in the Mott gap with sufficiently strong randomness, the nature of the low-lying excitations is crucial to understand the phase transition. In order to study the low-lying excitations, we calculate the one-particle Green's function $G_{ij\sigma}=\langle c^{\dagger}_{i\sigma} c_{j\sigma}\rangle$. The feature of $G_{ij\sigma}$ in metallic states is clear in the momentum space representation, which is the momentum distribution function $n_{\sigma}(k)$. Metallic nature of the system is reflected by the singularity of $n_{\sigma}(k)$ at $k=k_F$. For example, it is a step function in the Fermi liquid (Fermi surface) and, even in the Tomonaga-Luttinger liquid (doped Hubbard chain), the derivative of $n_{\sigma}(k)$ is diverging at $k=k_F$ (quasi-Fermi surface). On the other hand, in the Mott insulator (half-filled Hubbard chain), the derivative is finite. We may summarize that the formation of (quasi-)Fermi surface, as temperature is lowered, implies metallic nature of the system. Figure 3 shows momentum distribution function $n_{\sigma}(k)$ at $T=0.2t$ for several randomness strength. By performing calculations with different temperatures, we confirmed that the temperature is sufficiently low that the results reflect the ground-state properties. Although the charge gap is closed for $w/t \gtrsim 1.5$ as discussed above, the momentum distribution function is almost unchanged and no singularity appears at k_F even for $w/t=2.0$. It is in contrast to the transition from the Mott insulator to the Luttinger liquid in the pure Hubbard model when the system is doped. It suggests that the low-lying excitations created by randomness are localized.

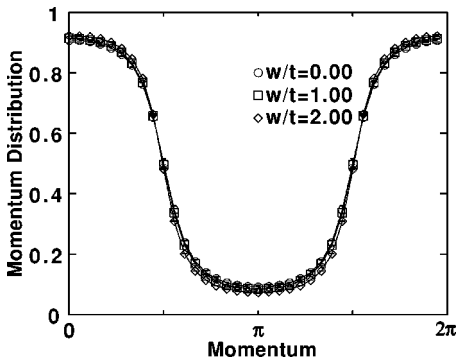

FIG. 3. The momentum distribution function ($L=36$ and $U/t=4$). Average over about 10 realizations of randomness is performed. There is no singularity at $k=k_F$ even for $w/t=2.0$ where the charge gap is closed as shown in the charge compressibility.

In summary, we have studied effects of randomness in the interacting fermionic system with charge gap (Mott gap). The strong randomness closes the charge gap and low-lying states are created, while (quasi-)Fermi surface is not formed. It implies that the transition is an insulator to an insulator transition. The transition point may be continuously connected to the metal-insulator transition point in the pure system, then it gives a new example of quantum-phase transitions in low-dimensional random fermionic systems. These phenomena may give a clue for the understanding of several aspects in quantum-phase transitions in low-dimensional random systems.

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