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Finite-size scaling for Mott metal-insulator transition on a half filled nonpartite lattice

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We combine the finite-size scaling method with a multistage real-space renormalization-group procedure to examine the Mott metal-insulator transition (MIT) on a nonpartite lattice. Based on the Hubbard model, we have found that there exists a critical point $U/t=12.5$ for the MIT with the correlation length exponent $\nu=1$. At the critical point, the charge gap scales with the system size as $\triangle_g \sim 1/L^{0.91}$.

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Ever since the experimental observations of the metallic behavior in two-dimensional electron gas with high-mobility Si metal-oxide-semiconductor field-effect transistor,[1] there has been an intensive interest in the investigations of electronic transport properties in such systems.[2,3] The significance of this discovery is that it has taken us to a different interaction regime where the electron correlations begin to play a very important role. For example, in disordered systems, when the electron-electron interactions E_{ee} are much stronger than the Fermi energy E_f, namely, E_{ee}/E_f lies in the range 5–50, they can show metallic properties.[3] These contradict the conventional prevailing noninteracting-electron scaling theory, which states that for two-dimensional (2D) systems, any disorder will localize all states and there should be no metal-insulator transition(MIT).[4] Hence the early experiments have stimulated a spate of new experimental results and MIT has been found in various 2D systems, such as *p*-type SiGe structures,[5] *p*-type GaAs/AlGaAs heterostructures,[6] *n*-type AlAs heterostructures,[7] *n*-type GaAs/AlGaAs heterostructures,[8] etc.; but there have been no satisfactory theoretical explanations of these phenomena. In the domain of disordered system with no or weak electron interactions, where Anderson MIT dominates,[9] the scaling theory of Abraham holds well and has been studied in detail.[4] When disorder effects are comparable to the influence of the electron interactions, the theory becomes very subtle and the nature of MIT is still an open question, which is actually becoming a central problem in condensed-matter physics.[10,11] If we go a little further, one may ask the question: what will happen in the strong-coupling regime, namely, the systems having very strong electron interactions with little or no disorder? Actually, this is the regime of the famous Mott MIT.[12] Although there has been much work in this direction,[13] not much study is carried out for the correlation induced or fixed density MIT in 2D systems from the viewpoint of the finite-size scaling (FSS) analysis.[15] However, the FSS study for Anderson MIT has a noteworthy history.[16,17] Hence, the main motivation of this study is to develop the FSS for Mott MIT .

The model we use is the Hubbard model,[18]

$$H=-t\sum_{\langle i,j\rangle,\sigma}[c_{i\sigma}^{+}c_{j\sigma}+\text{H.c.}]+U\sum_{i}n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i}(n_{i\uparrow}+n_{i\downarrow}), \tag{1}$$

where t is the nearest-neighbor hopping term, U is the local repulsive interaction, and μ is the chemical potential. $c_{i\sigma}^{+}(c_{i\sigma})$ creates (annihilates) an electron with spin σ in a Wannier orbital located at site i; the corresponding number operator is $n_{i\sigma}=c_{i\sigma}^{+}c_{i\sigma}$ and $\langle\rangle$ denotes the nearest-neighbor pairs. H.c. denotes the Hermitian conjugate.

For half filled system, Eq. (1) can be rewritten as

$$H=-t\sum_{\langle i,j\rangle,\sigma}[c_{i\sigma}^{+}c_{j\sigma}+\text{H.c.}]+U\sum_{i}\left(\frac{1}{2}-n_{i\uparrow}\right)\left(\frac{1}{2}-n_{i\downarrow}\right)+K\sum_{i}I_i, \tag{2}$$

with $K=-U/4$ and I_i is the unit operator. For the lattice structure, we use the nonpartite triangular lattice, the MIT emerges at finite $U=U_c$. It is well known that MIT on square lattice can only take place at $U=0$ due to the perfect nesting of the Fermi surface. Our work has also replicated this result. If we do not study the exotic case with $U<0$, which is possible in a strongly polarizable medium, the square lattice is not an optimal option for our purpose. Furthermore, the physical quantity that will be examined here is the charge gap $\triangle_g$, which is defined as

$$\triangle_g=E(N_e-1)+E(N_e+1)-2E(N_e), \tag{3}$$

where $E(N_e)$ denotes the lowest energy for the N_e-electron system. In our case, N_e is equal to the site number N_s of the lattice. This quantity is the discretized second derivative of the ground-state energy with respect to the number of particles, i.e., the inverse compressibility.

Conventionally, Monte Carlo and exact diagonalization methods are the two most used methods to carry out finite-size scaling analysis, but both methods involve too intensive calculations, especially for large-size systems. In this study, we develop a multistage block renormalization-group (RG) method to address this problem.

The essence of real-space RG method is to map the original Hamiltonian to a new Hamiltonian with much fewer degrees of freedom, which keeps the physical quantities we are interested in unchanged.[19] The mapping can be iterated until the final Hamiltonian can be easily handled. The crucial step in this method is how to relate the parameters between the old and the new Hamiltonians. This can be realized by divid-

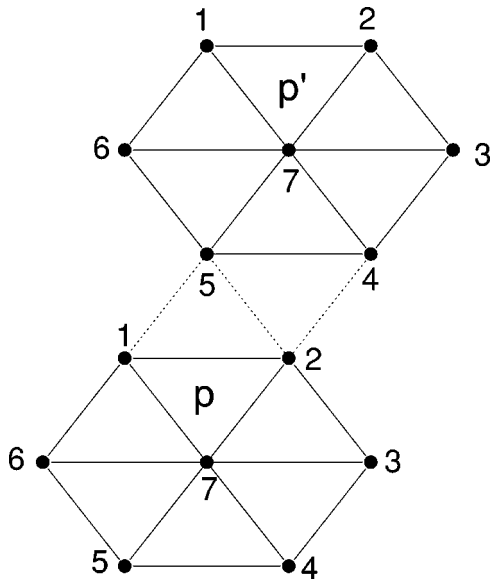

FIG. 1. Schematic diagram of the triangular lattice with hexagonal blocks. Only two neighboring blocks p and p' are drawn here. The dotted lines represent the interblock interactions and solid line the intrablock ones.

ing the original lattice into blocks and then build a new Hamiltonian upon blocks, namely, regard each block to be an effective site.

Figure 1 shows schematically the hexagonal block structure that we use in our calculations and the coupling between blocks. For each block, we solve it numerically in the subspaces of six electrons with three spin up and three spin down, seven electrons with four spin up and three spin down, seven electrons with three spin up and four spin down, and eight electrons with four spin up and four spin down. In all the subspaces, we keep the lowest-energy nondegenerate state, which is also required to belong to the same irreducible representations of $C_{6\nu}$ symmetry group. It should be mentioned here that if the degeneracy is involved, one possible solution might be to average the renormailzed parameters over the degenerated states. The kept states will then be taken as the four states for an effective site. If we denote the energies corresponding to the first two states by E_1 and E_2, after some intensive calculations, we can obtain the new Hamiltonian for the effective lattice, which has the same structure as the original Hamiltonian,[20]

$$H' = -t' \sum_{\langle i,j\rangle,\sigma} [c'^{+}_{i\sigma} c'_{j\sigma} + \text{H.c.}] + U' \sum_i \left(\frac{1}{2} - n'_{i\uparrow}\right)\left(\frac{1}{2} - n'_{i\downarrow}\right) + K' \sum_i I_i, \tag{4}$$

where the prime $'$ denotes the operator action upon the block states and

$$t' = \nu \lambda^2 t, \tag{5}$$

$$U' = 2(E_1 - E_3), \tag{6}$$

$$K' = (E_1 + E_3)/2. \tag{7}$$

The above equations are the so-called RG flow equations. Usually, they are iterated until we get the fixed point. The charge gap for an infinite lattice can then be written as,[20]

$$\Delta_g = \lim_{n\to\infty} U^{(n)}. \tag{8}$$

Because of the implicit functional in Eqs. (5)–(7), it is very difficult to obtain any other useful information except the critical transition point U_c. However, instead of letting RG flow to infinity for a fixed initial parameter (U,k,t), we can stop the RG flow at some stage. Thus the energy gap obtained from Eq. (3) will correspond to a system of fixed size. For example, if we stop the RG flow at the first iteration, then the obtained t' and U' will be for hexagonal block mapped from a system of 7^2 sites. Since we can solve the hexagonal block Hamiltonian exactly, the energy gap for a system of 49 sites can be obtained easily. Thus, we can study the variations of Δ_g as a function of the system size of $7^1, 7^2, \ldots, 7^7$. We call this procedure a multistage real-space RG method, which is well adapted to start the finite-size scaling analysis.

In Fig. 2(a), we present the size dependence of the scaled $\triangle_g/t$ on U/t. But from this figure, it is not easy to decide the location of the transition point for $\triangle_g$. To explicitly display the critical phenomenon, we present in Fig. 2(b) the scaling of $\triangle_g$ with respect to N at $N=N_e=N_s$. Now it is very easy to obtain the critical value of $(U/t)_c = 12.5$, which is the crossing point of all the curves corresponding to different system sizes. The same value is obtained by letting RG equations flow to infinity.[20] In Fig. 2(c), we show that all the data collapse to one curve once one carries out a second step of scaling with $U/t-(U/t)_c$ by N. It is an obvious evidence for the occurrence of a quantum phase transition as the tuning parameter U varies. Hence we can write down the following equation:

$$\triangle_g N^{0.405} = f[qN^{0.5}], \tag{9}$$

where $f(x)$ is a universal function independent of the system size and $q=U/t-(U/t)_c$. By using $N=L^2$ for 2D systems, the above equation can be rewritten as

$$\triangle_g = L^{-0.91} f[qL], \tag{10}$$

from which we can get two scaling relationships for the charge gap. One is the finite-size scaling at the transition point, i.e., when $q=0$, $\triangle_g \sim 1/L^{0.91}$. As shown in Ref. 14 in the Anderson MIT, when the electron correlation energy dominates the Fermi energy, the average inverse compressibility $(=\Delta_g)$ exhibits a scaling as $1/L$ with respect to the system size. Here it shows a slower decay as L increases. The other one is the bulk scaling around the transition point for the infinite system, $\triangle_g \sim q^{0.91}$. According to the scaling analysis of the Gutzwiller solution for the Mott MIT for the

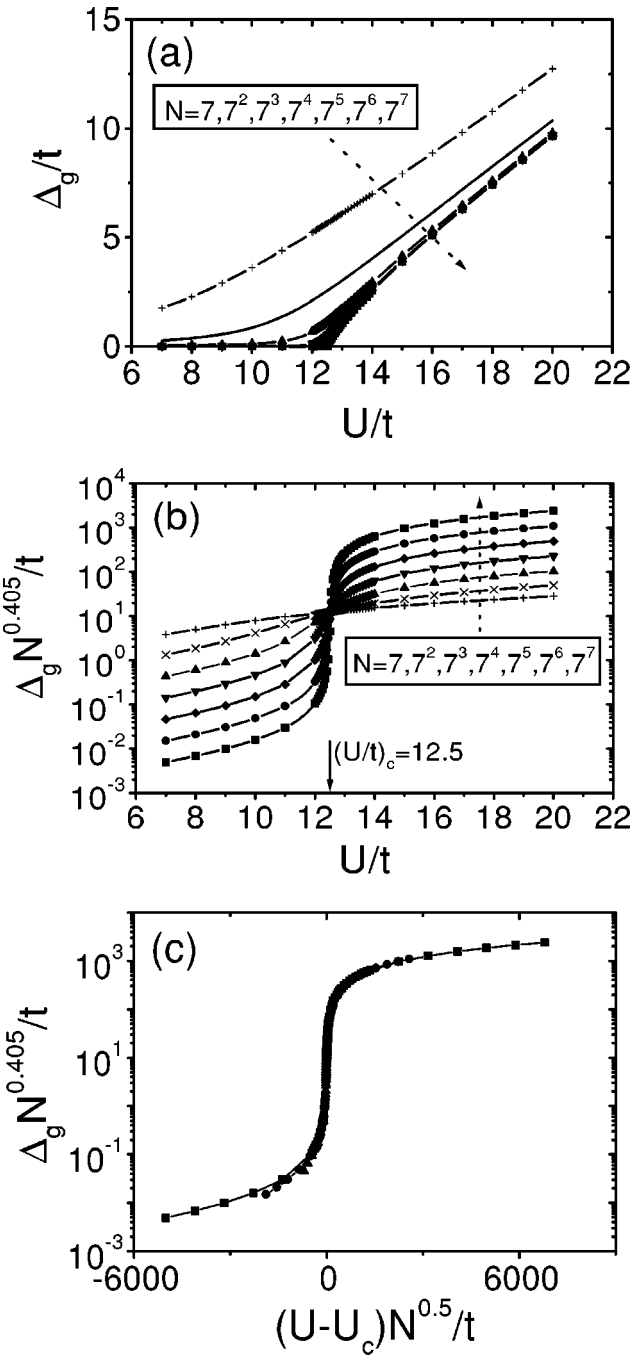

FIG. 2. Variations of the charge gap Δ_g against the on-site electron iteration U for different system sizes, i.e. the number of sites: 7 (cross +), 7^2 (cross ×), 7^3 (up triangle), 7^4 (down triangle), 7^5 (diamond), 7^6 (circle), 7^7 (square). More points are calculated around the transition point. In (a), no scaling is utilized. In (b), the charge gap is scaled by $1/N^{0.405}$ to display clearly the phase transition. In (c), all the data are collapsed onto one curve by scaling both axes with respect to N.

Hubbard model, $\triangle_g \sim q^{0.5}$.[15] Since the Gutzwiller solution is a mean-field approximation, the upper critical dimension for it to give a correct description of this critical phenomenon is $d_c=3$, it is understandable that our 2D results cannot be merged into the one obtained by mean-field theory.

By introducing a critical exponent $y_\triangle$ for $\triangle_g$, the one-parameter scaling theory gives

$$\triangle_g = q^{y_\triangle} f\left(\frac{L}{\xi}\right), \tag{11}$$

in which $\xi = q^{-\nu}$ is the correlation length with ν being the corresponding critical exponent and L denotes the system size. By using $N=L^2$ for 2D systems, the above equation can be rewritten as

$$\triangle_g = N^{-(y_\triangle/2\nu)} f(qN^{1/2\nu}). \tag{12}$$

Comparing Eqs. (9) and (10), we can obtain

$$y_\triangle = 0.91, \quad \nu = 1. \tag{13}$$

By relating $y_\triangle$ to the dynamic exponent z, $y_\triangle = z\nu$, thus $z \approx 0.91$. Because of the approximate properties of our method, it is difficult to make a judgement purely from $\nu = 1$ whether it violates the Chayes limit criterion $2/d$. More detailed work is desired before a definite conclusion can be built.

For filling-control or density-driven MIT, there are two types of universality classes.[13] One is characterized by $z = 1/\nu = 2$,[21] which is the case for all 1D systems as well as for several transitions at higher dimensions, such as the transitions between insulator with diagonal order of components and metal with diagonal order components and small Fermi volume. Another one is characterized by $z = 1/\nu = 4$.[22] Numerical calculations have shown that Hubbard model on a square lattice is an example of this class.[22] For Anderson MIT, analytical, numerical, and experimental studies have produced $\nu > 1$, such as $\nu = 1.35$,[23] 1.54,[24] and 1.62.[25]

Our work leads to $z = 0.91$ and $\nu = 1$, which implies the possibility of an eventual new universality class for MIT. This might be understandable since the MIT studied here is driven by a different mechanism, i. e., electron-electron correlations with a fixed density. It is interesting to note that the ν and z we have obtained are quite near the critical values for the energy gap of the one-dimensional Ising model in a transverse field, which can be solved exactly with $\nu = z = 1$.[26] A modified real-space RG method[27] is also tried on this model and similar results are obtained. As we know, the Ising model is a special case of the Heisenberg model, which is a limiting case of the Hubbard model when $U \gg t$. This is exactly the strong-coupling regime that has been examine in this study.

Recently, Lee *et al.*[28] have investigated experimentally the dynamic behavior of morphous niobium-silicon alloys near a zero-temperature 2D MIT critical point, where a different universality class with $z = 2$ and $\nu = 1$ is obtained. The difference between this scaling and the conventional Anderson scaling is attributed to the electron-electron correlations. This conclusion is consistent with our finding with respect to the correlation length critical exponent ν. The difference in estimating the dynamical critical exponents z might be due to the negligence of the disorders in our study.

In summary, by using a multistage real-space renormalization-group method we show that the finite-size

scaling can be applied to the Mott MIT. We have found that at the transition point, the charge gap scaled with size as $\triangle_g \sim 1/L^{0.91}$ and the dynamic and correlation length critical exponents are found to be $z=0.91$ and $\nu=1$, respectively. The method presented here is very general and can be used to study many other properties of the system if they are properly defined, for example, the magnitude of the local momentum. It can also be used to study the quasiparticle weight in the metallic phase close to the MIT.

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