More Accurate Determination of Mott Metal-Insulator Transition in Strongly Correlated Electronic Systems

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The Mott metal-insulator transition is at the heart of the essential physics in a strong correlation system as many novel quantum phenomena occur at the metallic phase near the Mott metal-insulator transition. We investigate the Mott metal-insulator transition in a strong correlation system based on the Hubbard model. The average number of the bound electrons evaluated by the dynamical mean-field theory is employed to depict the Mott metal-insulator transition. In comparison with the corresponding quasiparticle coherent weight, the average number of bound electrons is a more proper order parameter to accurately determine the critical point of the Mott metal-insulator transition. Moreover, this order parameter also gives a consistent description of two distinct forms of the critical points in the Mott metal-insulator transition.

PACS numbers: 71.30.+h, 71.27.+a, 71.50.+t

Introduction. The Mott metal-insulator transition (MIT) [1–3] driven by a competition between the kinetic energy \( t \) of the electrons and the Coulomb repulsive interaction \( U \) between electrons on a same lattice site is a paradigmatic example of the strong electron correlation effect. In particular, it has been shown experimentally that the unconventional superconductivity and many other exotic quantum phenomena occur at the metallic phase near the Mott MIT [3]. This is why the accurate determination of the critical point of the Mott MIT is crucial to deeply understand the essential physics of the novel quantum phenomena in a strong correlation system.

Although the intense efforts at the experimental and theoretical levels have been put forth in order to understand the physical origin of the Mott MIT together with the associated novel quantum phenomena [3], the accurate determination of the critical point of the Mott MIT still is a challenging issue. In the early studies, it has been shown in the Gutzwiller approximation that the quasiparticle coherent weight can be identical as the order parameter to determine the critical point of the Mott MIT, where the quasiparticle coherent weight \( Z_F \) disappears and the effective mass diverges as \( 1/Z_F \) when the Coulomb interaction approaches the critical point of MIT [4, 5]. This is followed a fact that the quasiparticle coherent peak of zero-energy at the Fermi energy comes mainly from scattering of electrons on the local-spin fluctuations, and then its disappearance at the critical point of MIT can be also tracked by analyzing the energy dependence of the electron self-energy at different Coulomb repulsive interactions between electrons [6]. Later on, the systematic analysis within the framework of the dynamical mean-field theory [7] (DMFT) indicates that at low temperatures, the opening of the gap and the vanishing of the quasiparticle coherent peak do not happen at the same critical value of \( U_c \), instead, MIT is found as a function of \( U/t \), with the corresponding metallic and insulating solutions coexisting between \( U_{c2} \) and \( U_{c1} \), respectively. Since then, a series of studies focused on the region of the metallic and insulating solutions coexisting between \( U_{c2} \) and \( U_{c1} \) has been made [8–14]. However, these studies also indicate that the quasiparticle coherent weight \( Z_F \) as an order parameter may not be able to mark off these two distinct forms of the critical points in MIT. In this case, a natural question is raised: is there a more proper order parameter to define the existence of two distinct forms of the critical points in Mott MIT?

In this paper, we study the Mott MIT in a strong correlation system by using the DMFT approach with the Lanczos method as impurity solver, and show that the average number of bound electrons is a more proper order parameter to accurately determine the critical points of the Mott MIT. In particular, the average number of bound electrons as the proper order parameter can give a consistent description of two distinct forms of the critical points in the Mott MIT.

Models and Methods. The Hubbard model is the simplest model that captures the essential physics of MIT. The Hamiltonian of the one-band Hubbard model is given by [15–18],

\[
H = -t \sum_{\langle ij \rangle \sigma} d_{i \sigma}^\dagger d_{j \sigma} - \mu \sum_{i \sigma} d_{i \sigma}^\dagger d_{i \sigma} + \frac{U}{2} \sum_{i \sigma} n_{i \sigma} n_{i \bar{\sigma}}, \tag{1}
\]

where the summation \( \langle ij \rangle \) is over all sites \( i \), and for each site \( i \), restricted to its nearest-neighbor (NN) sites \( j \), \( t \) denote the electron NN hopping amplitude, \( U \) is the onsite Coulomb repulsion between electrons, \( \mu \) is the chemical potential. \( d_{i \sigma}^\dagger (d_{i \sigma}) \) is the creation (annihilation) operator for an electron with spin \( \sigma \) at lattice site \( i \), and \( n_{i \sigma} \) is the occupation number operator of electrons at lattice site \( i \). Unless explicitly stated, we set \( t = 1 \) as the energy scale in this paper.

In the framework of DMFT, the one-band Hubbard model (1) on a Bethe lattice of infinite connectivity \((z \to \infty)\) is mapped onto an effective single impurity
model by dropping the nonlocal contribution to the electron self-energy,

\[ H_{imp} = \sum_{m\sigma} \varepsilon_{m\sigma} c_{m\sigma}^\dagger c_{m\sigma} + \sum_{m\sigma} V_{m\sigma} c_{m\sigma}^\dagger d_{\sigma} + d_{\sigma}^\dagger c_{m\sigma} \]

\[ + \sum_{\sigma} (\varepsilon - \mu) d_{\sigma}^\dagger d_{\sigma} + \frac{U}{2} \sum_{\sigma} n_{\sigma} n_{\sigma}, \quad (2) \]

which becomes exact in the limit of infinite lattice coordination [19], where \( d_{\sigma}^\dagger \) (\( d_{\sigma} \)) is creates (annihilates) a particle in the \textit{impurity orbital} and \( c_{m\sigma}^\dagger \) (\( c_{m\sigma} \)) creates (annihilates) an electron in a \textit{conduction band}. The \textit{impurity orbital} and \textit{conduction band} are coupled each other via effective parameters \( \varepsilon_{m\sigma} \) and \( V_{m\sigma} \), which are determined by performing self-consistent DMFT calculations utilizing an impurity solver. In the following discussions, we introduce the local electron Green’s function \([20, 21]\),

\[ G_{\sigma}(\tau) = - < T_{\tau} d_{\sigma}(\tau) d_{\sigma}^\dagger(0) >, \quad (3) \]

with imaginary time \( \tau = it \). This local electron Green’s function (3) in momentum-space can be obtained by the Fourier transformation as,

\[ \mathcal{G}(i\omega_{n}) = \int_{0}^{\beta} d\tau e^{i\omega_{n}\tau} G(\tau), \]

\[ G(\tau) = - \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_{n}\tau} \mathcal{G}(i\omega_{n}), \quad (5) \]

where \(-\beta \leq \tau \leq \beta \) and \( \omega_{n} = (2n+1)\pi/\beta \) with \( n = 0, \pm 1, \pm 2, \cdots \). The spin indexes are omitted in the above equations because we consider the paramagnetic phases. After the Fourier transformation, the local Green’s function reads,

\[ \mathcal{G}(i\omega_{n}) = \sum_{k} \frac{1}{i\omega_{n} + \mu - \varepsilon_{k} - \Sigma(i\omega_{n})}, \quad (6) \]

with the noninteracting electron energy \( \varepsilon_{k} \) and the momentum-independent self-energy of infinite dimensional system \( \Sigma(i\omega_{n}) \) [22, 23]. The local properties of the Hubbard model on the Bethe lattice can be obtained via a single-site impurity problem supplemented by the following self-consistency relation [24, 25],

\[ G_{0}^{-1}(i\omega_{n}) = i\omega_{n} + \mu - \Sigma(i\omega_{n}), \quad (7) \]

where \( G_{0} \) is the bare Green’s function. The self-consistency relation ensures that the on-site (local) component of the Green’s function \( \Sigma(i\omega_{n}) = \sum_{k} \mathcal{G}(k, i\omega_{n}) \) coincides with the Green’s function \( \mathcal{G}(i\omega_{n}) \) calculated from the effective action.

The Green’s function \( G_{imp}(i\omega_{n}) \) of the impurity model (2) is then calculated by the \textit{Lanczos} method [26, 27], which can be expressed as [7, 24, 28],

\[ G_{imp}(i\omega_{n}) = G^{+}(i\omega_{n}) + G^{-}(i\omega_{n}), \quad (8) \]

with \( G^{+}(i\omega_{n}) \) and \( G^{-}(i\omega_{n}) \) that are given by,

\[ G^{+}(i\omega_{n}) = \frac{\langle \phi_{0}|d d^\dagger|\phi_{0} \rangle}{i\omega_{n} - a_{0}^{(+)} - b_{1}^{(+)} - \cdots}, \]

\[ G^{-}(i\omega_{n}) = \frac{\langle \phi_{0}|d^\dagger d|\phi_{0} \rangle}{i\omega_{n} + a_{0}^{(-)} - b_{1}^{(-)} - \cdots}, \quad (9, 10) \]

where \( a_{n} (b_{n}) \) is the \( n \)th subdiagonal element of the tridiagonal Hamiltonian obtained by the \textit{Lanczos} method, and \( |\phi_{0} \rangle \) is the ground state of the Hamiltonian (2). In our calculations, we choose \( \beta = 512 \) to assure the accuracy of the self-consistency calculations, especially in the low-energy region.

The Green’s function behaves differently depending on whether the eigenstates are localized or extended [29], which helps us to obtain the interaction effects on the phase transitions. In a noninteracting system, the fermion distribution function can be obtained generally by \( n_{F}(\omega_{k}) = \frac{1}{\beta} \sum_{n} e^{i\omega_{n}\alpha_{k}} G(0, \omega_{n}) \). It is worth noticing that \( G(0) \) is ambiguous, which will get quite different results by approaching \( \tau = 0 \) from the positive or negative direction. Extended to the purely localized Green’s function \( G(i\omega_{n}) \) obtained by the DMFT procedure, we introduce,

\[ n_{b} = - \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_{n}0^{+}} G(i\omega_{n}), \quad (11) \]

which is so-called the \textit{average number of bound electrons} of a given site. The factor \( e^{-i\omega_{n}0^{+}} \) is introduced to ensure the convergence of the summations. Equation (11) and (5) in the limit \( \tau = 0^{+} \) have the same summation form, except for a minus sigh.

To evaluate the frequency summations over the Matsubara Green’s functions, we need to further simplify the above formula by considering the interacting Matsubara Green’s functions at the poles, which holds,

\[ \mathcal{G}(i\omega_{n}) = \mathcal{G}(-i\omega_{n})^{*}, \]

\[ \omega_{n} = \frac{(2n+1)\pi}{\beta}, \quad n = 0, 1, 2, \cdots. \quad (12) \]

With the help of the above equation (12), the average number of bound electrons of a given site \( n_{b} \) directly from the summation of positive frequency for the effective on-site problem.

\[ n_{b} = - \frac{2}{\beta} \text{Re} \sum_{n=0}^{\infty} e^{-i\omega_{n}0^{+}} \mathcal{G}(i\omega_{n}) \]

which therefore shows that we can get the average number of bound electrons of a given site directly from the summation of positive frequency for the effective on-site problem.
Mott MIT depicted by average number of bound electrons. We define the quasiparticle coherent weight \( Z_F \) as \([21, 30] \):

\[
\frac{1}{Z_F} = 1 - \frac{\partial}{\partial \omega} \text{Re} \Sigma(\omega)|_{\omega=0} \approx 1 - \frac{\text{Im} \Sigma(i\omega_0)}{\omega_0}. \tag{14}
\]

In the following discussions, we study the Mott MIT of the Hubbard model at half-filling in terms of the evolution of the average number of bound electrons of a given site \( n_b \) with \( U \). In Fig. 1 we plot \( n_b \) as a function of \( U \), where the red dashed-line indicates the position of the critical point of the Mott MIT. For a better comparison, the evolution of the quasiparticle coherent weight \( Z_F \) (blue solid-line) with \( U \) is also presented in Fig. 1. Apparently, \( Z_F \) smoothly decreases with increasing \( U \), and then it disappears around the critical point \( U_c = 6.4 \) of MIT, in good agreement with the results obtained in the previous studies. It should be emphasized that within the framework of DMFT \([24, 30] \), when \( U \) is much smaller than \( U_c \), \( Z_F \) still has an accuracy of up to 0.3\%. However, the systematic errors of \( Z_F \) increase heavily near the critical point of MIT, leading to a difficult problem for the accurate determination of the critical point of MIT. In fact, the critical point of MIT in terms of \( Z_F \) can only be determined within a small range of \( U \). On the other hand, in a striking contrast to the evolution of \( Z_F \) with \( U \), \( n_b \) is exactly equal to zero in the metallic phase, where \( U < U_c \). However, at the critical point \( U_c = 6.4 \) of MIT, it jumps abruptly from \( n_b = 0 \) in the metallic phase to \( n_b \approx 1 \) in the insulating phase. As shown in Fig. 1, our results present clearly that the average number of bound electrons of a given site \( n_b \) is very sensitive to the existence of the resonant-peak at Fermi level, which is a more proper order parameter to accurately depict the critical point of the Mott MIT.

Two classes of solutions. Now we turn to discuss two classes of solutions: (i) the solution from the metallic phase towards the critical point of MIT (the metallic-phase solution); and (ii) the solution from the insulating phase towards to the critical point of MIT (the insulating-phase solution), and then show that the average number of bound electrons \( n_b \) as the order parameter of MIT can give a natural explanation of the difference between the metallic and insulating solutions. We have made a series of calculations for \( n_b \), and the results of the metallic solution of \( n_b \) (red dotted-line) and the insulating solution (blue solid-line) are plotted in Fig. 2, where \( U_{c1} = 4.7 \) denoted by blue solid-line and \( U_{c2} = 6.4 \) denoted by red dashed-line are the critical points of the insulator to metal transition and metal to insulator transition, respectively. Hence the results in Fig. 2 show that apart from a metallic phase at the weak interaction \((U < U_{c1}) \) and a insulating phase at the strong interaction \((U > U_{c2}) \), there is an intermediate interaction regime \((U_{c1} < U < U_{c2}) \), where the metallic solution coexists with the insulating solution. Within this intermediate interaction regime, \( n_b \) as a function of \( U \) exhibits a hysteretic behavior since both metallic and insulating solutions are found to be attractive points of a particle-hole symmetry system \([14] \). The present results in Fig. 1 and Fig. 2 therefore show that \( n_b \) is a more suitable order parameter to give a more proper description of the Mott MIT in a strong correlation system.

Finally, we estimate the cutoff effect. This follows a fact that although the summation of Matsubara frequency in equation (13) is from zero to infinity, the actual calculation is performed numerically with the infinitude of Matsubara frequency \( n = 0, 1, 2, \ldots, \infty \to n = 0, 1, 2, \ldots, n_{\text{max}} \) replaced by a finite \( n_{\text{max}} \). In this case,
we have made a series of calculations for \( n_b \) as a function of \( U \) at different cutoff \( n_{\text{max}} \), and the results are plotted in Fig. 3, where the critical points at \( n_{\text{max}} = 2048 \), \( n_{\text{max}} = 8192 \), \( n_{\text{max}} = 32768 \), and \( n_{\text{max}} = 65536 \) are very close to each other, indicating that for the large enough \( n_{\text{max}} \), the error bars are small enough. In particular, \( U_c \) can be extrapolated as \( U_c = 6.32 \) in the case of \( n_{\text{max}} = \infty \).

**Conclusions.** Based on the one-band Hubbard model, we study the Mott MIT in a strong correlation system by using the combined dynamical mean-field approach and Lanczos technique. Our results show very clearly that the average number of bound electrons as a more proper order parameter can correctly depict the Mott MIT in a strong correlation system, including the accurate determination of the critical points as well as the consistent description of two distinct forms of the critical points. The average number of bound electrons is a universal order parameter of strong correlation systems, and can be used to discuss the novel physics in orbital-selective Mott insulators [31] and cuprate superconductors [32, 33]. In particular, it may be applied to explain the hysteresis observed experimentally from the Mott-field effect transistors [34, 35], and these related works are under investigation now.

**ACKNOWLEDGEMENTS**

This work is supported by the Fundamental Research Funds for the Central Universities of China No. JN200208. YS is supported by the National Natural Science Foundation of China (NSFC) under Grants No. 11474023. SF is supported by the National Key Research and Development Program of China, and NSFC under Grant Nos. 11974051 and 11734002.

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