Mott Transition and Superconductivity in the two-band Hubbard model in Infinite dimensions

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(Received)

Abstract

Electronic states in the two-band Hubbard model in infinite dimensions are investigated by using the exact diagonalization method. In the half-filled case, the phase boundary separating the metallic and insulating regimes is obtained as a function of the on-site repulsive interaction U and the charge-transfer energy Δ. The Mott metal-insulator transition is observed when U is varied for the case with $U < \Delta$ (Mott-Hubbard type), while it is observed when Δ is varied for the case with $U > \Delta$ (charge-transfer type). In the doped case, on-site paring susceptibility is calculated at finite temperature and the critical temperature of the superconductivity is found in a charge-transfer type while not in a Mott-Hubbard type.

Keywords: Metal-Insulator transition; Two-band Hubbard Model; Infinite Dimensions; exact diagonalization;

Since the discovery of the high-temperature superconductors, a considerable number of theoretical works have been performed to clarify properties of the strongly correlated electron systems. In particular, the dynamical mean field theory (DMFT) in the limit of infinite dimensions $d = \infty$ has received much attention due to a successful description of electron correlation. [1] In the DMFT, a lattice problem is reduced to an impurity problem embedded in an effective medium by neglecting the momentum dependence of the self-energy. Various methods, which are the exact diagonalization method, quantum Monte Carlo method and perturbation method, allow us to solve the corresponding impurity problem. The DMFT is exact in the limit of $d = \infty$ and believed to be good approximation in high dimensions.

A detailed analysis of the $d = \infty$ single-band Hubbard model shows that the metal-insulator transition occurs as the first order phase transition at finite temperatures. [2] A coexistence region of the metallic and insulating solutions is observed near the transition point. At zero temperature, the coexistence region is observed for $1.2 \lesssim U/W \lesssim 1.5$, [3] where U and W are the on-site repulsive interaction and the bandwidth respectively. The magnetic phase diagram is also obtained as a function of doping, temperature and U. Away from half-filling, the antiferromagnetic transition temperature decreases with increasing doping. A commensurate order changes to an incommensurate state at a value of the doping which depends on U. [4] The superconducting phase is absent in this model. [5]

In spite of the well understanding of the single-band Hubbard model, the electronic states, especially the metal-insulator transition of the two-band Hubbard model in infinite dimensions is much less known. [6–8] In this work, we study the electronic states of the model by using the DMFT with the exact diagonalization method. The phase diagram of the metal-insulator transition is obtained as a function of U and the charge-transfer energy Δ at the half-filling. In the doped case, we discuss the critical temperature of the superconductivity by calculating paring susceptibilities.

We consider the two-band Hubbard model on a Bethe lattice with infinite connectivity $z = \infty$. The Hamiltonian

is given by

$$H = \sum_{i,j,\sigma}(t_{ij} d^\dagger_{i\sigma} p_{j\sigma} + h.c.) + \epsilon_p \sum_{j,\sigma} p^\dagger_{j\sigma} p_{j\sigma} + \epsilon_d \sum_{i,\sigma} d^\dagger_{i\sigma} d_{i\sigma} + U_d \sum_i n^d_{i\uparrow} n^d_{i\downarrow}, \quad (1)$$

where $d^\dagger_{i\sigma}$ and $p^\dagger_{j\sigma}$ are creation operators for an electron (or hole) with spin σ in the d- orbital at site i and in the p-orbital at site j, respectively. $n^d_{i,\sigma} = d^\dagger_{i\sigma} d_{i\sigma}$. The charge-transfer energy Δ is defined by $\Delta = \epsilon_p - \epsilon_d > 0$. $t_{ij} = t_{pd}/\sqrt{z}$ represents the transfer energy between the nearest neighbor d and p orbitals and we set $t_{pd} = 1$ in the present study. In the limit $z \to \infty$, the self-energy becomes purely site-diagonal and the DMFT becomes exact.

In the DMFT, the effective action of the impurity model is given by

$$S = U_d \int_0^\beta d\tau n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) - \int_0^\beta \int_0^\beta d\tau d\tau' \sum_\sigma d^\dagger_\sigma(\tau) D_0^{-1}(\tau - \tau') d_\sigma(\tau'). \quad (2)$$

where the Weiss function $D_0(i\omega)$ includes effects of the interaction at all the sites except the impurity site. The local Green's function for the d-electron $D(\tau - \tau') = - < Td(\tau) d^\dagger(\tau') >_S$ is calculated with this action. In the case with $z = \infty$ Bethe lattice, the self-consistency equations for the local Green's functions are given by [6]

$$\begin{aligned} D_0(i\omega_n)^{-1} &= i\omega_n + \mu - \varepsilon_d - t^2_{pd} P(i\omega_n), \\ P(i\omega_n)^{-1} &= i\omega_n + \mu - \varepsilon_p - t^2_{pd} D(i\omega_n), \end{aligned} \quad (3)$$

where μ is the chemical potential and ω_n is the Matsubara frequency, $\omega_n = (2n+1)\pi/\beta$. $P(i\omega)$ is the local Green's function for the p-electron. To solve the impurity problem for a given $D_0(i\omega)$, we use the exact diagonalization method. The self-consistency equations (3) lead a new $D_0(i\omega)$ and we repeat the calculation of the impurity problem. This process is iterated until the solutions converge.

In the exact diagonalization method, we approximately solve the impurity Anderson model by the exact diagonalization of a finite-size cluster; [7, 8]

$$H_{And} = \varepsilon_0 \sum_\sigma n_{d\sigma} + \sum_{l=2,\sigma}^{N_s} \varepsilon_l c^\dagger_{l\sigma} c_{l\sigma} + \sum_{l=2,\sigma}^{N_s} V_l (d^\dagger_\sigma c_{l\sigma} + c^\dagger_{l\sigma} d_\sigma) + U_d n^d_\uparrow n^d_\downarrow, \quad (4)$$

where ε_0 is the impurity level and ε_l $(l = 2, 3, ..., N_s)$ are levels of the conduction electron hybridized with the impurity by V_l. We regard the non-interacting Green's function $G^0_{And}(i\omega_n)$ as the Weiss function $D_0(i\omega)$ in the action eq.(3). Then, the interacting Green's function $G_{And}(i\omega_n)$ corresponds to the local Green's function $D(i\omega)$ in the original lattice problem. Here, $G^0_{And}(i\omega_n) = [i\omega_n - \varepsilon_0 - \sum_{l=1}^{N_s} \frac{V_l^2}{i\omega_n - \varepsilon_l}]^{-1}$. For a given $D_0(i\omega)$, we determine $2N_s - 1$ parameters $\varepsilon_0, \varepsilon_l, V_l (l = 2, 3, ..., N_s)$ to make $G^0_{And}(i\omega_n)$ as close to $D_0(i\omega)$ as possible. Using these parameters, we diagonalize the finite cluster of the impurity Anderson model, and calculate $G_{And}(i\omega_n)$ $(D(i\omega_n))$. At finite temperature, the Green's function is calculated from a complete set of eigenstates $|i>$ with eigenvalues E_i according to

$$D(i\omega_n) = \frac{1}{\Xi} \sum_{i,j} \frac{| < i|d^\dagger_\sigma|j > |^2}{i\omega_n - E_i + E_j} [\exp(-\beta E_i) + \exp(-\beta E_j)],$$

with $\Xi = \sum_i \mathrm{e}^{-\beta E_i}$. Using the Lanczos method with the continued-fraction expansions, we also calculate the zero temperature Green's function. In this case, we replace the Matsubara frequencies by a fine grid of imaginary frequencies, which correspond to a fictitious inverse temperature $\tilde{\beta}$ $(\omega_n = (2n+1)\pi/\tilde{\beta})$. Here, $\tilde{\beta}$ determines a low-frequency cut-off. [7]

First, we consider the metal-insulator transition at zero temperature in the half-filled case with the total number per unit cell $n = n_d + n_p = 1$. It is well known that the system such as two-band Hubbard model indicates a transition from a metallic to an insulating state. [9] For the case with $U_d < \Delta$ (Mott-Hubbard type), the metal-insulator transition is observed when U_d is varied. If we assume $t_{pd} \ll \Delta$, d-electrons exclusively contribute to the bare band near the fermi level. In this case, the transition occurs when U_d is comparable to the bare bandwidth as observed in the single-band Hubbard model.

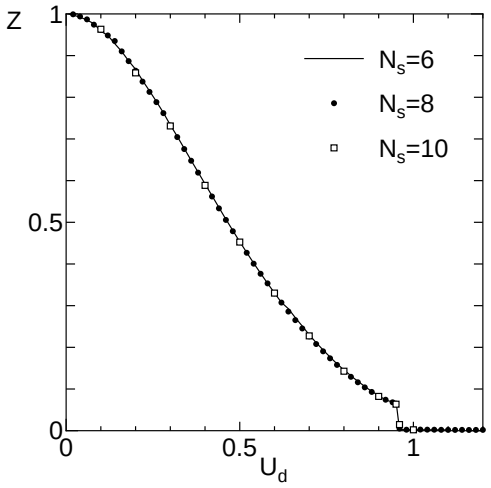

Fig. 1. The quasiparticle weight Z as a function of U_d at $\Delta = 6$, $n = 1$ and $T = 0$ for the system size $N_s = 6, 8, 10$. The fictitious inverse temperature is set to be $\tilde{\beta} = 200$.

In Fig.1, we show the quasiparticle weight Z as a function of U_d at $\Delta = 6$ for the system size $N_s = 6, 8, 10$, where we define $Z^{-1} = 1 - \frac{d\Sigma(i\omega_n)}{di\omega_n}|_{i\omega_n \to 0} \simeq 1 - [\mathrm{Im}\Sigma(i\pi T) - \mathrm{Im}\Sigma(-i\pi T)]/2\pi T$. The metal-insulator transition occurs at a critical value $U_d^c = 0.96$. Taking into account of the bare bandwidth $W = [(\Delta^2 + 16t_{pd}^2)^{\frac{1}{2}} - \Delta]/2 \sim 0.6$, the value of $U_d^c/W \sim 1.6$ is close to that in the single-band Hubbard model ($U_c/W = 1.47$). [3] We also find a coexistence of metallic ($Z \neq 0$) and insulating ($Z = 0$) solutions for $0.78 < U_d < 0.96$ as observed in the single-band Hubbard model for $1.25 < U/W < 1.47$. [3, 10]

The size dependence of Z is very small and negligible except for the proximity of the transition point. The curve Z seems to jump at U_c, but it is related with the value of the fictitious inverse temperature $\tilde{\beta}$. In order to check the influence of $\tilde{\beta}$ on Z, we calculate U_d dependence of Z for various $\tilde{\beta}$ near the critical point as shown in Fig.2. The magnitude of the jump decreases with increasing $\tilde{\beta}$. It suggests that Z becomes zero smoothly at $U = U_d^c$ in the limit $\tilde{\beta} \to \infty$. The critical value U_d^c also depends on $\tilde{\beta}$, however, the variance of U_d^c is small and about 0.05.

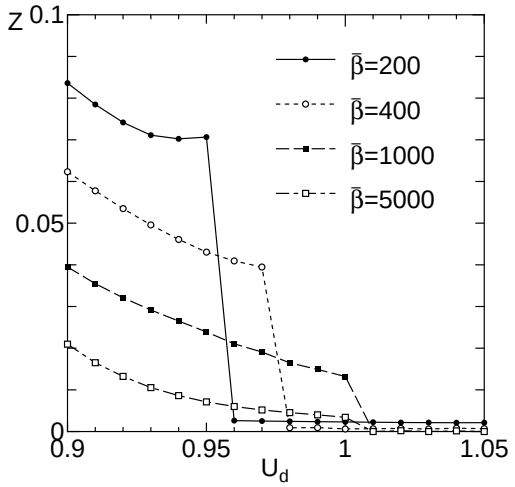

Fig. 2. The quasiparticle weight Z as a function of U_d at $\Delta = 6$, $n = 1$, $T = 0$ and $N_s = 6$ for several values of the fictitious inverse temperature $\tilde{\beta}$.

For the case with $U_d > \Delta$ (charge-transfer type), the metal-insulator transition is observed when Δ is varied. When $t_{pd} \ll \Delta < U_d$, d-sites are almost singly occupied and p-sites are nearly empty. The electron transfer between d- and p-orbitals costs an energy $\sim \Delta$ while the kinetic energy gains $\sim t_{pd}^2/\Delta$. Therefore, we have a charge-transfer type insulator for $t_{pd} << \Delta$. In Fig.3, we show the quasiparticle weight Z and the number of p-electron n_p as functions of Δ at $U_d = 6$ for the system size $N_s = 6, 8$. The metal-insulator transition occurs at a critical value $\Delta_c = 2.23$. A coexistence of metallic and insulating solutions for $1.88 < \Delta < 2.23$ is visible in the Δ-dependence of n_p as shown in Fig.3.

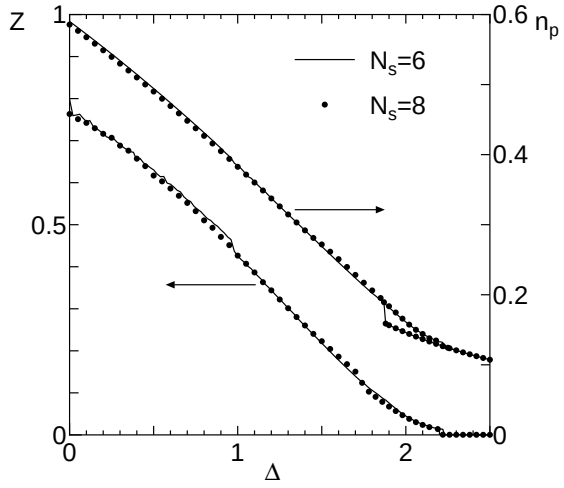

Fig. 3. The quasiparticle weight Z and the number of p-electron n_p as functions of Δ at $U_d = 6$, $n = 1$ and $T = 0$ for the system size $N_s = 6, 8$. The fictitious inverse temperature is set to be $\tilde{\beta} = 200$.

Phase diagram of the metallic ($Z \neq 0$) and insulating ($Z = 0$) regions is shown in Fig.4. Based on the above argument, the critical value U_d^c is expected to decrease with increasing Δ and $U_d^c \sim t_{pd}^2/\Delta \to 0$ in the limit $\Delta \to \infty$ in the Mott-Hubbard type. On the other hand, the critical value Δ_c may be finite and of order of t_{pd} in the limit $U_d \to \infty$ in the charge-transfer type. The coexistence of metallic and insulating solutions observed at the proximity of the phase boundary. It extends continuously from the Mott-Hubbard type to the charge-transfer type.

Finally, we discuss the superconductivity away from half-filling. The on-site paring susceptibility χ of the model (1) is given by [1, 6]

$$\chi = \frac{1}{N}\int_0^\beta d\tau \sum_{ij} < T d_{i\uparrow}(\tau) d_{i\downarrow}(\tau) d_{j\downarrow}^\dagger(0) d_{j\uparrow}^\dagger(0) >$$

$$= T \sum_{\nu,\nu'} [\alpha^{-1/2}\{I - \Lambda\}^{-1} \cdot \Lambda \cdot \alpha^{-1/2}]_{\nu,\nu'}, \qquad (5)$$

where $[\Lambda]_{\nu,\nu'} = t_{pd}^4 |P(i\nu)| [\tilde{\chi}_{loc}]_{\nu,\nu'} |P(i\nu')|$, and $[\alpha]_{\nu,\nu'} = t_{pd}^4 |P(i\nu)|^2 \delta_{\nu,\nu'}$. Here, $\tilde{\chi}_{loc}$ is the local paring susceptibility on a d-orbital given by

$$[\tilde{\chi}_{loc}]_{\nu,\nu'} = T^2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 e^{i\nu(\tau_1 - \tau_2)}$$

$$\times e^{i\nu'(\tau_3 - \tau_4)} < T d_\uparrow(\tau_1) d_\downarrow(\tau_2) d_\downarrow^\dagger(\tau_3) d_\uparrow^\dagger(\tau_4) > . \qquad (6)$$

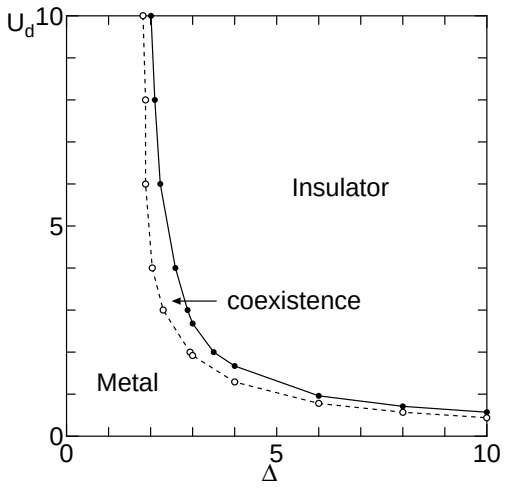

Fig. 4. The phase boundary separating the metallic and insulating regimes (solid line) as a function of U_d and Δ at $n = 1$ and $T = 0$ for the system size $N_s = 6$ and the fictitious inverse temperature $\tilde{\beta} = 200$. The coexistence region exists between solid and dashed lines.

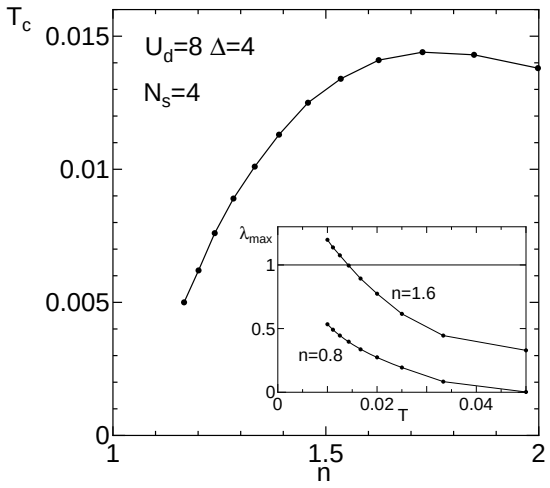

Fig. 5. The critical temperature T_c of the singlet superconductivity as a function of filling n at $U_d = 8$ and $\Delta = 4$ for the system size $N_s = 4$. The inset shows the largest eigenvalue λ_{max} as a function of temperature T at the same parameters.

To calculate $\tilde{\chi}_{loc}$ within the exact diagonalization method, we use a spectral representation of r.h.s. in eq.(6) by inserting a complete set of eigenstates $|i>$.

When the largest eigenvalue of Λ approaches unity, the paring susceptibility diverges. It signals the transition into the superconducting state from the normal state. In the inset in Fig.5, we plot the temperature dependence of the largest eigenvalue of Λ, λ_{max}, in a case with charge-transfer type, $U_d = 8$ and $\Delta = 4$, for the system size $N_s = 4$. The value of λ_{max} increases with decreasing T and exceeds unity at a certain critical temperature $T_c = 0.014$ for $n = 1.6$. Fig.5 shows the critical temperature T_c for the singlet pairing as a function of filling n in the hole doping case (hole picture). T_c increases with increasing n and has a maximum at $n \sim 1.7$. On the other hand, in the electron doping case, T_c is considerably suppressed (see for $n = 0.8$ in the inset in Fig.5). Furthermore, we can not find a finite T_c in the Mott-Hubbard type. These results seem to be consistent with the results of the single-band Hubbard model [5] and of the high-T_c superconductors except for the doping dependence of T_c.

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