Critical Behaviour near the Mott Transition in a Two-band Hubbard Model

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The Mott metal-insulator transition in the two-band Hubbard model in infinite dimensions is studied by using the linearized dynamical mean-field theory. The discontinuity in the chemical potential for the change from hole to electron doping is calculated analytically as a function of the on-site Coulomb interaction U, and the charge-transfer energy Δ between the d- and p-orbitals, transfer integrals t_{pd}, t_{pp}, t_{dd} between p-d, p-p and d-d sites respectively. The critical behaviour of the quasiparticle weight is also obtained analytically.

KEYWORDS: Mott transition, metal−insulator transition, two-band Hubbard model, dynamical mean-field theory, infinite dimensions

§1. Introduction

The Mott metal−insulator transition (MIT) is observed in various transition metal oxides and have been extensively studied for years. The dynamical mean-field theory (DMFT),[1,2] which becomes exact in the infinite spatial dimensions, has been used in various models and have given plausible results for the MIT. However, it is difficult to obtain the critical behaviour of the MIT numerically as the quasiparticle peak becomes extremely sharp in the limit of the MIT. There is an alternative way to resolve the adifficulty. The linearized DMFT (LDMF)[3–6] is an approximate but analytical method which becomes the most correct on the MIT point.

There are two types of the MIT in real materials: the Mott-Hubbard (MH) type in which the energy gap is given roughly by the Coulomb interaction and the charge-transfer (CT) type in which the energy gap is given roughly by the charge transfer energy. In order to describe the two types of the MIT, we need at least the two-band Hubbard model which is characterized by the Coulomb interaction U, charge transfer energy Δ and p-d, p-p and d-d transfer integrals t_{pd}, t_{pp} and t_{dd}.[5]

The critical behaviour of the MIT has been studied using the LDMF for the single-band Hubbard model.[3,6] It has also been studied for the two-band Hubbard model in our previous paper.[4] However, effects of t_{pp} and t_{dd} were not considered there, which are not negligible in actual compounds but make important contribution to the critical behaviour near the MIT, as found to be significant to determine the phase boundary of the MIT.[5] In the present paper, we study the discontinuity in the chemical potential and the critical behaviour of the MIT in the two-band Hubbard model in the presence of t_{pp} and t_{dd}.

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§2. Formulation

We consider the two-band Hubbard model,[5]

$$H = \frac{t_{pd}}{\sqrt{q}} \sum_{\langle i,j\rangle,\sigma} (d^\dagger_{i\sigma} p_{j\sigma} + h.c.) + U \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow} + \frac{t_{dd}}{q} \sum_{\langle i,i'\rangle,\sigma} (d^\dagger_{i\sigma} d_{i'\sigma} + h.c.) + \epsilon_{d0} \sum_{i,\sigma} d^\dagger_{i\sigma} d_{i\sigma} + \frac{t_{pp}}{q} \sum_{\langle j,j'\rangle,\sigma} (p^\dagger_{j\sigma} p_{j'\sigma} + h.c.) + \epsilon_{p0} \sum_{j,\sigma} p^\dagger_{j\sigma} p_{j\sigma}, \quad (2.1)$$

where $d^\dagger_{i\sigma}$ and $p^\dagger_{j\sigma}$ are creation operators for an electron with spin σ in the d-orbital at site i and in the p-orbital at site j, respectively. t_{pd}, t_{dd} and t_{pp} are the transfer integrals between the nearest neighbor p-d, p-p and d-d orbitals, respectively. In eq. (2.1), we assume that p- and d-orbitals are on different sub-lattices of a bipartite lattice, more explicitly, a Bethe lattice with connectivity q. In the limit $q = \infty$, the self-consistency equations for the local Green's functions are given by[2]

$$\mathcal{G}_0(z)^{-1} = z - \epsilon_d - t^2_{pd} G_p(z) - t^2_{dd} G_d(z), \quad (2.2)$$

$$G_p(z)^{-1} = z - \epsilon_p - t^2_{pd} G_d(z) - t^2_{pp} G_p(z), \quad (2.3)$$

where $G_p(z)$ is the local Green's function for the p-electron and $G_d(z)$ is that for the d-electron; $\epsilon_d \equiv \epsilon_{d0} - \mu = -\mu$ and $\epsilon_p \equiv \epsilon_{p0} - \mu = \Delta - \mu$, where we set $\epsilon_{d0} = 0$ and the CT energy Δ is defined by $\Delta \equiv \epsilon_p - \epsilon_d > 0$.

In the LDMF, the two-band Hubbard model eq. (2.1) is mapped onto a two-site Anderson model

$$H_{2-\text{site}} = \epsilon_f \sum_\sigma f^\dagger_\sigma f_\sigma + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow + \epsilon_c \sum_\sigma c^\dagger_\sigma c_\sigma + V \sum_\sigma (f^\dagger_\sigma c_\sigma + c^\dagger_\sigma f_\sigma), \quad (2.4)$$

with $\epsilon_c = 0$ and $\epsilon_f = \epsilon_d = -\mu$. In the model eq. (2.4), the non-interacting impurity Green's function is: $\mathcal{G}_0(z)^{-1} = z - \epsilon_f - \frac{V^2}{z}$. In the limit $V \to 0$, the local Green's functions are given by $G_d(z) = \frac{Z_d}{z}$ and $G_p(z) = \frac{Z_p}{z}$,[4,5] near the Fermi level with small weights $Z_d \to 0$ and $Z_p \to 0$.

Then the self-consistency equations (2.2) and (2.3) are reduced to a simple equation

$$t_{pd}^2 Z_p + t_{dd}^2 Z_d = V^2. \tag{2.5}$$

To second order in V, the quasiparticle weights for the d-electron and the p-electron are given by[7)]

$$Z_d = F(U,\mu)V^2, \tag{2.6}$$

$$Z_p = A(t_{pd}, t_{pp}, U, \Delta, \mu)V^2, \tag{2.7}$$

where

$$F(U,\mu) = \frac{5}{2\mu^2} + \frac{5}{2(U-\mu)^2} + \frac{4}{\mu(U-\mu)}, \tag{2.8}$$

$$A(t_{pd}, t_{pp}, U, \Delta, \mu) = \frac{t_{pd}^2 F(U,\mu)}{E_p^2 - t_{pp}^2}, \tag{2.9}$$

and

$$E_p = \Delta - \mu - \frac{t_{pp}^2}{\Delta - \mu} - t_{pd}^2 \left\{ -\frac{1}{2\mu} + \frac{1}{2(U-\mu)} \right\}. \tag{2.10}$$

Substituting eqs.(2.6) and (2.7) with eqs.(2.8) and (2.9) into eq. (2.5) we obtain an equation to determine the MIT point,

$$P(t_{pd}, t_{pp}, t_{dd}, U, \Delta, \mu) = 1, \tag{2.11}$$

where

$$P = t_{pd}^2 A(t_{pd}, t_{pp}, U, \Delta, \mu) + t_{dd}^2 F(U,\mu). \tag{2.12}$$

After self-consistency cycle, V increase exponentially with iteration number for $P > 1$, and then the single pole approximation breaks down resulting in the metallic solution, on the other hand $P < 1$ correspond to the insulating solution. In eq. (2.11), P includes the chemical potential μ which has to be determined explicitly to obtain the critical values of the MIT. We can use a certain condition to determine μ, based on the fact that at the MIT point P has a minimum value as a function of μ.[4)] This condition gives

$$\frac{\partial}{\partial \mu} P(t_{pd}, t_{pp}, t_{dd}, U, \Delta, \mu) = 0. \tag{2.13}$$

§3. Discontinuity in the Chemical Potential

By solving eqs. (2.11) and (2.13), the MIT phase boundary is determined and shown in Fig. 1 (see $\Delta\mu = 0$). In the insulating regime, the chemical potential $\mu_\pm$ in the limit $n \to 1 \pm 0_+$ is obtained from eq. (2.11): $P|_{\mu=\mu_\pm} = 1$,[4)] which yields the discontinuity in the chemical potential, $\Delta\mu = \mu_+ - \mu_-$. In Fig. 1, we show the contour map for $\Delta\mu$ on the Δ-U plane, where the diagonal dotted line represents a boundary separating the CT and the MH regimes, and the dashed lines are the critical values of U_c and Δ_c in the limit of $\Delta \to \infty$ and $U \to \infty$, respectively. The discontinuity in the chemical potential smoothly connects the Mott-Hubbard type and the charge-transfer type insulators. In the limit $\Delta \to \infty$, the critical value of $U_c = 6\ t_{dd}$ is the same as that for the corresponding single-band Hubbard model.[3,6)]

§4. Critical Behaviour near the Mott MIT

We discuss the critical behaviour in the vicinity of the Mott MIT at half-filling in the two-band Hubbard model. In this case, we need the result of the quasiparticle weight for the d-electron up to fourth order in V ,

$$Z_d = F(U,\mu)V^2 - G(U,\mu)V^4, \tag{4.1}$$

where F is given in eq. (2.8) and

$$G(U,\mu) = \frac{29}{2\mu^4} + \frac{24}{\mu^3(U-\mu)} + \frac{22}{\mu^2(U-\mu)^2} + \frac{24}{\mu(U-\mu)^3} + \frac{29}{2(U-\mu)^4}. \tag{4.2}$$

The quasiparticle weight for the p-electron Z_p is also calculated up to fourth order in V,

$$Z_p = A(t_{pd}, t_{pp}, U, \Delta, \mu)V^2 - B(t_{pd}, t_{pp}, U, \Delta, \mu)V^4, \tag{4.3}$$

where A is given in eq. (2.9) and

$$B(t_{pd}, t_{pp}, U, \Delta, \mu) = t_{pd}^2 \frac{G}{E_p^2 - t_{pp}^2} + t_{pd}^4 \frac{2F\,B_1 E_p}{(E_p^2 - t_{pp}^2)^2} + t_{pd}^4 \frac{F^2\{2t_{pp}^2 + 3B_2 E_p(\Delta-\mu)\}}{(E_p^2 - t_{pp}^2)^3(\Delta-\mu)}, \tag{4.4}$$

with

$$B_1 = \frac{-3\,U^3 + 7\,U^2\,\mu - 3\,U\,\mu^2 + 2\,\mu^3}{\mu^3\,(U-\mu)^3}, \tag{4.5}$$

$$B_2 = 1 + t_{pd}^2 \left\{ \frac{1}{2\mu^2} + \frac{1}{2(U-\mu)^2} \right\} + \frac{{t_{pp}}^2}{(\Delta-\mu)^2}. \tag{4.6}$$

Substituting V^2 from the self-consistency equation (2.5) into eqs. (4.1) and (4.3), we obtain

$$Z_d = F(U,\mu)\frac{P-1}{Q}, \tag{4.7}$$

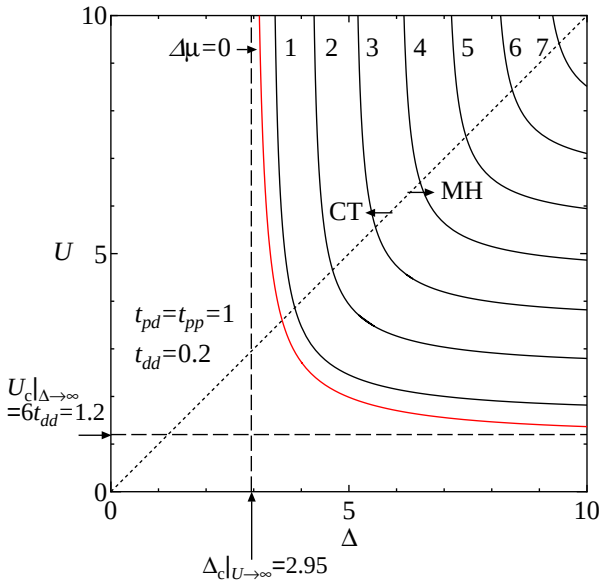

Fig. 1. The contour map for the discontinuity in the chemical potential $\Delta\mu = 0, 1, 2, 3, 4, 5, 6, 7$ at $t_{pd} = t_{pp} = 1$ and $t_{dd} = 0.2$. The dotted line represents a boundary separating the MH and CT regime.

where

$$Q = t_{pd}^2 B(t_{pd}, t_{pp}, U, \Delta, \mu) + t_{dd}^2 G(U, \mu). \quad (4.8)$$

At the MIT point with the critical values U_c, Δ_c and μ_c, eqs. (4.7) yield $Z_d = 0$ from eq. (2.11). When Δ or U decreases from the MIT point, the quasiparticle weight for the d-electron Z_d eq. (4.7) increases as

$$Z_d = C_\Delta \left(1 - \frac{\Delta}{\Delta_c}\right), \quad (4.9)$$

$$Z_d = C_U \left(1 - \frac{U}{U_c}\right), \quad (4.10)$$

near the MIT point at half-filling, respectively. The coefficients C_Δ and C_U are shown in Figs. 2(a) and (b).

When t_{pp} increases, the p-component of the quasiparticle weight increases, then, C_Δ increases and C_U decreases (compare the dotted line with the solid line in Figs. 2(a) and (b)). On the other hand, when t_{dd} increases, the d-component of the quasiparticle weight increases, then, C_Δ decreases and C_U increases (compare the dashed line with the solid line in Figs. 2(a) and (b)).

In the CT regime ($U > \Delta$), the MIT occurs at $\Delta = \Delta_c$ when Δ is varied for a fixed U. As Δ decreases below Δ_c for a fixed U, the quasiparticle weight increases as given in eq. (4.9). With increasing U_c (decreasing Δ_c), the coefficients both C_Δ and C_U decrease due to the increasing correlation effect as seen in Figs.2(a) and (b).

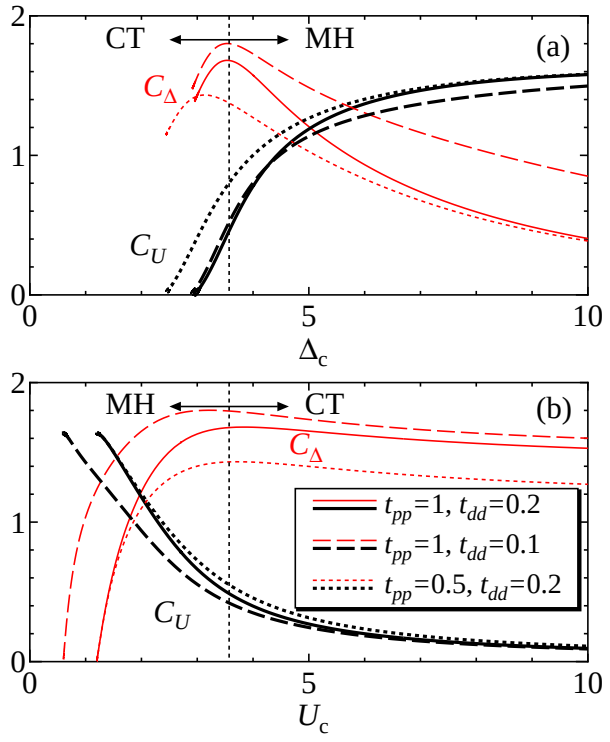

Fig. 2. The coefficients C_Δ (thin lines) and C_U (thick lines) of the quasiparticle weights for the d-electrons $Z_d = C_\Delta \left(1 - \frac{\Delta}{\Delta_c}\right)$ and $Z_d = C_U \left(1 - \frac{U}{U_c}\right)$, respectively, as functions of Δ_c (a) and U_c (b) for several values of t_{pp} and t_{dd} with $t_{pd} = 1$. The thin vertical dotted line shows a boundary of MH and CT for $t_{pp} = 1$ and $t_{dd} = 0.2$.

In the limit $U_c \to \infty$, the coefficients are

$$C_\Delta = 1.31, \quad C_U = 0, \quad (4.11)$$

for $t_{pd} = t_{pp} = 1$ and $t_{dd} = 0.2$.

In the MH regime ($U < \Delta$), the MIT occurs at $U = U_c$ when U is varied for a fixed Δ. As U decreases below U_c for a fixed Δ, the quasiparticle weight increases as given in eq. (4.10). With increasing Δ_c (decreasing U_c), C_U increases due to the decreasing correlation effect, while C_Δ decrease due to the decreasing p-component of the quasiparticle weight (See Figs.2(a) and (b)). In the limit $\Delta_c \to \infty$, the coefficients are

$$C_\Delta = 0, \quad C_U = \frac{18}{11}, \quad (4.12)$$

for $t_{pd} = t_{pp} = 1$ and $t_{dd} = 0.2$. In the limit $\Delta_c \to \infty$, the effect of the p-band becomes irrelevant and, then, $C_\Delta = 0$ and $C_U = \frac{18}{11}$ is the same value as that for the single-band Hubbard model.[3] We note that, even in this limit, C_Δ is finite and $C_U \neq \frac{18}{11}$ in the case with $t_{dd} = 0$, because the electron has to transfer between d and p orbitals through the hopping integral t_{pd} and the effect of the p-band is still relevant as shown in Ref. 4.

§5. Discussion

In the real materials, the ratio of the transfer integrals are estimated as: La_2CuO_4, $t_{pd} : t_{pp} = 1 : 0.50$,[8] $LaTiO_3$, $t_{pd} : t_{pp} = 1 : 0.15$, $LaNiO_3$, $t_{pd} : t_{pp} = 1 : 0.27$[9,10] (no data for t_{dd}). There is little data for the critical behaviour of the MIT when U or Δ is varied at the half-filling because of the difficulty of the experiments.[11] Further progress in both theoretical and experimental study for the critical behaviour of the MIT is expected.

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