Crossover between Mott-insulator and band-insulator in the two-orbital Hubbard model

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Abstract. Electronic states of the two-orbital Hubbard model are investigated by means of the composite operator method. In addition to the transfer within the same kind of orbital, we introduce the off-diagonal transfer $t'_0$, which provides the mixing of orbitals. In the $t'_0 = 0$ case, the system shows the orbital selective Mott transition at $U = 4$. Upon adding $t'_0$, the band gap goes wider. This increase of the gap originates from the crossover between the Mott-insulator and the band-insulator.

1. Introduction
The two-orbital Hubbard model has recently been in the limelight as a model for studying phenomena which originate from the orbital degeneracy. One of the most prominent feature of this system is the orbital selective Mott transition (OSMT). The one band possesses the energy gap with the strong Coulomb interaction, while the other stays metallic. Up to now, the OSMT has studied by DMFT [1, 2], slave-spin mean-field theory [3], Gutzwiller variational method [4], and composite operator method [5, 6].

Recently, Koga et al. introduced the local mixing of orbitals in this system [2]. Even though orbitals are orthogonal, they can mix with each other because of the deformation of crystal. The local mixing $V$ was introduced to study such a situation. In this paper, we also study the effects of orbital mixing. However, the interaction is not $V$ but $t'_0$, which provides the off-diagonal transfer in this system.

2. Model and formulation
The two-orbital Hubbard Hamiltonian reads as

$$H = H_0 + H_t + H_U + H_U' + H_J$$

with

$$H_0 = \sum_{\gamma,i,\sigma} \left( e_\gamma - \mu \right) c_{\gamma\sigma}^\dagger(i)c_{\gamma\sigma}(i),$$

$$H_t = \sum_{\gamma\gamma',ij,\sigma} t_{ij}^{(\gamma\gamma')} c_{\gamma\sigma}^\dagger(i)c_{\gamma'\sigma}(j),$$

$$H_U = U \sum_{\gamma,i} n_{\gamma\uparrow}(i)n_{\gamma\downarrow}(i),$$
\[ H_{U'} = U' \sum_{i,\sigma} n_{1\sigma}(i)n_{2\sigma'}(i), \]

\[ H_J = -\frac{1}{2} J \sum_{i,\nu} n_{1\nu}(i)n_{2\nu}(i) + J \sum_i \left[ p^\dagger_i(i)p_2(i) + p_i^\dagger(i)p_1(i) \right]. \]

c_{\gamma\sigma}(i) and c_{\gamma\sigma}(i) are creation and annihilation operators of electrons with spin \( \sigma \) at the orbital \( \gamma = 1, 2 \) and the site \( i = (i, t) \), respectively. \( n_{\gamma\sigma}(i) = c^\dagger_{\gamma\sigma}(i)c_{\gamma\sigma}(i) \), \( \epsilon_\gamma \) is the energy level of the orbital \( \gamma \), \( \mu \) is the chemical potential. \( t^{(\gamma\gamma')}_i \) provides the transfer between \( \gamma \)-orbital at site \( i \) and \( \gamma' \)-orbital at site \( j \). \( U \) and \( U' \) are the intra- and inter-orbital Coulomb interaction, respectively. \( H_J \) describes the inter-orbital interaction in the charge (\( \nu = 0 \)), spin (\( \nu = 1, 2, 3 \)) and pair (\( \gamma = 1 \)) channels. In the present research, we investigate the degenerate case, \( \epsilon_1 = \epsilon_2 \). \( t^{(\gamma\gamma')}_i \) has a form \( t^{(\gamma\gamma')}_i = -z (\delta_{\gamma\gamma'}t_0 + \delta_{ \gamma'\gamma} t'_0) \alpha_{ij} \). \( z \) is the coordination number, \( \alpha_{ij} \) presents the connection with nearest-neighbor sites. \( t_0 \) provides the hopping between \( i \) and \( j \) site within the same kind of orbital. \( t' \) provides the mixing of different kind of orbitals \( \gamma = 1 \leftrightarrow 2 \) between \( i \) and \( j \) site. \( \bar{\gamma} \) denotes \( \bar{\gamma} = 1 (\gamma = 2) \) and \( \bar{\gamma} = 2 (\gamma = 1) \). In general, the density of states (DOS) has a van Hove singularity according to the geometry of a lattice. In this research, we use the semi-circular approximation for simplicity, which corresponds to the case of Bethe lattice.

We introduce the Hubbard operators for each orbitals,

\[ \psi_\sigma(i) = \begin{pmatrix} \psi_\gamma^{(1)}(i) \\ \psi_\gamma^{(2)}(i) \\ \psi_\gamma^{(3)}(i) \\ \psi_\gamma^{(4)}(i) \end{pmatrix} \]

where \( \psi_\gamma^{(1)}(i) = \xi_{\gamma\sigma}(i) = c_{\gamma\sigma}(1 - n_{\gamma\sigma}(i)) \) and \( \psi_\gamma^{(2)}(i) = \eta_{\gamma\sigma}(i) = c_{\gamma\sigma}n_{\gamma\sigma}(i) \). The equations of motions are

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \psi_{\gamma\sigma}(i) = (\epsilon_{\gamma} - \mu) \psi_{\gamma\sigma}(i) - z t_\gamma \left( c^\dagger_{\gamma\sigma}(i) + \pi_{\gamma\sigma}(i) \right) - z t'_0 \left( c^\dagger_{\gamma\sigma}(i) + \pi'_{\gamma\sigma}(i) \right) + U' \psi_{\gamma\sigma}(i)n_{\gamma\sigma}(i) - J \left( \xi_{\gamma\sigma}(i)c^\dagger_{\gamma\sigma}(i) + \eta_{\gamma\sigma}(i)n_{\gamma\sigma}(i) + \eta'_{\gamma\sigma}(i)c_{\gamma\sigma}(i)c_{\gamma\sigma}(i) \right),
\]

where

\[
\pi_{\gamma\sigma}(i) = -n_{\gamma\sigma}(i)c_{\gamma\sigma}(i) + c^\dagger_{\gamma\sigma}(i)c_{\gamma\sigma}(i) - c_{\gamma\sigma}(i)c_{\gamma\sigma}(i),
\]

\[
\pi'_{\gamma\sigma}(i) = -n_{\gamma\sigma}(i)c_{\gamma\sigma}(i) + c^\dagger_{\gamma\sigma}(i)c_{\gamma\sigma}(i) - c_{\gamma\sigma}(i)c_{\gamma\sigma}(i).
\]

c_{\gamma\sigma}(i) denotes \( c_{\gamma\sigma}(i) = \sum_{\alpha} \alpha c_{\gamma\sigma}(j) \).

Within the composite operator method [7, 8], the retarded Green’s function takes a form

\[
G(\omega, k) = \frac{1}{\omega - E(k)} I(k),
\]

where \( I(k) = i \mathcal{F}\{\{\psi, \psi^\dagger\}\} \) and \( E(k) = m(k)I^{-1}(k) \) with \( m(k) = \mathcal{F}\{i \frac{\partial}{\partial t} \psi, \psi^\dagger\} \). \( \mathcal{F} \) is the Fourier transform. \( I(k) \) is a diagonal matrix with \( I_{11} = 1 - \langle n_{1-\sigma} \rangle, I_{22} = \langle n_{1-\sigma} \rangle, I_{33} = 1 - \langle n_{-\sigma} \rangle \) and

\[
\langle n_{1-\sigma} \rangle = \langle n_{1-\sigma} \rangle = \langle n_{-\sigma} \rangle = \langle n_{-\sigma} \rangle.
\]
Figure 1. The density of states for $\gamma = 1$ band (solid line) and $\gamma = 2$ band (dashed line). Parameters are shown in the text.

$I_{44} = \langle n_{2-\sigma} \rangle$. Whereas, each element of $m(k)$ has a somewhat complicated form which will be presented in elsewhere.

$I$ and $m(k)$ contain some correlation functions which are directly calculated by Green’s function itself self-consistently. Furthermore, there are some correlation functions which are out of the scheme of self-consistency. For example,

$$p_{\gamma\sigma} = \langle n_{\gamma-\sigma} n_{\gamma-\sigma}^\alpha \rangle + \langle c_{\gamma-\sigma}^\dagger c_{\gamma-\sigma}(c_{\gamma-\sigma}^\dagger c_{\gamma-\sigma})^{\alpha} \rangle - (c_{\gamma\sigma} c_{\gamma-\sigma} (c_{\gamma-\sigma} c_{\gamma\sigma})^{\alpha}). \tag{8}$$

To evaluate such quantities, the hermite condition of the Green’s function and/or the algebra-constraint of operators are available [8]. Here, we apply the algebra-constraint, $\langle \xi^\dagger \eta \rangle = 0$.

3. Results and discussion

In figure 1, we present the DOS for each orbital. We use the energy unit $D_1 = 1$, where $D_\gamma$ denotes the band width of $\gamma$ orbital in the tight-binding limit, $-D_\gamma \leq \omega \leq D_\gamma$. We adopt the different band width for two orbitals such as $D_2 / D_1 = 2$. $U' = 0.75U$ and $J = 0.125U'$, they satisfy the condition of $U' = U - 2J$. Temperature is $T = 1/6$.

First, we consider the $t' = 0$ case. At $U = 1$, the DOS has a original band width $D_2 / D_1 = 2$, though they show a tail structure because of the effects of correlation $U$. Upon increasing $U$, each band goes wider. At $U = 4$, $\gamma = 1$ band starts to split, which means the OSMT. Next, we study the effects of $t'$. At $U = 1$ and $2$, DOS show a metallic state having a finite intensity at $\omega = 0$. Upon increasing $t'$, the band width goes wider showing the resonance peak at $\omega = 0$. With the further increase of $t'$, the $\gamma = 1$ band starts to split at the end ($U = 2$ and $t' = 1$).
This split comes from the mixing of two orbitals, that is to say, the band-insulator. In $U = 4$ and 6 case, this tendency becomes more prominent. As seen in the figure, $\gamma = 1$ band shows the Mott-insulator at $t'' = 0$. Upon increasing $t''$, the band gap goes wider. From the results in $U = 2$ case, we can deduce that the system goes to the band-insulator also for $U = 4$ and 6 cases. This means that, with increasing $t''$, there is the crossover between the Mott-insulator and the band-insulator.

In summary, we have investigated the electronic states of the two-orbital Hubbard model by means of the composite operator method. In addition to the diagonal-transfer, we have introduced the off-diagonal one which provides the mixing of orbitals. This mixing promotes the band splitting showing the crossover between the Mott-insulator and the band-insulator. This crossover also affects to the physical quantities related to the correlation $U$ such as double occupancy, which will be presented in elsewhere.

References
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