Effects of degenerate orbitals on the Hubbard model

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Strongly correlated electron systems with degenerate orbitals have attracted much interest. One of typical examples is the transition metal compound LiV$_2$O$_4$,$^{1}$(U' = 3.0) where the heavy-fermion behavior was observed down to very low temperatures. It was suggested that $t_{2g}$ orbitals as well as geometrical frustration are important to understand the ground state stabilized against other ordered states.$^{2}$ Another example is the $f$-electron system CeTIn$_5$ (T = Co, Ir, Rh) $^{3,4,5}$ where the superconducting state competes with the magnetically ordered state. It was claimed that the effective Hamiltonian for this compound may be described by the degenerate Hubbard model.$^{6}$ Therefore, it is desirable to investigate low-energy properties of the degenerate Hubbard model systematically. In our previous paper,$^{7}$ we studied the ground-state properties of the degenerate Hubbard model by means of the dynamical mean field theory (DMFT) combined with the exact diagonalization method.$^{8}$ It was found that if the intra- and inter-band Coulomb interactions are nearly equal, the metallic ground state is stabilized up to fairly large interactions due to orbital fluctuations. Shown in Fig. 1 is a more precise phase diagram newly obtained by DMFT with the exact diagonalization. However, we were not able to systematically deal with dynamical properties in the previous paper because of the limitation inherent in the exact diagonalization of small clusters. We address this problem here by combining the quantum Monte Carlo simulations with DMFT. This also enables us to explore finite-temperature properties, which are useful to reveal the many-body character in correlated electron systems.

We consider a correlated electron system with two-fold degenerate orbitals, which may be described by the Hubbard Hamiltonian,

$$
H = \sum_{k,\alpha,\sigma} (\epsilon_k - \mu) c_{k\alpha\sigma}^{\dagger} c_{k\alpha\sigma} + \sum_{\alpha} U n_{\alpha\uparrow} n_{\alpha\downarrow} + U' \sum_{i,\sigma,\sigma'} n_{i\sigma} n_{i2\sigma'}
$$

(1)

where $c_{i\alpha\sigma}^{\dagger}(c_{i\alpha\sigma})$ creates (annihilates) an electron with spin $\sigma(=\uparrow, \downarrow)$ and orbital $\alpha(=1, 2)$ at the $i$th site, and $n_{i\sigma\sigma'} = c_{i\sigma\sigma'}^{\dagger} c_{i\sigma\sigma'}. \epsilon_k$ represents the dispersion relation, $\mu$ the chemical potential, $U$ and $U'$ the intra-band and inter-band Coulomb interaction. We use the semicircular density of states $\rho(\omega) = 2/\pi D \sqrt{1 - (\omega/D)^2}$ for simplicity. We focus here on the symmetric case by setting $\mu = U + U'$. In the following, we take the bandwidth $D$ as unity.

To discuss how two kinds of Coulomb interactions affect the stability of the metallic state, we use DMFT,$^{8}$ which can incorporate local electron correlations precisely. This method has been applied to the degenerate Hubbard model by several groups.$^{7, 9-12}$ In this paper, we exploit the quantum Monte Carlo simulations based on the Hirsch-Fye algorithm$^{13}$ to clarify finite-temperature properties of the degenerate model.

In Fig. 2, we show the density of states deduced by applying the maximum entropy method to the Monte Carlo data. When $U' = 0.0$, the system is reduced to the single-band Hubbard model, where the metal-insulator transition occurs at a critical point $U_c = 2.94.^{14}$ In the case $(U, U') = (3.0, 0.0)$, the system is in the insulating phase close to the transition point. Nevertheless we can clearly observe the formation of the Hubbard gap with the decrease of temperature $T$. Introducing

Fig. 1. Quasi-particle weight for the degenerate Hubbard model calculated by the DMFT within the exact diagonalization. $Z = 0 \ (Z \neq 0)$ corresponds to the insulating (metallic) phase.

Fig. 2. Density of states for the degenerate Hubbard model ($U = 3.0$). The data are for inverse temperature $T^{-1} = 1, 2, 4, 8$ and 16 from the top to the bottom.
the interband Coulomb interaction $U'$, the sharp quasiparticle peak appears around the Fermi surface in the case $(U, U') = (3.0, 3.0)$. This implies that orbital fluctuations induced by the interband Coulomb interaction drives the system to the metallic phase. In fact, the local charge susceptibility is increased up to $U \sim U'$ at low temperatures, as seen in Fig. 3. These results are consistent with the previous results. Further increase in the interband interaction suppresses spin fluctuations, leading the system to another type of the Mott insulator in the region of $U' > U$ (see Fig. 1).

To characterize the nature of two types of the Mott insulators, we investigate the temperature dependence of the local spin and orbital susceptibilities, which are defined as,

\[ \chi_s = \int_0^\beta d\tau \{ n_\uparrow(0) - n_\downarrow(0) \} \{ n_\uparrow(\tau) - n_\downarrow(\tau) \} \]

\[ \chi_o = \int_0^\beta d\tau \{ n_1(0) - n_2(0) \} \{ n_1(\tau) - n_2(\tau) \} \]

where $\beta = T^{-1}$, $n_\sigma = \sum_\alpha n_{\alpha,\sigma}$, $n_{\alpha} = \sum_\sigma n_{\alpha,\sigma}$ and $\tau$ is an imaginary time. We show the results obtained by the quantum Monte Carlo simulations within DMFT in Fig. 4. Let us first look at Figs. 4 (a) and (b) for $U' = 0$ (equivalent to the single band model). Since the introduction of the intra-orbital interaction $U$ sharpens the quasi-particle peak, this gives rise to the increase of the spin susceptibility $\chi_s$ at low temperatures. On the other hand, the formation of the Hubbard gap suppresses not only the charge susceptibility, but also the orbital susceptibility $\chi_o$. As seen from Figs. 4 (c) and (d), we encounter quite different behavior in the susceptibilities, when the interband interaction $U'$ is increased. Namely, the spin susceptibility is suppressed, while the orbital susceptibility is enhanced at low temperatures. We have checked that this tendency holds for larger $U'$ beyond the condition $U' \sim U$.

Therefore in the metallic phase close to the Mott insulator in the region of $U > U'(U < U')$, spin (orbital) fluctuations are enhanced whereas orbital (spin) fluctuations are suppressed with the decrease of temperature. These analyses shed some light on the reason why the metallic phase is particularly stable along the line $U = U'$. On this line, spin and orbital fluctuations are almost equally enhanced, and this subtle balance is efficient to stabilize the metallic phase. When the ratio of interactions deviates from this condition, the system prefers either of two types of the Mott insulating phases.

In this paper, we have restricted our discussions to the paramagnetic phase. As mentioned above, spin and/or orbital fluctuations are particularly enhanced in the metallic phase close to the Mott insulator, which would trigger a quantum phase transition to a certain ordered phase. This problem is to be addressed in the future work. Nevertheless, we think that the general feature about the stability of metallic phase near $U \sim U'$ may hold even in those cases.

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