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Ferromagnetism and Superconductivity in the One-dimensional Multi-orbital Hubbard Model

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Abstract

Using the numerical diagonalization method, we investigate the ferromagnetism and the superconductivity in the multi-orbital Hubbard model in one-dimension. To examine the superconductivity, we calculate the critical exponent K_ρ based on the Luttinger liquid theory and the anomalous flux quantization in the superconducting region. Analyzing the value of K_ρ, we obtain the phase diagram on the $U' - J$ parameter plane including the superconducting phase and the fully polarized ferromagnetic phase.

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Keywords: multi-orbital Hubbard model; numerical diagonalization; Hund's rule coupling; superconductivity; ferromagnetism

Multi-orbital Hubbard models have attracted much interest due to various interesting phenomena such as ferromagnetism and superconductivity. Many works [1–4] have studied the model in the case of the crystal-field splitting $\Delta = 0$. They revealed that Hund's rule coupling J plays a crucial role in ferromagnetism. In the previous work[5], we studied this model at finite Δ. We found that the fully polarized ferromagnetism becomes unstable when J is smaller than a certain critical value of order of Δ. Further, we obtained the superconducting (SC) phase for the singlet ground state in the vicinity of the partially polarized ferromagnetism. However, the superconductivity in the case of $\Delta = 0$ has not been sufficiently considered in these studies.

In the present work, we investigate the one-dimensional multi-orbital Hubbard model, paying attention to relationship between the superconductivity and the Hund's rule coupling J using the numerical diagonalization method. We consider the following Hamiltonian:

$$H = -t \sum_{i,m,\sigma} (c^\dagger_{i,m,\sigma} c_{i+1,m,\sigma} + h.c.) + U \sum_{i,m} n_{i,m,\uparrow} n_{i,m,\downarrow} + U' \sum_{i,\sigma} n_{i,a,\sigma} n_{i,b,-\sigma} + (U' - J) \sum_{i,\sigma} n_{i,a,\sigma} n_{i,b,\sigma} - J \sum_{i,m} (c^\dagger_{i,a,\uparrow} c_{i,a,\downarrow} c^\dagger_{i,b,\downarrow} c_{i,b,\uparrow} + h.c.) - J' \sum_{i,m} (c^\dagger_{i,a,\uparrow} c^\dagger_{i,a,\downarrow} c_{i,b,\uparrow} c_{i,b,\downarrow} + h.c.), \quad (1)$$

where $c^\dagger_{i,m,\sigma}$ is the creation operator of an electron with spin σ in the orbital m $(= a, b)$ at site i. The interaction parameters U, U', J and J' stand the intra- and inter-orbital direct Coulomb interactions, the exchange (Hund's rule) coupling and the pair-transfer, respectively. We set $U = U' + 2J$ and $J' = J$, hereafter.

We numerically diagonalize the Hamiltonian eq. (1) up to 6 sites (12 orbitals) using the standard Lanczos algorithm. To reduce the finite size effect, we use the Moebius boundary condition, which is known to work well for systems with doubly degenerate conduction bands such as the t-J ladder model [6].

Figure 1 shows the value of K_ρ as a function of U' for $J = 0$ at the electron density $n = 1$ (4 electrons/4 sites). We also plot the results from the Green's function Monte Carlo (GFMC) method [7] and a weak coupling estimation for K_ρ [5]. These results are in good agreement with each other. As U' increases, K_ρ decreases from unity for $U' = 0$ to ~ 0.42 for $U' = 4$. In the case with $J = 0$, the Hamiltonian eq.(1) is equivalent to the SU(4) Hubbard model which shows the metal-insulator transition (MIT) at a critical interaction where K_ρ=0.5 [7,8]. In the present model, the critical interaction is $U'_c \sim 3$ as shown in Fig. 1.

In Fig. 2, K_ρ is plotted as a function of U' in the cases with $J = U'/2$, $J = U'$ and $J = 2U'$ at $n = 1$ (4 elec-

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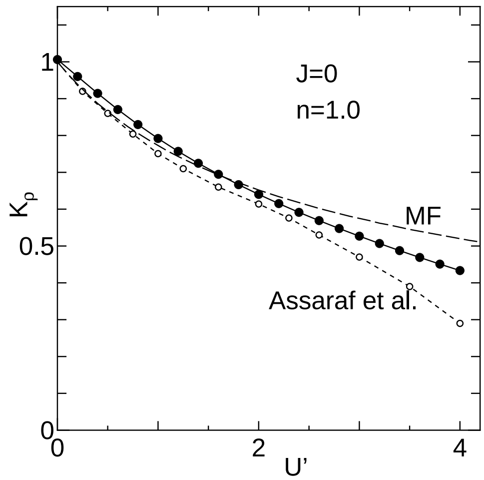

Fig. 1. K_ρ as a function of U' for $J = 0$ at $n = 1$. The dashed line represents a weak coupling estimation for K_ρ. The open circles are the GFMC results obtained by Assaraf *et al.* [7].

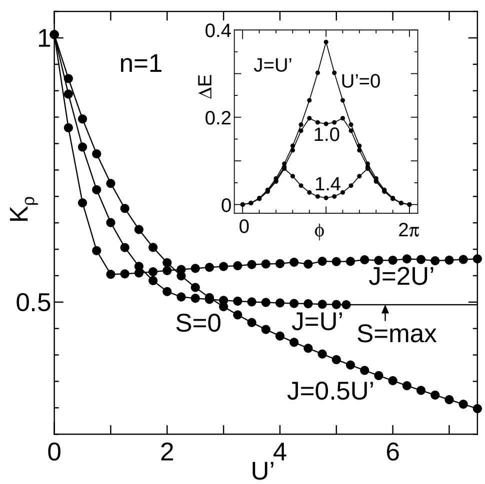

Fig. 2. K_ρ as a function of U' in the cases with $J = U'/2$, $J = U'$ and $J = 2U'$ at $n = 1$. Inset shows the energy difference $E_0(\phi) - E_0(0)$ as a function of an external flux ϕ at $n = 1$.

trons/4 sites). In the region $K_\rho > 0.5$, the SC correlation is expected to be the most dominant as compared with the CDW and SDW correlations [9]. To confirm the SC state, we calculate the lowest energy of the singlet state $E_0(\phi)$ as a function of an external flux ϕ at $n = 1$ (6 electrons/6 sites). As shown in the inset of Fig.2, the anomalous flux quantization occurs in the region $K_\rho > 0.5$. Within the bosonization method [8], this SC state with $K_\rho > 0.5$ is identified as the triplet SC with spin gap, while the state with $K_\rho < 0.5$ is the spin gapped insulator. These results are consistent with the recent DMRG results for the MIT [3] and for the SC state [10].

In Fig. 3, we show the phase diagram on the $U' - J$ parameter plane at $n = 1$ (4 electrons/4 sites). In the paramagnetic state (S=0), we plot the phase boundary separating the SC region with $K_\rho > 0.5$ and the insulating region with $K_\rho < 0.5$. This SC phase diagram is again confirmed by the external flux dependence: the anomalous flux quan-

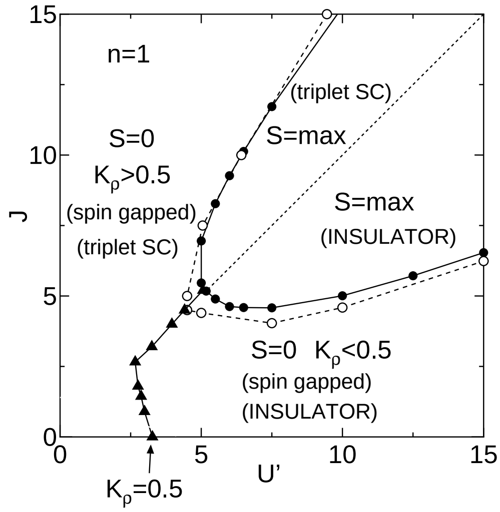

Fig. 3. Phase diagram on the $U' - J$ parameter plane at $n = 1$. The open circles are the DMRG results for the ferromagnetic phase boundary and the dotted line is the DMRG result for the MIT boundary in the ferromagnetic state [3].

tization takes place in the SC region as shown in the inset of Fig.2, while it disappears in the insulating region with large U' (not shown).

We also plot the ferromagnetic phase boundary in Fig. 3. A complete ferromagnetism with S=max. appears around $J \simeq U'$ in the strong coupling regime. This result is in good agreement with the DMRG result obtained by Sakamoto *et al.* [3] as shown in Fig. 3. In this ferromagnetic region, Sakamoto *et al.* also claimed that the system shows the triplet SC for $J > U'$, while it becomes insulator for $J < U'$. The SC phase boundary in the ferromagnetic region is smoothly connected to that in the paramagnetic region as shown in Fig. 3. These results tell us that the Hund's rule coupling J plays important roles not only for the ferromagnetism but also for the superconductivity.

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