Superconductivity in the One-Dimensional Two-Orbital Hubbard Model with Finite Band Splitting

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Abstract. Using the numerical diagonalization method, we investigate superconductivity and related ferromagnetism in the one-dimensional two-orbital Hubbard model with a finite band splitting at less than half filling. We obtain the superconducting (SC) region with the Luttinger liquid parameter $K_\rho > 1$ and confirm the anomalous flux quantization in the SC state. It is found that the SC phase appears near the partially polarized ferromagnetic phase. We also calculate the various paring correlation functions to clarify the nature of the SC phase. Detailed analysis of these functions indicates that the triplet paring between the nearest neighbor sites is relevant to the superconductivity. It suggests that the ferromagnetic fluctuation plays an important role for the superconductivity.

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1. Introduction

The orbital degrees of freedom in strongly correlated electron systems are expected to play an important role for various interesting phenomena such as the metal-insulator transition, ferromagnetism and superconductivity. [1, 2, 3, 4, 5, 6] In the previous work[7], we studied the multi-orbital Hubbard model in one-dimension using the numerical diagonalization method. We found that the fully polarized ferromagnetism becomes unstable against the partially polarized ferromagnetism when the exchange (Hund's rule) coupling J is larger than value of order of the crystal-field splitting Δ. The superconducting(SC) phase was observed for the singlet ground state in the vicinity of the partially polarized ferromagnetism.

However, the nature of the superconductivity has not been sufficiently considered in that work. In the present work, we investigate the same model to clarify the possible mechanisms of superconductivity, particularly paying attention to the symmetry of paring. We analyze the various paring correlation functions and discuss relationship between the ferromagnetism and the superconductivity.

2. Model Hamiltonian and Luttinger Liquid Relation

We consider the following Hamiltonian for the one-dimensional multi-orbital Hubbard model:

$$
\begin{aligned}
H = & -t \sum_{i,m,\sigma} (c^\dagger_{i,m,\sigma} c_{i+1,m,\sigma} + h.c.) + U \sum_{i,m} n_{i,m,\uparrow} n_{i,m,\downarrow} \\
& + U' \sum_{i,\sigma} n_{i,u,\sigma} n_{i,l,-\sigma} + (U' - J) \sum_{i,\sigma} n_{i,u,\sigma} n_{i,l,\sigma} + \frac{\Delta}{2} \sum_{i,\sigma} (n_{i,u,\sigma} - n_{i,l,\sigma}) \\
& - J \sum_{i,m} (c^\dagger_{i,u,\uparrow} c_{i,u,\downarrow} c^\dagger_{i,l,\downarrow} c_{i,l,\uparrow} + h.c.) - J' \sum_{i,m} (c^\dagger_{i,u,\uparrow} c^\dagger_{i,u,\downarrow} c_{i,l,\uparrow} c_{i,l,\downarrow} + h.c.) \qquad (1)
\end{aligned}
$$

where $c^\dagger_{i,m,\sigma}$ stands for the creation operator of an electron with spin σ in the orbital m $(= u, l)$ at site i and $n_{i,m,\sigma} = c^\dagger_{i,m,\sigma} c_{i,m,\sigma}$. Here, t represents the hopping integral between the same orbitals and we set $t = 1$ in this study. The interaction parameters U, U', J and J' stand for the intra- and inter-orbital direct Coulomb interactions, the exchange (Hund's rule) coupling and the pair-transfer, respectively. Δ denotes the energy difference between the two atomic orbitals, that is, crystal-field splitting. For simplicity, we impose the relations, $J = J'$ and $U = U' + 2J$. In the noninteracting case ($U = U' = J = 0$), the Hamiltonian eq. 1 yields a dispersion relation $\epsilon^\pm(k) = -2t\cos(k) \pm \frac{\Delta}{2}$, where k is the wave vector and $\epsilon^+(k)$ ($\epsilon^-(k)$) represents the upper (lower) orbital band energy. When the lowest energy of the upper orbital band, $\epsilon^+(0)$, is larger than the Fermi energy, E_{k_F}, electrons occupy only the lower orbital band with $k_F = \frac{\pi n}{2}$ and the model is regarded as a single component electron system. Hereafter, we mainly treat the case with $\epsilon^+(0) \geq E_{k_F}$.

We numerically diagonalize the model Hamiltonian up to 9 sites (18 orbitals) and obtain the value of K_ρ from the ground state energy of finite size systems using the standard Lanczos algorithm. We use the periodic(antiperiodic) boundary condition for the lower (upper) orbital band at $N_e = 4m + 2$ and the antiperiodic(periodic) boundary condition for the upper (lower) orbital band at $N_e = 4m$, where N_e is the total electron number and m is an integer. This choice of the boundary condition removes accidental degeneracy and shows smaller finite size effect than another boundary condition.

According to the Luttinger liquid theory, the critical exponents of various types of correlation functions are determined by a single parameter K_ρ.[8, 9] It is predicted that SC correlation is dominant for $K_\rho > 1$ (the correlation function decays as $\sim r^{-(1+\frac{1}{K_\rho})}$ in the Tomonaga-Luttinger (TL) regime and as $\sim r^{-\frac{1}{K_\rho}}$ in the Luther-Emery (LE) regime), whereas the CDW or SDW correlations are dominant for $K_\rho < 1$ (the correlation functions decay as $\sim r^{-(1+K_\rho)}$ in the TL regime and as $\sim r^{-K_\rho}$ in the LE regime). Here, the LE regime is characterized by a gap in the spin excitation spectrum, while in

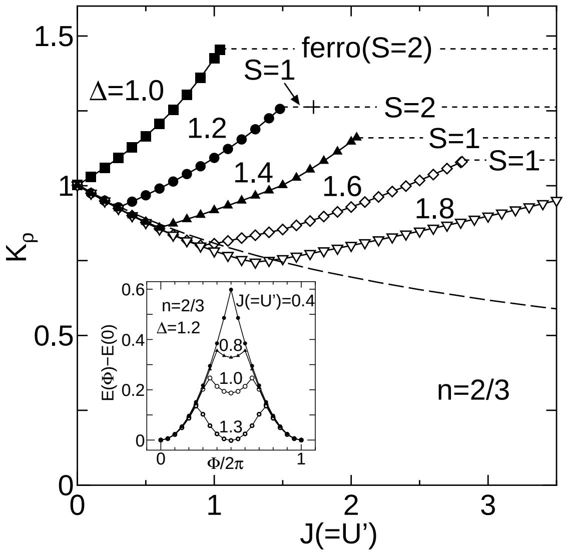

Figure 1. (a) K_ρ as a function of $J(=U')$ for $n = 2/3$(6electrons/9sites) at $\Delta = 1.0, 1.2, 1.4, 1.6,$ and 1.8. The singlet ground state changes into the partially polarized ferromagnetic (S=1 or 2) state at $U' \simeq 1.1$, 1.5, 2.1 2.8 and 4.1 for $\Delta =$ 1.0, 1.2, 1.4, 1.6 and 1.8, respectively. The dashed line represents a weak coupling estimation for K_ρ. Inset shows the energy difference $E_0(\phi) - E_0(0)$ as a function of an external flux ϕ for $n = 2/3$(6electrons/9sites) at $\Delta = 1.2$.

the TL regime, the excitation is gapless. In the case of non-interacting fermion systems, the exponent K_ρ is always unity. Thus, the effective interaction between quasi-particles is attractive for $K_\rho > 1$ whereas that is repulsive for $K_\rho < 1$.

3. Numerical Results

Figure 1 shows the value of K_ρ as a function of $J(= U')$ for several values of Δ at the electron density $n = 2/3$(6electrons/9sites). The broken line represents the weak coupling approximation for K_ρ.[7] As J increases, K_ρ decreases for a small J, while it increases for a large J, and then becomes larger than unity. In the region $K_\rho > 1$, the SC correlation is expected to be the most dominant compared with the CDW and SDW correlations. When J is larger than a certain critical value, the ground state changes into the partially ferromagnetic state with S=1 or S=2 from the singlet state S=0.

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. As shown in the inset of Fig. 1, the anomalous flux quantization occurs clearly at $J \sim 1.3$, where K_ρ is about 1.2. When $J = 0.4$, K_ρ is less than unity and the anomalous flux quantization is not found. We have also confirmed that the superconductivity does not vanish even if the pare-transfer term is omitted. It suggests that the superconductivity is caused by not the pair-transfer J' but the exchange interaction J.

In Fig.2, we show various types of SC paring correlation functions $C(r)$ in detail for $n = 2/3$(6electrons/9sites) at $\Delta = 1.2$ and $J(= U') = 1.48$. The paring correlation functions are defined by

$$S_{\rm ll}(r) = \frac{1}{N_u}\sum_i < c^\dagger_{i,l,\uparrow}c^\dagger_{i,l,\downarrow}c_{i+r,l,\downarrow}c_{i+r,l,\uparrow} >, \tag{2}$$

$$S_{\rm uu}(r) = \frac{1}{N_u}\sum_i < c^\dagger_{i,l,\uparrow}c^\dagger_{i,u,\downarrow}c_{i+r,u,\downarrow}c_{i+r,u,\uparrow} >, \tag{3}$$

$$\begin{aligned} S_{\rm l-l}(r) &= \frac{1}{2N_u}\sum_i < (c^\dagger_{i,l,\uparrow}c^\dagger_{i+1,l,\downarrow} - c^\dagger_{i,l,\downarrow}c^\dagger_{i+1,l,\uparrow}) \\ &\times (c_{i+r+1\downarrow}c_{i+r,l,\uparrow} - c_{i+r+1,l,\uparrow}c_{i+r,l,\downarrow}) >, \end{aligned} \tag{4}$$

$$\begin{aligned} S_{\rm u-u}(r) &= \frac{1}{2N_u}\sum_i < (c^\dagger_{i,u,\uparrow}c^\dagger_{i+1,u,\downarrow} - c^\dagger_{i,u,\downarrow}c^\dagger_{i+1,u,\uparrow}) \\ &\times (c_{i+r+1,u,\downarrow}c_{i+r,u,\uparrow} - c_{i+r+1,u,\uparrow}c_{i+r,u,\downarrow}) >, \end{aligned} \tag{5}$$

$$\begin{aligned} S_{\rm ul}(r) &= \frac{1}{2N_u}\sum_i < (c^\dagger_{i,l,\uparrow}c^\dagger_{i+1,u,\downarrow} - c^\dagger_{i,l,\downarrow}c^\dagger_{i+1,u,\uparrow}) \\ &\times (c_{i+r+1,u,\downarrow}c_{i+r,l,\uparrow} - c_{i+r+1,u,\uparrow}c_{i+r,l,\downarrow}) >, \end{aligned} \tag{6}$$

$$\begin{aligned} T_{\rm l-l}(r) &= \frac{1}{2N_u}\sum_i < (c^\dagger_{i,l,\uparrow}c^\dagger_{i+1,l,\downarrow} + c^\dagger_{i,l,\downarrow}c^\dagger_{i+1,l,\uparrow}) \\ &\times (c_{i+r+1\downarrow}c_{i+r,l,\uparrow} + c_{i+r+1,l,\uparrow}c_{i+r,l,\downarrow}) >, \end{aligned} \tag{7}$$

$$\begin{aligned} T_{\rm u-u}(r) &= \frac{1}{2N_u}\sum_i < (c^\dagger_{i,u,\uparrow}c^\dagger_{i+1,u,\downarrow} + c^\dagger_{i,u,\downarrow}c^\dagger_{i+1,u,\uparrow}) \\ &\times (c_{i+r+1,u,\downarrow}c_{i+r,u,\uparrow} + c_{i+r+1,u,\uparrow}c_{i+r,u,\downarrow}) >, \end{aligned} \tag{8}$$

$$\begin{aligned} T_{\rm ul}(r) &= \frac{1}{2N_u}\sum_i < (c^\dagger_{i,l,\uparrow}c^\dagger_{i+1,u,\downarrow} + c^\dagger_{i,l,\downarrow}c^\dagger_{i+1,u,\uparrow}) \\ &\times (c_{i+r+1,u,\downarrow}c_{i+r,l,\uparrow} + c_{i+r+1,u,\uparrow}c_{i+r,l,\downarrow}) >, \end{aligned} \tag{9}$$

where $C(r) = S_{\rm ll}(r)$, $S_{\rm uu}(r)$, $S_{\rm l-l}(r)$, $S_{\rm u-u}(r)$ and $S_{\rm ul}(r)$ denote the singlet paring correlation functions on the same site in the lower orbital, on the same site in the upper orbital, between the nearest neighbor sites in the lower orbital, between the nearest neighbor sites in the upper orbital, between lower and upper orbitals on the same site, respectively. Further, $T_{\rm l-l(r)}$, $T_{\rm u-u}(r)$ and $T_{\rm ul}(r)$ are the triplet paring correlation functions between the nearest neighbor sites in the lower orbital, between the nearest neighbor sites in the upper orbital and between lower and upper orbitals on the same site, respectively.

The absolute value of $T_{\rm u-u}(r)$ is small, but the correlation as a function of r is the slowest to decay. This result seems to suggest that the relevant paring of the superconductivity is the triplet paring between the nearest neighbor sites in *upper* orbital. and the ferromagnetic fluctuation near the ferromagnetic phase may cause the paring. To show the behavior of the correlation functions more clearly, we calculate the ratio $R(r)$ of the paring correlation functions at $J(= U') = 1.48$ and that of $J(= U') = 0.3$ as $R(r) = \frac{C(r)_{\rm J=1.48}}{C(r)_{\rm J=0.3}}$. Although the correlation function $C(r)$ decays as distance r increases, the function $R(r)$ for relevant paring is expected to increase with r, because the value of K_ρ at $J = 1.48$ is larger than that at $J = 0.3$, where K_ρ is

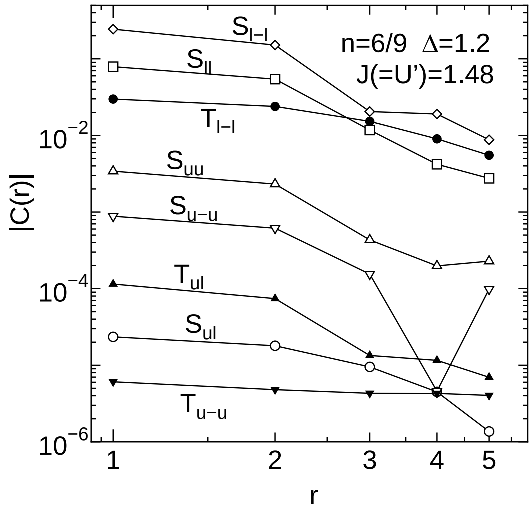

Figure 2. The singlet paring correlation functions $C(r) = S_{\rm ll}(r)$, $S_{\rm l-l}(r)$, $S_{\rm uu}(r)$, $S_{\rm u-u}(r)$, $S_{\rm ul}(r)$ and the triplet correlation functions $T_{\rm l-l}(r)$, $T_{\rm u-u}(r)$, $T_{\rm ul}(r)$, respectively(see text). Here we show the absolute value of the correlation functions at $\Delta = 1.2$ and $J(= U') = 1.48$ for n=2/3(6electrons/9sites).

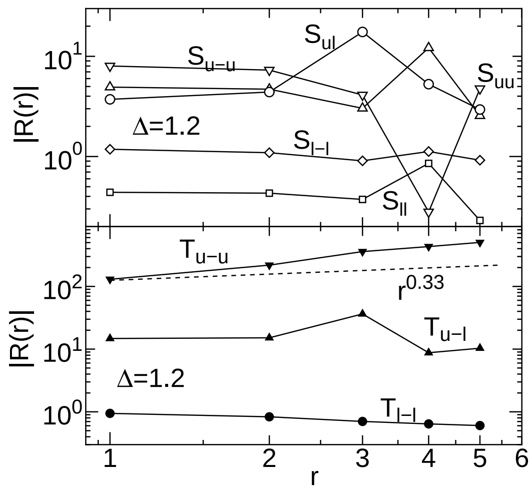

Figure 3. The ratio of the singlet paring correlation functions $R(r) = C(r)_{J=1.04}/C(r)_{J=0.2}$ for $S_{\rm l-l}(r)$, $S_{\rm uu}(r)$, $S_{\rm u-u}(r)$, $S_{ul}(r)$ and that of the triplet correlation functions for $T_{\rm l-l}(r)$, $T_{\rm u-u}(r)$, $T_{\rm ul}(r)$ with the power-low $r^{0.33}$, respectively(see text). The broken line represents the power-low $r^{0.33}$ predicted by the Luttinger liquid relation.

about at 1.26 and 0.93, respectively. Then, the behavior of $R(r)$ is expected to $\sim r^{0.33}$.

In fig.3, we show $R(r)$ for $S_{\rm ll}(r)$, $S_{\rm l-l}(r)$, $S_{\rm uu}(r)$, $S_{\rm u-u}(r)$ and $S_{\rm ul}$, (upper panel) and the triplet paring correlation functions $T_{\rm l-l}(r)$, $T_{\rm u-u}(r)$ and $T_{\rm ul}(r)$ with the power-low $r^{0.33}$ predicted by the Luttinger liquid relation (lower panel), respectively. It indicates that the function $R(r)$ for $T_{\rm u-u}$ is much enhanced especially for longer range paring correlation. On the other hand, the remains are not enhanced or decay as r increases.

These results suggest that the paring correlation function in upper orbital $T_{\mathrm{u-u}}(r)$ is most relevant paring to the superconductivity. Although the system size is too small to compare the slope of the function $R(r)$ with the power-low enhancement $\sim r^{0.33}$ directly, the behavior of $T_{\mathrm{u-u}}$ seems to be roughly consistent with the result of the Luttinger liquid relation.

4. Summary and Discussion

We have investigate the superconductivity and the related ferromagnetism of the Hubbard model with two-fold orbital degeneracy with paying attention to the effect of the interplay between the Coulomb interactions and the band splitting. To obtain reliable results, we have used the numerical diagonalization method and calculated the critical exponent K_ρ based on the Luttinger liquid theory. In the vicinity of the partially polarized ferromagnetism, we have found the SC phase, when J exceeds about the energy of Δ. These behaviors seem to be very similar to the result of $n > 1$ at $\epsilon^+(0) \geq E_{k_F}$ as shown in our previous work[7]. It suggests that the nature of the SC phase may not much depend on n so long as the band splitting Δ is sufficiently large and electrons occupy only the lower orbital band.

In order to clarify the nature of the superconductivity, we also obtained the various paring correlation functions. The analysis of these functions indicates that triplet paring between the nearest neighbor sites in upper orbital $T_{\mathrm{u-u}}(r)$ is relevant to the superconductivity. These results suggests that the ferromagnetic fluctuation produces the triplet superconductivity, In the $\Delta = 0$ case, the triplet SC phase with the spin gap has been already discussed in the recent bosonization method[4, 5] and numerical method[6, 10]. At this stage, we can not clarify the relationship between both triplet SC phases. Further study is needed and we would like to address it in future.

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