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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 a superconducting (SC) region with the Luttinger liquid parameter $K_\rho > 1$ and confirm anomalous flux quantization in the SC state. It is found that the SC phase appears near the partially polarized ferromagnetic phase. We also calculate various pairing correlation functions to clarify the nature of the SC phase. Detailed analysis of these functions indicates that the triplet pairing between the nearest neighbour sites is relevant to the superconductivity. This suggests that ferromagnetic fluctuation plays an important role for the superconductivity.

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 [1–6]. In a previous work [7], we studied the multi-orbital Hubbard model in one dimension, using the numerical diagonalization method. We found that fully polarized ferromagnetism becomes unstable against partially polarized ferromagnetism when the exchange (Hund's rule) coupling J is larger than the value of the order of the crystal-field splitting Δ. A superconducting (SC) phase was observed for the singlet ground state in the vicinity of the partially polarized ferromagnetism.

However, the nature of the SC phase was not sufficiently considered in that work. In the present work, we investigate the same model to clarify possible mechanisms of the superconductivity, particularly paying attention to the symmetry of pairing. We analyse the various pairing correlation functions and discuss the 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:

$$H = -t\sum_{i,m,\sigma}(c^{\dagger}_{i,m,\sigma}c_{i+1,m,\sigma} + \text{h.c.}) + U\sum_{i,m} n_{i,m,\uparrow}n_{i,m,\downarrow} + U'\sum_{i,\sigma} n_{i,u,\sigma}n_{i,l,-\sigma} + (U'-J)\sum_{i,\sigma} n_{i,u,\sigma}n_{i,l,\sigma} + \frac{\Delta}{2}\sum_{i,\sigma}(n_{i,u,\sigma} - n_{i,l,\sigma}) - J\sum_{i,m}(c^{\dagger}_{i,u,\uparrow}c_{i,u,\downarrow}c^{\dagger}_{i,l,\downarrow}c_{i,l,\uparrow} + \text{h.c.}) - J'\sum_{i,m}(c^{\dagger}_{i,u,\uparrow}c^{\dagger}_{i,u,\downarrow}c_{i,l,\uparrow}c_{i,l,\downarrow} + \text{h.c.}) \quad (1)$$

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 non-interacting case ($U = U' = J = 0$), the Hamiltonian equation (1) yields a dispersion relation $\epsilon^{\pm}(k) = -2t\cos(k) \pm \frac{\Delta}{2}$, where k is the wavevector 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 and the model is regarded as a single component electron system. Hereafter, we mainly treat the case with $\epsilon^{+}(0) \geqslant E_{k_F}$.

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 other boundary conditions.

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 the 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 CDW and/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 the TL regime, the excitation is gapless. In the case of non-interacting systems, the exponent K_ρ is always unity. Thus, the effective interaction between quasi-particles is attractive for $K_\rho > 1$ whereas it 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 $n = 2/3$ (6 electrons/9 sites). The dashed 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

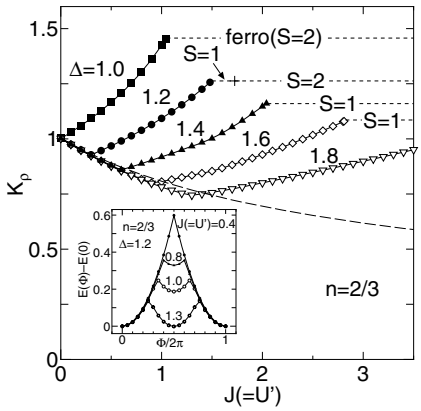

Figure 1. K_ρ as a function of J $(=U')$ for $n = 2/3$ (6 electrons/9 sites) at $\Delta = 1.0$, 1.2, 1.4, 1.6, and 1.8. The singlet ground state changes into the partially polarized ferromagnetic ($S = 1$ or 2) state at $U' \simeq 1.1$, 1.5, 2.1 2.8 and 4.1 for $\Delta = 1.0$, 1.2, 1.4, 1.6 and 1.8,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

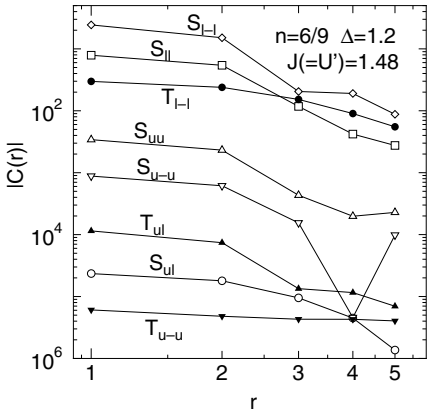

Figure 2. The singlet pairing correlation functions $C(r) = S_{ll}(r)$, $S_{l-l}(r)$, $S_{uu}(r)$, $S_{u-u}(r)$, $S_{ul}(r)$ and the triplet correlation functions $T_{l-l}(r)$, $T_{u-u}(r)$, $T_{ul}(r)$, respectively (see text). Here we show the absolute value of the correlation functions at $\Delta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

J is larger than a certain critical value, the ground state changes into the partially polarized ferromagnetic state with total spin $S = 1$ or $S = 2$ from the singlet state with $S = 0$.

To confirm the superconductivity, 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 figure 1, 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 SC state does not vanish even if the pair-transfer term J' is omitted. This suggests that the superconductivity is caused not by the pair-transfer but by the exchange interaction.

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

are defined by

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

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

$$S_{\mathrm{l-l}}(r) = \frac{1}{2N_u}\sum_i \langle (c^\dagger_{i,l,\uparrow} c^\dagger_{i+1,l,\downarrow} - c^\dagger_{i,l,\downarrow} c^\dagger_{i+1,l,\uparrow}) \times (c_{i+r+1\downarrow} c_{i+r,l,\uparrow} - c_{i+r+1,l,\uparrow} c_{i+r,l,\downarrow})\rangle, \tag{4}$$

$$S_{\mathrm{u-u}}(r) = \frac{1}{2N_u}\sum_i \langle (c^\dagger_{i,u,\uparrow} c^\dagger_{i+1,u,\downarrow} - c^\dagger_{i,u,\downarrow} c^\dagger_{i+1,u,\uparrow}) \times (c_{i+r+1,u,\downarrow} c_{i+r,u,\uparrow} - c_{i+r+1,u,\uparrow} c_{i+r,u,\downarrow})\rangle, \tag{5}$$

$$S_{\mathrm{ul}}(r) = \frac{1}{2N_u}\sum_i \langle (c^\dagger_{i,l,\uparrow} c^\dagger_{i+1,u,\downarrow} - c^\dagger_{i,l,\downarrow} c^\dagger_{i+1,u,\uparrow}) \times (c_{i+r+1,u,\downarrow} c_{i+r,l,\uparrow} - c_{i+r+1,u,\uparrow} c_{i+r,l,\downarrow})\rangle, \tag{6}$$

$$T_{\mathrm{l-l}}(r) = \frac{1}{2N_u}\sum_i \langle (c^\dagger_{i,l,\uparrow} c^\dagger_{i+1,l,\downarrow} + c^\dagger_{i,l,\downarrow} c^\dagger_{i+1,l,\uparrow}) \times (c_{i+r+1\downarrow} c_{i+r,l,\uparrow} + c_{i+r+1,l,\uparrow} c_{i+r,l,\downarrow})\rangle, \tag{7}$$

$$T_{\mathrm{u-u}}(r) = \frac{1}{2N_u}\sum_i \langle (c^\dagger_{i,u,\uparrow} c^\dagger_{i+1,u,\downarrow} + c^\dagger_{i,u,\downarrow} c^\dagger_{i+1,u,\uparrow}) \times (c_{i+r+1,u,\downarrow} c_{i+r,u,\uparrow} + c_{i+r+1,u,\uparrow} c_{i+r,u,\downarrow})\rangle, \tag{8}$$

$$T_{\mathrm{ul}}(r) = \frac{1}{2N_u}\sum_i \langle (c^\dagger_{i,l,\uparrow} c^\dagger_{i+1,u,\downarrow} + c^\dagger_{i,l,\downarrow} c^\dagger_{i+1,u,\uparrow}) \times (c_{i+r+1,u,\downarrow} c_{i+r,l,\uparrow} + c_{i+r+1,u,\uparrow} c_{i+r,l,\downarrow})\rangle, \tag{9}$$

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

The absolute value of $T_{\mathrm{u-u}}(r)$ is small, but the correlation shows the slowest decay as a function of r. This result seems to suggest that the relevant pairing of the superconductivity is the triplet pairing between the nearest neighbour sites in the *upper* orbital. To indicate the behaviour of the correlation functions more clearly, we calculate the ratio $R(r)$ between the pairing correlation function at $J\ (=U') = 1.48$ and that of $J\ (=U') = 0.3$, that is, $R(r) = \frac{C(r)_{\mathrm{J}=1.48}}{C(r)_{\mathrm{J}=0.3}}$. Although the correlation function $C(r)$ decays as the distance r increases, the function $R(r)$ for the relevant pairing 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 about at 1.26 and 0.93, respectively. Then, the behaviour of $R(r)$ is expected to be $\sim r^{0.33}$.

In figure 3, we show $R(r)$ for $S_{\mathrm{ll}}(r)$, $S_{\mathrm{l-l}}(r)$, $S_{\mathrm{uu}}(r)$, $S_{\mathrm{u-u}}(r)$ and S_{ul} (upper panel) and the triplet pairing correlation functions $T_{\mathrm{l-l}}(r)$, $T_{\mathrm{u-u}}(r)$ and $T_{\mathrm{ul}}(r)$ with the power-law $r^{0.33}$ predicted by the Luttinger liquid relation (lower panel), respectively. It indicates that the function $R(r)$ for $T_{\mathrm{u-u}}$ is much enhanced, especially for longer range pairing correlation. However, all remains of $R(r)$ except for $T_{\mathrm{u-u}}(r)$ are not enhanced. These results suggest

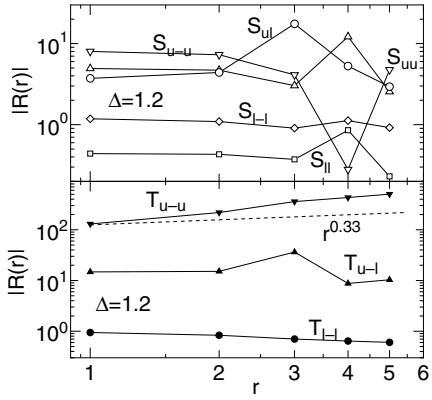

Figure 3. The ratio of the singlet pairing correlation functions $R(r) = C(r)_{J=1.48}/C(r)_{J=0.3}$ for $S_{l-l}(r)$, $S_{uu}(r)$, $S_{u-u}(r)$, $S_{ul}(r)$ and that of the triplet correlation functions for $T_{l-l}(r)$, $T_{u-u}(r)$, $T_{ul}(r)$, respectively (see text). The broken line represents the power-law $r^{0.33}$ predicted by the Luttinger liquid relation.

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

4. Summary and discussion

We have investigated the superconductivity and the related ferromagnetism of the Hubbard model with two-fold orbital degeneracy, 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 behaviours seem to be very similar to the result of the electron density $n > 1$ at $\epsilon^+(0) \geqslant E_{k_F}$, as shown in our previous work [7]. This suggests that the nature of the SC phase may not depend much 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 pairing correlation functions. The analysis of these functions indicates that triplet pairing is relevant to the superconductivity. This suggests that the ferromagnetic fluctuation may produce the SC state. In the $\Delta = 0$ case, the triplet SC phase with spin gap has been already discussed in the bosonization method [4, 5] and numerical methods [6, 10]. At this stage, we cannot clarify the relationship between both triplet SC phases. Further study is needed and we would like to address it in the future.

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