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Large triplet pairing mixing in the FFLO state of spin fluctuation mediated superconductivity in Q1D systems

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ABSTRACT

We study the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) state of spin fluctuation mediated superconductivity and focus on the effect of coexisting charge fluctuations. We find that (i) consecutive transitions from singlet pairing to FFLO and further to $S_z = 1$ triplet pairing can generally take place upon increasing the magnetic field when strong charge fluctuations coexist with spin fluctuations and (ii) the enhancement of the charge fluctuations lead to a significant increase of the parity mixing in the FFLO state, where the triplet/singlet component ratio in the gap function can be close to unity. We propose that such consecutive pairing state transition and strong parity mixing in the FFLO state may take place in a quasi-one-dimensional organic superconductor $(TMTSF)_2X$.

1. Introduction

One of the interesting aspects of the FFLO (Fulde–Ferrell–Larkin–Ovchinnikov) state [1] is mixing of even and odd parity pairing states. Phenomenological studies have shown that the mixing of the singlet and triplet pairings stabilizes the FFLO state [2]. Recent microscopic studies on the Hubbard model have shown that the $S_z = 0$ triplet pairing is mixed with singlet pairing in the FFLO state of the Hubbard model on the two-leg ladder-type lattice [3], and also on the square lattice, where *d*-wave superconductivity is mediated by spin fluctuations [4,5].

In this context, a Q1D organic superconductor $(TMTSF)_2X$ is an interesting material to investigate the possibility of the FFLO state and its nature. The possibility of the spin triplet pairing has previously been suggested experimentally for $(TMTSF)_2X$ ($X = PF_6$ [6], ClO_4 [7]), but on the other hand, recent experiments suggest the possibility of the FFLO state as mentioned above [8]. Theoretically, various studies have investigated the possibility of triplet pairing [9] and the FFLO state [10]. In particular, three of the present authors have previously shown that the triplet *f*-wave pairing can compete with the singlet *d*-wave pairing in the Q1D system because of the disconnectivity of the Fermi surface when $2k_F$ spin and $2k_F$ charge fluctuations coexist [11]. The coexistence of the charge fluctuations and the spin fluctuations is supported from the fact that diffuse X-ray scattering experiments observe the coexistence of $2k_F$ charge density wave (CDW) and the $2k_F$ spin density wave (SDW) in the vicinity of the superconducting phase in $(TMTSF)_2PF_6$ [12,13]. Moreover, we have recently found that this kind of triplet pairing due to the coexistence of $2k_F$ spin + $2k_F$ charge fluctuations is strongly enhanced by the magnetic field [14].

In the present study, we study the FFLO state of spin fluctuation mediated superconductivity by applying random phase approximation (RPA), and focus on the effect of the charge fluctuations. We find that (i) consecutive transition from singlet pairing to FFLO and further to $S_z = 1$ triplet pairing can generally take place upon increasing the magnetic field in the vicinity of SDW and CDW coexisting phase, and (ii) the enhancement of the charge fluctuations leads to a significant increase of the parity mixing in the FFLO state, where the triplet/singlet component ratio in the gap function can be close to unity. Based on a calculation on a model for $(TMTSF)_2X$, we propose that such consecutive pairing state transitions and the strong parity mixing in the FFLO state may actually be taking place in this materials.

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2. Formulation

The anisotropic extended Hubbard model that takes into account the Zeeman effect shown in Fig. 1a is given by

$$H = \sum_{i,j,\sigma} t_{ij\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow} + \sum_{i,j,\sigma,\sigma'} V_{ij} n_{i\sigma} n_{j\sigma'}, \quad (1)$$

where $t_{ij\sigma} = t_{ij} + h_z \mathrm{sgn}(\sigma)\delta_{ij}$, where the hopping t_{ij} is considered only for intrachain (t_x) and the interchain (t_y) nearest neighbors. $t_x = 1.0$ is taken as the energy unit. U is the on-site repulsion and the off-site repulsions V_{ij} are taken as V_x, V_{x2} and V_{x3}, which are first, second and third nearest neighbor intra-chain interactions, and V_y is the interchain interaction. We ignore the orbital effect, assuming that the magnetic field is applied parallel to the conductive x–y plane.

We use the RPA that takes account of the Zeeman effect [14] to obtain the pairing interactions, and solve the linearized gap equation within the weak coupling theory which takes account of the center of mass momentum Q_c (the total momentum $2Q_c$)

$$\lambda^{\sigma\sigma'}_{Q_c} \phi^{\sigma\sigma'}(k) = \frac{1}{N} \sum_{q} V^{\sigma\sigma'}(k,q) \frac{f(\xi_\sigma(q_+)) - f(-\xi_{\sigma'}(-q_-))}{\xi_\sigma(q_+) + \xi_{\sigma'}(-q_-)} \phi^{\sigma\sigma'}(q), \quad (2)$$

where $q_\pm = q \pm Q_c$, $\lambda^{\sigma\sigma'}_{Q_c}$ is the eigenvalue of this linearized gap equation, $V^{\sigma\sigma'}(k,q)$ is the pairing interaction that is obtained by RPA and $\phi^{\sigma\sigma'}(k)$ is the gap function, $\xi_\sigma(q)$ is the band dispersion from the chemical potential and $f(\xi)$ is the Fermi distribution function. The center of mass momentum $\mathbf{Q}_c$ which gives the maximum value of $\lambda^{\sigma\bar{\sigma}}_{Q_c}$ lies along the x-direction because of the nesting of the Fermi surface and $\lambda^{\sigma\sigma}_{Q_c}$ takes its maximum at $\mathbf{Q}_c = (0,0)$ because the electrons do not scatter between the different directional spins in this channel.

In the opposite spin pairing, we define the singlet and the $S_z = 0$ triplet component of the gap function as

$$\phi_{\mathrm{SS}}(k) = \left[\phi^{\uparrow\downarrow}(k) - \phi^{\downarrow\uparrow}(k)\right]/2,$$
$$\phi_{\mathrm{ST^0}}(k) = \left[\phi^{\uparrow\downarrow}(k) + \phi^{\downarrow\uparrow}(k)\right]/2. \quad (3)$$

In our calculation, the spin singlet and the spin triplet component of the gap function in the FFLO state is essentially d-wave and f-wave as schematically shown in Fig. 1b, so we write the singlet d-wave ($S_z = 0$ triplet f-wave) component of the FFLO state gap as $\phi_{\mathrm{SS}d}$($\phi_{\mathrm{ST}f^0}$) in Eq. (3). The eigenvalue of each pairing state is determined as follows. $\lambda^{\sigma\bar{\sigma}}_{Qc}$ with $\mathbf{Q}_c = (0,0)$ gives the eigenvalue of the singlet d-wave $\lambda_{\mathrm{SS}d}$($S_z = 0$ triplet f-wave $\lambda_{\mathrm{ST}f^0}$) when $\phi_{\mathrm{ST}f^0} = 0$($\phi_{\mathrm{SS}d} = 0$), while $\lambda^{\sigma\bar{\sigma}}_{Qc\neq 0}$ gives λ_{FFLO}. $\lambda^{\sigma\sigma}_{Qc}$ with $\mathbf{Q}_c = (0,0)$ gives the eigenvalue for the $S_z = +1$($S_z = -1$) triplet f-wave $\lambda_{\mathrm{ST}f^{+1}}$($\lambda_{\mathrm{ST}f^{-1}}$).

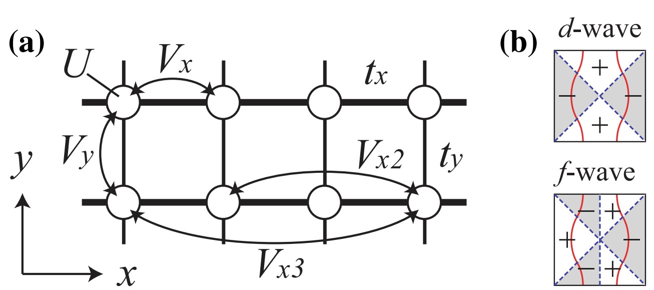

Fig. 1. (a) The model in this study. (b) The schematic figure of the gap for d-wave (upper) and f-wave (lower); the red solid curves are the Fermi surface and the blue dashed lines are the nodes of gap. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3. Results

First, to make the argument general, we concentrate on a simple model with only the on-site $U = 1.5$ and the nearest neighbor repulsion V_x in the x-direction. When V_x is large, $2k_F$ charge fluctuations tends to develop for band fillings close to half filling, so we take the band filling $n = 1.1$, where n = number of electrons/number of sites. Here we fix the value of t_y at 0.5, although this value does not have a specific meaning, and similar results can be obtained for other values of t_y. The temperature is fixed at $T = 0.01$ here. System size is taken as 2048×64 sites here.

In Fig. 2, we show the magnetic field dependence of Q_{cx} of the FFLO state, the parity mixing rate $\phi_{\mathrm{ST}f^0}/\phi_{\mathrm{SS}d}$ and the eigenvalues of the gap equation for (a) $V_x = 0$ and (b) $V_x = 0.65$. Note that we

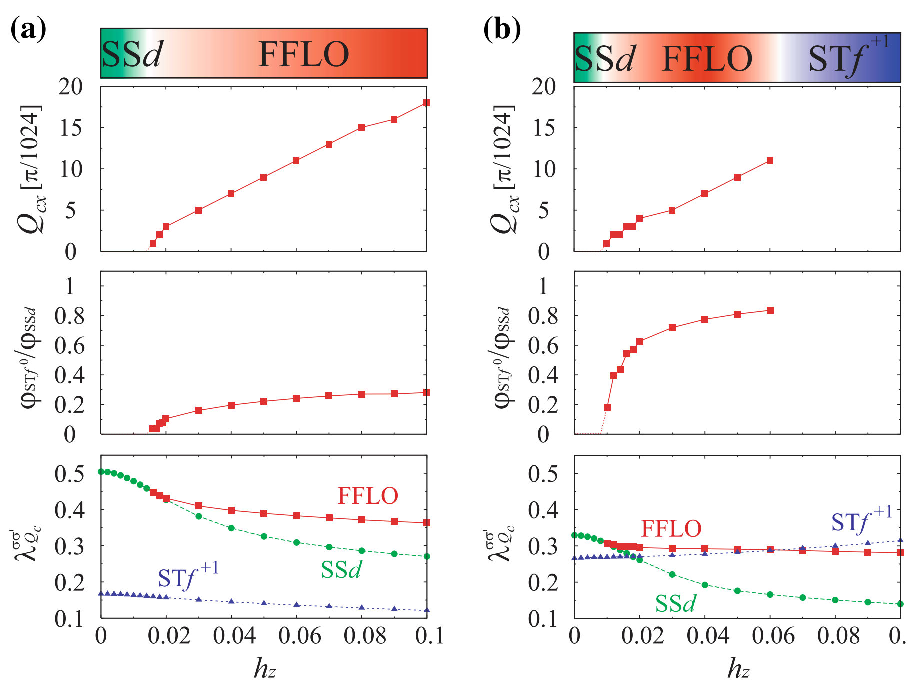

Fig. 2. The h_z-dependence of the Q_{cx} (upper), the $S_z = 0$ triplet/singlet ratio in the FFLO state (center) and the each eigenvalues (lower) for (a) $V_x = 0$ and (b) $V_x = 0.65$.