Journal of Physics and Chemistry of Solids 69 (2008) 3289–3292

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

Study on the competition between density waves, singlet, and triplet pairing superconductivity in organic conductors $(TMTSF)_2X$

Hirohito Aizawa [a,*], Kazuhiko Kuroki [a], Yukio Tanaka [b]

[a] Department of Applied Physics and Chemistry, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan

[b] Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan

ARTICLE INFO

PACS:
74.70.Kn
74.20.Rp
74.20.Mn

Keywords:
A. Organic compounds
D. Charge-density waves
D. Magnetic properties
D. Spin-density waves
D. Superconductivity

ABSTRACT

We study the effect of dimerization of TMTSF molecules and the effect of magnetic field (Zeeman splitting) on the phase competition in quasi one-dimensional organic superconductors $(TMTSF)_2X$ by applying the random phase approximation method. As for the dimerization effect, we conclude that due to the decrease of the dimerization, which corresponds to applying the pressure and cooling, spin and charge density wave states are suppressed and give way to a superconducting state. As for the magnetic field effect, we find generally that spin-triplet pairing mediated by a coexistence of $2k_F$ spin and $2k_F$ charge fluctuations can be strongly enhanced by applying magnetic field rather than triplet pairing due to a ferromagnetic spin fluctuations. Applying the above idea to $(TMTSF)_2X$ compounds, a magnetic field induced singlet–triplet transition is consistent with above mechanism in $(TMTSF)_2ClO_4$.

1. Introduction

Organic conductors $(TMTSF)_2X$ ($X = PF_6$, ClO_4, etc.) exhibit various fascinating phenomena such as spin density wave (SDW), charge density wave (CDW), superconductivity (SC) [1,2] and more. $(TMTSF)_2PF_6$ exhibits a coexistence of $2k_F$-SDW and $2k_F$-CDW at ambient pressure [3,4]. Applying pressure suppresses the $2k_F$-SDW + $2k_F$-CDW state and the SC takes place at low temperature. As for possible origins that degrade the SDW state when the pressure is applied, the effect of Umklapp processes [5–8], Fermi surface nesting [9], etc. have been discussed.

The symmetry of the superconducting gap of $(TMTSF)_2X$ has also been extensively discussed both experimentally and theoretically. Several experiments of the superconducting state have suggested the possibility of spin-triplet pairing, e.g. the upper critical field exceeds the Pauli paramagnetic limit [10,11] and the Knight shift is unchanged across T_c [12]. A very recent experiment on $(TMTSF)_2ClO_4$ has shown that the pairing occurs in the spin-singlet channel at low magnetic field, while a possible triplet pairing state or an FFLO state takes place at high fields [13]. These experiments suggest that the singlet-triplet pairing competition may be subtle in these compounds. Theoretically, some of the studies [14–19] have suggested that the presence of distant off-site interactions makes the competition subtle between spin-singlet *d*-wave and triplet *f*-wave pairing (see Fig. 1 (a)) due to coexisting $2k_F$ spin and $2k_F$ charge fluctuations in a quasi-one-dimensional(Q1D) system. As for the possibility of singlet to triplet pairing transition under high magnetic field was pointed out theoretically [20–22].

In the present study, we study two effects using the random phase approximation (RPA) method: (i) The effect of the dimerization of the molecules on the competition between the density waves (DW) and SC; the dimerization of the molecules is small but present in the actual materials, (ii) The magnetic field (Zeeman splitting) effect on the competition between spin-singlet and triplet pairings. We show generally that the effect of the Zeeman splitting on spin-triplet pairing mediated by coexisting $2k_F$ spin and $2k_F$ charge fluctuations can be much larger than that on the triplet pairing mediated by ferromagnetic spin fluctuations [23].

2. Formulation

Two band extended Hubbard model in this study is shown in Fig. 1(b), where t_{S1} is the intradimer nearest neighbor (n.n.) hopping parameter, t_{S2} is the interdimer n.n. hopping in the *x*-direction and t_y is the n.n. hopping in the *y*-direction. As for the interactions between electrons, we consider not only the on-site repulsion U but also n.n. off-site repulsion V_1, 2nd n.n. repulsion V_2 and 3rd n.n. repulsion V_3 in the *x*-direction and n.n. repulsion V_{p1} in the *y*-direction. To see the dimerization effect, we introduce a parameter $dt = |t_{S1} - t_{S2}|/(t_{S1} + t_{S2})$ that represents

* Corresponding author. Tel.: +81 42 443 5559.
E-mail address: aizawa@vivace.e-one.uec.ac.jp (H. Aizawa).

0022-3697/$ - see front matter
doi:10.1016/j.jpcs.2008.06.081

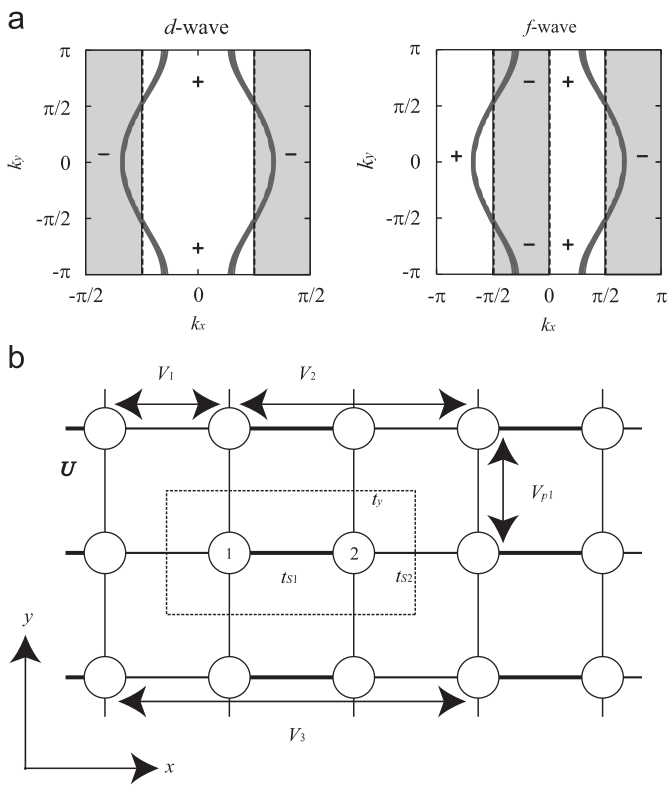

Fig. 1. (a) Gap function for spin-singlet d-wave(left) and spin-triplet f-wave(right), (b) the two band extended Hubbard model with $\frac{3}{4}$-filling electrons.

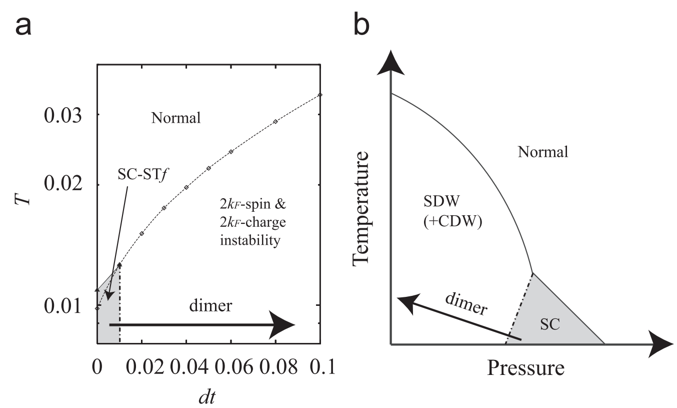

Fig. 2. (a) Calculated phase diagram in dt-T space and (b) schematic pressure-temperature phase diagram.

the magnitude of the dimerization. In this study, we set the hopping parameters as $t_{S1} = 1.0 + dt$, $t_{S2} = 1.0 - dt$, $t_y = 0.2$ and $0 \leqslant dt \leqslant 0.1$, where $(t_{S1} + t_{S2})/2$ is taken as the unit of energy. Furthermore, when we focus on the effect of the magnetic field $\mathbf{B}$ parallel to the x–y plane, the Zeeman splitting is taken into account in the band dispersion.

We use the RPA to obtain the pairing interactions mediated by spin and charge fluctuations, and plug them into the linearized gap equation, whose eigenvalue $\lambda(T)$ represents the strength of the pairing instability. We use the multi-band RPA [24] to treat the dimerization effect. Within the multi-band RPA, the spin susceptibility matrix is given as $\hat{X}^{\rm sp} = (\hat{I} - \hat{U}\hat{X}^0)^{-1}\hat{X}^0$, where $\hat{X}^0$ is the bare susceptibility matrix. We adopt the criterion that when the largest eigenvalue of $\hat{I} - \hat{U}\hat{X}^0$ becomes smaller than 0.005, the DW order sets in. To study the magnetic field effect, we apply RPA that takes into account the magnetic anisotropy [23]. To give a reference for the values of the magnetic field, we calculate the Pauli limit by $\mu B_{\rm P} = 1.75 k_{\rm B} T_{\rm c}/\sqrt{2}$. Although RPA is quantitatively insufficient for evaluating the absolute value of $T_{\rm c}$, we expect this approach to be valid for studying the *competition* between different pairing symmetries. In fact, we find very good agreement between the RPA results and the already known results obtained by dynamical cluster approximation (DCA) [25].

3. Dimerization effect

We first present the calculation result for the dimerization effect in the absence of the magnetic field. Interaction parameters are taken as $U = 1.7$, $V_1 = 0.9$, $V_2 = 0.45$, $V_3 = 0.1$ and $V_{p1} = 0.4$, where $2k_{\rm F}$-SDW + $2k_{\rm F}$-CDW may be present in this system since the interaction parameters satisfy the condition of $\hat{X}^{\rm sp}(\mathbf{Q}) = \hat{X}^{\rm ch}(\mathbf{Q})$ as $V_2 + V_{p1} = U/2$ [26–28]. The spin-triplet f-wave pairing can also be dominant over the spin-singlet d-wave pairing by satisfying this condition. Decreasing the dimerization parameter dt results in a suppression of the $2k_{\rm F}$-SDW + $2k_{\rm F}$-CDW, and the spin-triplet f-wave pairing state (SC-STf) appears as seen in Fig. 2(a), where we identify the regime of dt as SC if λ, the eigenvalue of the linearized BCS gap equation, exceeds unity before the DW order sets in. The obtained phase diagram is qualitatively consistent with the schematic P–T phase diagram as seen in Fig. 2(b) since applying pressure and cooling lead to a decrease of the dimerization [29]. As for the pairing symmetry competition, we find that the dimerization does not affect the condition for triplet f-wave pairing dominating over d-wave obtained in previous studies [17].

4. Magnetic field effect

We move on to the magnetic field effect on the pairing competition between the singlet d-wave and triplet f-wave pairings. Since we have found that the dimerization has no effect on the competition between d and f, we ignore the dimerization effect and focus on the Zeeman effect in the single band extended Hubbard model.

Within RPA that takes into account the magnetic anisotropy, the longitudinal susceptibility with parallel spins is given as

$$\chi^{\sigma\sigma} = \frac{(1 + \chi_0^{\bar{\sigma}\bar{\sigma}} V_{\mathbf{q}})\chi_0^{\sigma\sigma}}{(1 + \chi_0^{\sigma\sigma} V_{\mathbf{q}})(1 + \chi_0^{\bar{\sigma}\bar{\sigma}} V_{\mathbf{q}}) - (U + V_{\mathbf{q}})^2 \chi_0^{\sigma\sigma} \chi_0^{\bar{\sigma}\bar{\sigma}}} \tag{1}$$

and one with opposite spins is given as

$$\chi^{\sigma\bar{\sigma}} = \frac{-\chi_0^{\sigma\sigma}(U + V_{\mathbf{q}})\chi_0^{\bar{\sigma}\bar{\sigma}}}{(1 + \chi_0^{\sigma\sigma} V_{\mathbf{q}})(1 + \chi_0^{\bar{\sigma}\bar{\sigma}} V_{\mathbf{q}}) - (U + V_{\mathbf{q}})^2 \chi_0^{\sigma\sigma} \chi_0^{\bar{\sigma}\bar{\sigma}}}, \tag{2}$$

where $V_{\mathbf{q}}$ is the Fourier transform of the off-site interactions and $\chi_0^{\sigma\sigma}$ is the longitudinal bare susceptibility. Using these susceptibilities, we obtain the pairing interaction in the spin-triplet with $\mathbf{d} \perp \hat{z}$ channel as

$$\begin{aligned} V^{t\sigma\sigma}(\mathbf{q}) = {} & V(\mathbf{q}) - 2(U + V(\mathbf{q}))V(\mathbf{q})\chi^{\sigma\bar{\sigma}} \\ & - V(\mathbf{q})^2 \chi^{\sigma\sigma} - (U + V(\mathbf{q}))^2 \chi^{\bar{\sigma}\bar{\sigma}}, \end{aligned} \tag{3}$$

while the pairing interactions in the spin-singlet channel (V^s) and spin-triplet with $\mathbf{d} \| \hat{z}$ channel ($V^{t\sigma\bar{\sigma}}$) are represented by the ordinary RPA formula using longitudinal ($\chi_{\rm sp}^{zz}$) and transverse ($\chi_{\rm sp}^{+-}$) spin and charge ($\chi_{\rm ch}$) susceptibilities, although these susceptibilities are affected by the Zeeman effect [23].

Before giving the calculation results, we show generally using the above formula that the effect of the Zeeman splitting on the triplet pairing caused by the coexistence of $2k_{\rm F}$ spin and $2k_{\rm F}$ charge fluctuations can be very special. First, let us consider a case