Mechanism for the Singlet to Triplet Superconductivity Crossover in Quasi-One-Dimensional Organic Conductors

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Superconductivity of quasi-one-dimensional organic conductors with a quarter-filled band is investigated using the two-loop renormalization group approach to the extended Hubbard model for which both the single electron hopping $t$ and the repulsive interaction $V_{\perp}$ perpendicular to the chains are included. For a four-patches Fermi surface with deviations to perfect nesting, we calculate the response functions for the dominant fluctuations and possible superconducting states. By increasing $V_{\perp}$, it is shown that a $d$-wave (singlet) to $f$-wave (triplet) superconducting state crossover occurs, and is followed by a vanishing spin gap. Furthermore, we study the influence of a magnetic field through the Zeeman coupling, from which a triplet superconducting state is found to emerge.

KEYWORDS: singlet superconductivity, triplet superconductivity, organic conductors, extended-Hubbard model, renormalization group, quarter-filled, nesting deviations, Zeeman field

1. Introduction

Superconductivity in quasi-one-dimensional (quasi-1D) organic conductor, (TMTSF)$_2$X, has been studied extensively in the conditions where charge and spin fluctuations play an important role due to the low dimensionality of the Fermi surface.

The possibility for triplet state superconductivity, besides the singlet one, is an issue of current interest in these materials. From recent NMR measurements on (TMTSF)$_2$ClO$_4$, it has been suggested that spin-triplet superconductivity may emerge out of a singlet state under magnetic field. This can occur as a field-induced phase transition that can compete with a FFLO state under strong magnetic field. It is important for such a study to take into account the influence of low-dimensional fluctuations due to the strongly anisotropic band structure of (TMTSF)$_2$X. The existence of spin fluctuations is supported by the NMR experiments in the normal phase of these materials.

Several theoretical works have been devoted to the field-induced phase transition to the triplet superconducting (SC) state. Shimahara et al. pointed out such a transition using the RG technique for a many-chains quasi-1D system.

A similar transition has been shown to occur by Aizawa et al. using the RPA method for the extended Hubbard model that includes intersite repulsive interaction for longitudinal and transverse directions along the chains, and the Zeeman coupling of spins to a finite magnetic field. As shown for the Hubbard model with on-site repulsive interaction, the RPA approach, which sums up a higher order of perturbation for electron interactions, suggests the importance of the pairing interactions mediated by spin fluctuations. Thus it is of interest to further examine fluctuations of both density waves and superconducting pairings, where the spin gap is essential to the existence of a singlet superconducting state.

These features can be properly taken into account by the renormalization group (RG) method. The effect of a magnetic field on low-dimensional systems has been studied by the RG method mainly for the one-dimensional cases. Noticeable progress has been achieved in studying superconductivity in zero field for the case of quasi-1D systems with many chains. However, the different mechanisms by which triplet superconductivity can be stabilized in such systems, especially in finite magnetic field, have not been fully investigated within the RG scheme.

In the present work, we use the RG method up to the two-loop level to study the competition between the $d$-wave singlet SC state (SC$d$) and the $f$-wave triplet SC state (SC$f$) in quasi-1D systems with interchain electron hopping and repulsive interactions. It is demonstrated that superconductivity is driven by the interplay of interchain interaction and the nesting deviations. The crossover from the SC$d$ state to the SC$f$ state occurs with increasing the interchain repulsive interaction in the presence of nesting deviations. The effect that a Zeeman coupling to the magnetic field can have on the stability of the SC$d$ state and the emergence of a triplet SC$f$ state is studied in details. In §2, we give the formulation of the RG technique for a many-chains quasi-1D system at quarter-filling, in the presence of magnetic field and nesting deviations. Using a four-patches decomposition of the Fermi surface, we derive the flow equations for the SC$d$ and SC$f$ response functions in the superconductivity channel, and for the spin-density-wave (SDW) and charge-density-wave (CDW) responses in the staggered density-wave channel. In §3, the results for the possible states as a function of interchain Coulomb interaction, nesting deviations and magnetic field are presented. The conditions for the stability of the SC$f$ triplet state in the calculated phase diagrams are given. Summary and discussion are presented in §4.

2. Formulation

2.1 Model

In order to study the superconductivity for the (TMTSF)$_2$X salt, we consider the quasi-1D extended Hubbard model,
Expressing the interaction in terms of forward and backward scattering, eq. (3) is rewritten as

$$H_1 = \frac{2\pi v}{LN_{k_1,k_2,q}} \sum_{k_1,k_2,q,\sigma} G_{\sigma}(q) \sigma_{k_1,k_2} c_{\sigma}^\dagger(k_1)c_{\sigma}^\dagger(k_2-q)c_{\sigma}^\dagger(k_2-q)c_{\sigma}^\dagger(k_2),$$

(7)

where

$$G_{\sigma}(q) = G_{\sigma}^{\uparrow}(q) \delta_{\sigma_1,\sigma_2} \delta_{\sigma_3,\sigma_4} \delta_{\sigma_1,\sigma_2} - G_{\sigma}^{\downarrow}(q) \delta_{\sigma_1,\sigma_2} \delta_{\sigma_3,\sigma_4} \delta_{\sigma_1,\sigma_2}$$

(8)

The couplings $G_{\sigma}^{\uparrow}$ and $G_{\sigma}^{\downarrow}$ stand for the forward scattering with spin being anti-parallel and parallel, respectively. The amplitude $G_{\sigma}^{\uparrow}$ denotes that of the backward scattering with anti-parallel spins. The $8k_F$-Umklapp scattering due to the quarter-filling is discarded. The coupling constants depend on the wave vector perpendicular to the chains, and the definition is the same as in ref. 24. The bare scattering amplitudes, which correspond to the initial values for the RG equations, are given by

$$G_{\sigma}^{\uparrow}(q) = \frac{1}{2\pi v} (U + 2V^b_{\uparrow} \cos q),$$

(9a)

$$G_{\sigma}^{\downarrow}(q) = \frac{1}{2\pi v} \left[ U + 2V^b_{\downarrow} \cos (k_1 - k_2) \right],$$

(9b)

$$G_{\sigma}(q) = \frac{1}{2\pi v} \left[ 2V^1_{\uparrow} \cos (k_1 - k_2) - 2V^b_{\uparrow} \cos q \right].$$

(9c)

In the following, we shall only retain the backscattering part ($V^b_{\uparrow}$) and neglect the forward scattering contribution $V^1_{\uparrow}$ of eqs. (9a)-(9c); $V^b_{\uparrow}$ is known to be involved in the enhancement of $2k_F$ CDW fluctuations.

2.2 RG equations for the vertex couplings

We consider the partition function, which is represented in the path integral form,

$$Z = \int \mathcal{D} \psi^* \mathcal{D} \psi \, e^{\mathcal{S}\left[\psi^*, \psi\right]},$$

(10)

where $\mathcal{S}\left[\psi^*, \psi\right] = S_0[\psi^*, \psi] + S_1[\psi^*, \psi]$ is the action corresponding to the Hamiltonian (1). The fields $\psi^*(\psi)$ are the Grassmann variables for the electron degrees of freedom and $\mathcal{D} \psi^* \mathcal{D} \psi$ corresponds to the integration measure for the Grassmann variables. In the Fourier-Matsubara space, the free and interacting parts of the action $S_0[\psi^*, \psi]$ and $S_1[\psi^*, \psi]$ are respectively given by

$$S_0[\psi^*, \psi] = \sum_{k,\omega_n,\sigma} \left[ g^0_{\sigma,\sigma}(\mathbf{k},i\omega_n) \right] \psi^*_{\sigma,\sigma}(\mathbf{k},i\omega_n),$$

(11a)

$$S_1[\psi^*, \psi] = -T \sum_{i\omega_n,\sigma} H^1_{\sigma,\sigma}(\mathbf{k},i\omega_n),$$

(11b)

where $T$ is the temperature ($k_B = 1$ throughout this work) and $H^1_{\sigma,\sigma}(\mathbf{k},i\omega_n)$ is obtained by substituting the fermion operators for the Grassmann variable $g^0_{\sigma,\sigma}(\mathbf{k},i\omega_n)$, etc., where $\mathbf{k} = (k_1,k_2)$ and $\omega_n$ are $\mathbf{k}$ and $\omega_n$ being the Matsubara frequencies for fermions and bosons, respectively. The Green’s function for the free fermions is given by $g^0_{\sigma,\sigma}(\mathbf{k},i\omega_n) = [i\omega_n - \epsilon_{\sigma,\sigma}(\mathbf{k})]^{-1}$. In order to examine the behavior at low temperature, we proceed to implement...
the successive partial integrations of eq. (10) on high-energy shells. This leads to the renormalization of the inner shell action, the external momentum is fixed at the Fermi surface, i.e., $E_{\text{F}} = E_{\text{F}}^* < E_F$, while crossed lines represent electrons at higher energy or lower $l$ values.

The use of the linked cluster expansion allows one to write the result in the form

$$Z \propto \int [\mathcal{D} \psi^* \mathcal{D} \psi \exp \left\{ S_c[\psi^*, \psi] + \sum_{n=1}^{\infty} \frac{1}{n!} (S_{\text{pert}}^n)_{<,c} \right\}],$$

where $(\cdots)_c$ denotes the contribution of connected diagrams to the outer energy shell of width $E_{l+dl}$, where $dl \ll 1$. The action $S_{l+dl}$, at the step $l + dl$, thus contains additional renormalization terms, which for the coupling constants read

$$\delta G_{V}(q, k_2, l) = G_{V}(q, k_2, l + dl) - G_{V}(q, k_2, l) = \delta G_{V}^{\text{pert} = 2}(q, k_2, l) + \delta G_{V}^{\text{pert} = 3}(q, k_2, l) + \cdots,$$

where $\nu = 1, 2, \ldots$, and $l$. The logarithmic contributions at the one-loop level ($n = 2$) for $\delta G_{V}^{\text{pert} = 2}(q, k_2, l)$ are given by the diagrams shown in Fig. 2.

This renormalization consists of two parts, which come from the Peierls channel and Cooper channels, namely

$$\delta G_{V}^{\text{pert} = 2}(q, k_2, l) = F_{C}(q, k_2, l) + F_{P}(q, k_2, l).$$

The Peierls bubble $F_{P}^{V}(q, k_1, k_2)$ is given by

$$F_{P}(q, k_1, k_2) = \frac{2 \pi \nu T}{L_{N_{\perp}}} \sum_{i} \sum_{k_{i}} \sum_{t_{0i}} \frac{m_{p}^{V_{i}^{V_{1}^{V_{2}}}} G_{V_{1}^{V_{2}}}(q, k_{1}^{2}, k_{2})}{|e_{R}(k) - e_{L}(k) - E_{\text{F}}|} \times \sum_{i} \sum_{l_{i} = 1, 2} I_{p_{i}^{V_{1}^{V_{2}}}}(q, k_{1}^{2}, k_{2}, i, 0_{i}) \delta_{k, i}^{0} e_{L}(k - q, i) e_{0}(k - q, i),$$

where $I_{p_{i}^{V_{1}^{V_{2}}}}(q, k_{1}^{2}, k_{2}, i, 0_{i})$ is performed in the outer shell region. The summation is written as

$$\sum_{k_{i}^{2}} = 2 \sum_{k} \Theta(|e_{R}(k) - e_{L}(k) - E_{\text{F}}|),$$

and the sum of $\nu$, $\nu' (= 1, 2, 3, \ldots)$ is taken for the fixed $v$, as shown explicitly later. The quantity $m_{p}^{V_{1}^{V_{2}}}$ denotes the number of the permutation of Grassmann variable. $\sum_{k_{i}^{2}}$ is performed in the outer shell region. The summation is written as

$$\sum_{k_{i}^{2}} = 2 \sum_{k} \Theta(|e_{R}(k) - e_{L}(k) - E_{\text{F}}|).$$

In the above equations, $\sigma = \pm$ and $\eta$ are replaced by $\sigma = 1$ and $-1$, respectively. In a similar way, the Cooper bubble is calculated as follows:

$$F_{C}(q, k_1, k_2) = -\frac{2 \pi \nu T}{L_{N_{\perp}}} \sum_{i} \sum_{k_{i}} \sum_{t_{0i}} \frac{m_{p}^{V_{1}^{V_{2}}}}{2} G_{V_{1}^{V_{2}}}(q, k_{1}^{2}, k_{2}) \times \sum_{i} \sum_{l_{i} = 1, 2} I_{p_{i}^{V_{1}^{V_{2}}}}(q, k_{1}^{2}, k_{2}, i, 0_{i}) \delta_{k, i}^{0} e_{L}(k - q', -i0_{i}),$$

where $q' = q - k_1 - k_2$ and $F_{C}(q, k_1, k_2) = (-1)^{m_{p}^{V_{1}^{V_{2}}}} G_{V_{1}^{V_{2}}}(q - k_1^{2} - k_2, k_2) G_{V_{2}}(q - k_1^{2} - k_2, k_2).$
Fig. 3. (Color online) The RG equations for the coupling constants at the one-loop level. The slashed and crossed internal lines represent the electrons on the high-energy shell and within the shell, respectively. The diagrams with the slash and cross lines interchanged (not shown) are also taken into account.

and the summation $\sum_{k,k'}^{\nu} \sigma^i$ is given by substituting $\epsilon_{\nu,\sigma^i}(\mathbf{k} - \mathbf{q})$ for $\epsilon_{\nu,\sigma^i}(\mathbf{k} - \mathbf{q})$ in eq. (18). The Fermi surface of the external momentum is given by \((k_{F,\sigma_1}(k_1, k_1), (-k_{F,\sigma_2}(k_2 - q), k_2 - q))\) for the incoming states, and \((k_{F,\sigma_2}(k_2), k_2), (-k_{F,\sigma_2}(k_1 - q), k_1 - q))\) for the outgoing states. The longitudinal momentum vector $q''_i$ is also determined by the momentum conservation for respective vertex. Performing the Matsubara-frequency summation, eq. (24) is rewritten as

$$F^\nu_C(q,k_1,k_2) = \frac{2}{N_L} \sum_{\nu_1 \nu_2} F^\nu_{C(q,k_1,k_2)}$$

$$\times \int d\epsilon R, \sigma \left( \frac{f(\epsilon_{R,\sigma}(\mathbf{k})) - f(\epsilon_{\nu,\sigma^i}(\mathbf{k} - \mathbf{q})))}{\epsilon_{R,\sigma}(\mathbf{k}) + \epsilon_{\nu,\sigma^i}(\mathbf{k} - \mathbf{q})} \right) \times \Theta(|\epsilon_{\nu,\sigma^i}(\mathbf{k} - \mathbf{q})| - E_i).$$

(26)

At zero temperature, eq. (26) is calculated as

$$F^\nu_C(q,k_1,k_2) = \frac{1}{N_L} \sum_{\nu_1 \nu_2} \sum_k I^\nu_{C(q,k_1,k_2)}$$

$$\times \frac{1}{2} \sum_{i=1,2} I_C(q'_{k_1,k_1}, \sigma - \sigma_i),$$

(27)

where

$$I_C(q'_{k_1,k_1}, \sigma - \sigma_i) = \frac{2E}{2E + |Y_{q'_{k_1,k_1}, \sigma - \sigma_i}(l)|},$$

(28)

and

$$Y^C_{q'_{k_1,k_1}, \sigma - \sigma_i}(l) = \epsilon_{R,\sigma}(k) + \epsilon_{\nu,\sigma^i}(\mathbf{k} - \mathbf{q'})$$

$$+ 2t_1(l)[\cos k - \cos (k + \mathbf{q'})] + 2t_2(l)[\sin k - \sin (k + \mathbf{q'})] + h(l)\sigma - \sigma_i).$$

(29)

The functions $I_{p_{\nu_1 \nu_2}^l}(q,k_1,k_2,\sigma - \sigma_i)$ and $I_{C(q,k_1,k_1),\sigma - \sigma_i}$, which are equal to unity in the one-dimensional case and in the absence of the magnetic field, are reduced by $t_1$ and $t_2$ in the quasi-1D case.

The RG flow equations at the one-loop level are shown diagrammatically in Fig. 3. Including the two-loop corrections derived in the Appendix, the RG equations take the form

$$\frac{d}{dt} G^\nu_{v(q,k_1,k_2)} = \frac{1}{2N_L} \sum_{k} (1)_{v(q,k_1,k_2)}$$

$$- \frac{1}{8N_L} G^\nu_{v(q,k_1,k_2)} \sum_{q',k'} G^\nu_{v(q,k_1,k_2)}$$

$$+ \frac{1}{4N_L} \sum_{q',k'} \Xi^\nu_{v(q,k_1,k_2,1)} + (k_1 \leftrightarrow k_2),$$

(30)

where $\Xi^\nu_{v(q,k_1,k_2,1)}$ is the contribution from the one-loop RG, while $\Xi^\nu_{v(q,k_1,k_2,2)}$ and $\Xi^\nu_{v(q,k_1,k_2,3)}$ are the two-loop contributions coming from the self-energy and the vertex part, respectively (see Appendix). The quantity $\Xi^\nu_{v(q,k_1,k_2)}$ is written as

$$\Xi^\nu_{v(q,k_1,k_2,1)} = \Xi^\nu_{v(q,k_1,k_2,2)} = \Xi^\nu_{v(q,k_1,k_2,3)}$$

(31a)

$$\Xi^\nu_{v(q,k_1,k_2,1)} = \Xi^\nu_{v(q,k_1,k_2,2)} = \Xi^\nu_{v(q,k_1,k_2,3)}$$

(31b)

and

$$\Xi^\nu_{v(q,k_1,k_2,1)} = \Xi^\nu_{v(q,k_1,k_2,2)} = \Xi^\nu_{v(q,k_1,k_2,3)}$$

(31c)

where for $\lambda = P, C$,

$$I^0_{\lambda}(q,k_1,k_2) = \frac{1}{4} \sum_{i=1,2} I^0_{\lambda}(q,k_1,k_1,0),$$

(32a)

$$I^0_{\lambda}(q,k_1,k_1) = \frac{1}{4} \sum_{i=1,2} I^0_{\lambda}(q,k_1,k_1,2r) + I^0_{\lambda}(q,k_1,k_1,0),$$

(32b)

$$I^0_{\lambda}(q,k_1,k_1,2r) = \frac{1}{4} \sum_{r=-1}^{1} \sum_{i=1,2} I^0_{\lambda}(q,k_1,k_1,2r).$$

(32c)

Note that in the absence of interchain couplings, $\Xi^\nu_{v(q,k_1,k_1)}$ coincides with the expressions already obtained by Montambaux et al. at $h \neq 0$ in the 1D case.

2.3 RG equations for response functions

Now we calculate the response functions for CDW, SDW, SCd, and SSc. The composite fields of corresponding order parameters are defined as

$$\delta_{CDW}(q) = \sqrt{\frac{1}{LN_\perp} \sum_{k_1,\sigma} c^+_{k_1,\sigma}(k)c_{k_1,\sigma}(k - q)},$$

(33a)
\[ \frac{d}{dt} \chi_{\text{CDW}}(q \nu) = \frac{1}{\pi v^2} \chi_{\text{CDW}}(q \nu) I_2, \quad (36a) \]

\[ \frac{d}{dt} \chi_{\text{SDW}}(q \nu) = \frac{1}{\pi v^2} \chi_{\text{SDW}}(q \nu) I_2, \quad (36b) \]

\[ \frac{d}{dt} \chi_{\text{SCd}}(q \nu) = \frac{1}{\pi v^2} \chi_{\text{SCd}}(q \nu) I_2, \quad (36c) \]

\[ \frac{d}{dt} \chi_{\text{SCf}}(q \nu) = \frac{1}{\pi v^2} \chi_{\text{SCf}}(q \nu), \quad (36d) \]

where the respective three-point vertices \( z_{\mu} \) obey the RG equations:

\[ \frac{d}{dt} \ln \chi_{\text{CDW}}(q \nu) = -G_{1,1}(\pi,0,0) - G_{1,1}(\pi,0,\pi) \]

\[ + G_{\parallel,\parallel,0,0} + G_{\parallel,\parallel,0,\pi} I_2/2 I_2^2, \quad (37a) \]

\[ \frac{d}{dt} \ln \chi_{\text{SDW}}(q \nu) = -G_{2,1}(\pi,0,0) + G_{2,1}(\pi,0,\pi) I_2, \quad (37b) \]

\[ \frac{d}{dt} \ln \chi_{\text{SCd}}(q \nu) = -G_{1,1}(0,0,0) + G_{1,1}(\pi,0,\pi) \]

\[ + G_{2,1}(\pi,0,\pi) - G_{2,1}(0,0,0) I_2/2 I_2^2, \quad (37c) \]

\[ \frac{d}{dt} \ln \chi_{\text{SCf}}(q \nu) = G_{\parallel,\parallel,0,0} - G_{\parallel,\parallel,0,\pi}. \quad (37d) \]

The initial values are \( z_{\mu} \mid_{t=0} = 1 \). In the above equations, \( I_2 \) is defined by

\[ I_2 = \frac{E}{E + h(l)}, \quad (38) \]

Note that eq. (37b) represents the flow equation for the transverse SDW. The longitudinal SDW response is obtained by substituting \([G_{1,1}(\pi,0,0) + G_{1,1}(\pi,0,\pi)] + G_{2,1}(\pi,0,\pi) - G_{2,1}(0,0,0) I_2/2 I_2^2\) for the r.h.s. of eq. (37b). These two flow equations become equivalent in the absence of \( h \).

3. Singlet versus triplet superconductivity

For the numerical calculations that follow, parameters of the model are fixed at \( U = 4t_\parallel \) and \( t_1 = 2t_\parallel \) unless stated explicitly. The unit of the energy is \( t_1 \), which is set to unity \( t_1 = 1 \), and we take \( E = 2t_\parallel \). The scaling parameter \( l \) is replaced by \( l = \ln(E/T) \), where \( T \) can be squared with the actual temperature introduced in \$2.\)

In the following study of the four-patches Fermi surface, we will also examine the spin gap \( \Delta_\sigma \), which is governed by the combination of coupling constants\(^{29}\)

\[ G_{\sigma^+} = \frac{1}{2} [G_{2,1}(0,0,0) - G_{\parallel,\parallel,0,0,0} + G_{2,1}(\pi,0,0) - G_{\parallel,\parallel,0,\pi,0}] \quad (39) \]

For a non zero \( \Delta_\sigma \), the coupling \( G_{\sigma^+} \) takes a positive value at \( l = 0 \), but moves to a fixed point with a large negative value. At a qualitative level for the spin gap, we shall use \( \Delta_\sigma = E_{\sigma^-}(= E e^{-i_\sigma}) \) where \( E_\sigma \) is determined by the condition \( G_{\sigma^-}(l_\sigma) = -0.7 \).\(^{24}\) Thus a non zero spin gap is obtained for the couplings \( G_{2,1}(0,0,0) < 0, G_{\parallel,\parallel,0,0,0} > 0, G_{2,1}(\pi,0,0) < 0, \) and \( G_{\parallel,\parallel,0,\pi,0} > 0 \). Here we note that in the absence of magnetic field, the combination of couplings for the spin gap, eq. (39), can be rewritten as

\[ G_{\sigma^+} = \frac{1}{2} [G_{2,1}(0,0,0) + G_{1,1}(\pi,0,0)] \quad (40) \]

From \( G_{\sigma^+} \), the uniform susceptibility within RPA takes the
for the Hubbard ladder model with repulsive interactions. The SDW correlations, which are the most dominant fluctuation state in the absence of magnetic field is then either SC or CDW. This behavior resembles to that of the spin gap, \( \Delta_g \), as shown by the dashed line in Fig. 6. The existence of such a critical point of \( V^b_{\perp} \) has been also shown for two-coupled chains.\(^{29}\) A similar behavior shown by \( \Delta_g \) indicates that spin degrees of freedom are also critical at \( V^b_{\perp} \). The behavior around the quantum critical point, \( V^b_{\perp} \), is ascribed to the competition between SCd and CDW, which are associated to different spin gaps. The spin gap for SCd is formed by interchain pairing, whereas that of CDW results from intrachain interactions. Therefore \( \Delta_g \) vanishes at the critical point where the symmetry of the gap changes.

We now turn to the effect of magnetic field, \( h \), which brings new states due to its influence on the spin gap. When \( \Delta_g \) is destroyed by the magnetic field, the magnetic state is expected to be either the transverse SDW or SCf. Such a region actually exists when \( V^b_{\perp} \sim V^b_{\perp} \). The phase diagram in the \( V^b_{\perp} - t_1 \) plane is shown in Fig. 7. The boundary between SCd and SDW (and also between SCf and CDW) is estimated from the condition, \( \Delta_g \rightarrow 0 \). It is found that the effect of \( h \) on SCd is larger than it is for CDW. The SDW state thus takes place for \( V^b_{\perp} < V^b_{\perp} \), whereas the SCf state appears for \( V^b_{\perp} > V^b_{\perp} \). Moreover, \( V^b_{\perp} \) is a critical value for the crossover between SDW and SCf as the dominant fluctuations. In our two-loop approach, the fact that both SDW and SCf of Fig. 7 vanish for \( h = 0 \) is at variance with the emergence of SDW state found in ref. 25 at low temperature using one-loop RG.

3.2 Nesting deviations and superconductivity

We now examine the SC state in the presence of nesting deviations, which is the main subject of the present paper.
We look at the possible states at $t_{2}/t_{1} \neq 0$ and low temperature by choosing $V_{b}^{0} = 0.7$ (a), 0.88 (b), and 1.0 (c), namely for small, intermediate, and large interchain couplings. Figures 8 (a), (b), and (c) show the temperature dependence of coupling constants which give rise to the response functions for SC, SC′, and CDW respectively. The other couplings (not shown in the figures) only contribute a lesser degree to the response functions. These functions are traced in Figs. 9 (a)–(c).

For $V_{b}^{0} = 0.7$ [Fig. 8 (a)], the values of $G_{1,∥,(π,0,π)}$ and $G_{2,∥,(π,0,π)}$ at the fixed points are positive, while those of $G_{1,⊥,(0,0,0)}$ and $G_{2,⊥,(0,0,0)}$ are negative. The SC′ response function is then the strongest and becomes the dominant state. Since the coupling constant $G_{2,⊥,(0,0,0)}$ changes its sign and becomes relevant, a spin gap appears [see eq. (39)], which is crucial to SCd. As for the relevant coupling $G_{2,∥,(π,0,π)}(>0)$, it enhances both SDW and SCd, as seen from eqs. (37b) and (37c). Figure 9 (a) shows the temperature dependence of the response functions, where the SDW state is found to be the dominant state at high temperature, but becomes subdominant at low temperature. The amplitude of SDW correlations is reduced by nesting deviations. Thus it is found that SCd pairing is induced by spin fluctuations with the coupling $G_{2,∥,(π,0,π)}(>0)$.

For $V_{b}^{0} = 0.88$ [Fig. 8 (b)], the relevant couplings are given by $G_{∥,(π,0,π)}(>0)$ and $G_{∥,(0,0,0)}(<0)$ which are quite different from those obtained in (a) for weaker $V_{b}^{0}$; SC′ fluctuations are then dominant, as seen from eq. (37d). The spin gap vanishes since the combination of couplings given by eq. (39) remains positive. Thus if $Δ_{F} = 0$, the dominant contribution to the SC coupling comes from density fluctuations for which the relevant coupling with parallel spins, namely $G_{∥,(π,0,π)}(>0)$, is connected to charge fluctuations. It is worth noting that long wave length spin fluctuations also promote the SC′ state since $G_{∥,(0,0,0)} < 0$ suppresses the divergence of SC′ correlations and also the uniform spin susceptibility [eq. (41)], as it will be discussed later. The CDW fluctuations are well developed at temperatures just above the region where SCd is dominant [Fig. 9 (b)]. At these temperatures, the CDW response function is nearly the same as that of SDW, implying a coexistence of spin and charge fluctuations for intermediate $V_{b}^{0}$. We finally note that the dominance of SC′ state is obtained in the presence of nesting deviations ($t_{2}^{*} \neq 0$), which suppresses the divergence of CDW in the low temperature limit.

For $V_{b}^{0} = 1.0$ [Fig. 8 (c)], the relevant couplings are $G_{∥,(π,0,π)}(>0)$, $G_{∥,(0,0,0)}(>0)$, $G_{1,∥,(π,0,π)}(<0)$, and $G_{1,⊥,(π,0,π)}(<0)$, which lead to a CDW state as seen from eq.
density-wave correlations. The effect of but the CDW state is suppressed and the SC corresponding to the SC Fig. 11, the temperature dependence of this quantity is shown (a) is essential to the predominance of either SC or CDW.

The dominant states are summarized in the $V^b_T$ phase diagram of Fig. 10. This phase diagram shows some similarity with the one of Fig. 6 in the sense that the SDW state is found at high temperature, namely for $T \gtrsim t_2^*$. However, for $T \lesssim t_2^*$, the SCf state comes in between the regions of the SCd and CDW states. In the zone where $T \lesssim t_2^*$ and $V^b_\perp \gtrsim V^b_\parallel$, the CDW state is dominant and the SCf state is sub-dominant, but the CDW state is suppressed and the SCf state becomes dominant for $t_2^* \neq 0$ – a result well explained by the fact that nesting deviations have a detrimental influence primarily on density-wave correlations. The effect of $t_2^*$, when $V^b_\perp < V^b_{c,t}$, is small, because the SCd state is less affected by nesting deviations in that region.

At this point we would like to comment on the behavior of the uniform magnetic susceptibility, $\chi$, given by eq. (41). In Fig. 11, the temperature dependence of this quantity is shown for the $V^b_\perp = 0.7, 0.88$, and 1.0 cases considered above, which correspond to the SCd, SCf, and CDW states, respectively. It should be noticed that $\chi$, increases when the system is entering in the SCf state, indicating an enhancement of long wave length spin correlations. This contrasts with the cases where SCd and CDW states prevail and $\chi$, decreases rapidly due to the formation of a spin gap.

Now we study the effect of a magnetic field on the SCd state for the intermediate interchain interaction, namely in the region where the sub-dominant SCf state is close to SCd. Figure 12 shows the $T$ vs $h$ phase diagram for the most dominant states at $V^b_\perp = 0.78$. At low temperature, there is a crossover from SCd to the SCf state due to the suppression of the spin gap with $h$. In the inset, the temperature dependence of the response functions for SCd and SCf are shown at finite ($h=0.0002$) and zero magnetic field. The SCd correlations are strongly suppressed by $h$, while the magnetic field has essentially no influence on SCf correlations.

**4. Summary and Discussion**

We have examined by the two-loop RG method the singlet SCd and the triplet SCf superconducting states in the framework of a 4-patch model with nesting deviations. The triplet SCf state, which is absent in the model for intrachain interactions only, is found to develop from the combined effect of interchain repulsive interactions and nesting deviations.

It is of importance to return to the mechanism of formation of the superconducting state and examine the scattering processes that are pertinent to this state. This is shown in Fig. 13, where the symbol $\pm$ in the $k_z$-$k$ plane denotes the sign of the superconducting gap function for the SCd [i.e., $\cos k$ in eq. (33c) (a)] and SCf [i.e., $\sin k, \cos k$ in eq. (33c) (b)] phases. The scattering processes for parallel and anti-parallel spins are described by a dashed arrow, while the long continuous arrows stand for the nesting vector. The sign of the renormalized coupling constants are also stated in each case considered. A sign change of the gap function following the scattering occurs for positive renormalized coupling constants, while the sign remains the same for attractive ones. Thus all the scattering processes shown in Fig. 13 gain the energy.

Figure 13 (a) depicts scattering processes with anti-parallel spins leading to the SCd state. The interaction with interchain momentum transfer $\pi$, i.e., the interband scatterings, give rise to the repulsive couplings among which $G_{21}(r,0,\pi)$ is the dominant contribution and $G_{11}(r,0,\pi)$ also becomes relevant, leading to the growth of spin fluctuations as explained after eq.
(38). The sign of the gap function changes in these scattering process. For the couplings $G_{2\perp(0,0,0)}$ and $G_{1\perp(0,0,0)}$, which become attractive through the renormalization, the sign of the gap function remains the same in the scattering process.

We now turn to the SCf state, where the relation between the sign change of the gap function and the forward scattering process with parallel spins is shown in Fig. 13 (b) (upper panel). For the repulsive $G_{f\parallel(\pi,0,\pi)}$, the gap function is opposite in sign, whereas the sign is the same for the attractive $G_{f\parallel(0,0,0)}$. The backward scattering shown in the lower (b) panel also favors the SCf state, since the signs of the respective coupling constants, $-G_{f\parallel(\pi,0,\pi)} < 0$ and $-G_{f\parallel(0,0,0)} > 0$, are consistent with the change of the sign in the gap function.

We now comment on the crossover from the SCd to SCf states as a function of $V_{b}^{f}$. The $V_{b}^{f}$ dependence of relevant coupling constants at low temperature ($T = 10^{-3}$) is shown in Figs. 14 (a) and (b), which correspond to the SCd and SCf cases, respectively. For the SCd state, the coupling $G_{1\perp(0,0,0)}$ evolves from negative to positive values, suggesting a vanishing spin gap. The resultant reduction of the SCd state by $V_{b}^{\perp}$ is reasonable because the interchain spin singlet state is destroyed by the formation of CDW state for moderate $V_{b}^{\perp}$. With increasing $V_{b}^{\perp}$, the repulsive interactions $G_{2\perp(\pi,0,\pi)}$ and $G_{1\perp(\pi,0,\pi)}$ decrease and the amplitude of the SCd correlation is reduced.

In Fig. 14 (b), the coupling $G_{f\parallel(\pi,0,\pi)}$ increases from zero, while the coupling $G_{f\parallel(0,0,0)}$ decreases to negative value. Negative $G_{f\parallel(0,0,0)}$ indicates the absence of spin gap. These features yield in turn the development of the SCf state, as a consequence of charge fluctuations and nesting. From Fig. 14 (b), the $V_{b}^{f}$ interval, where $G_{f\perp} > 0$, suggests that the spin gap vanishes for $V_{b}^{\perp} \sim V_{b}^{f}$. However, it is found that the SCf state moves to the CDW state by noting that $G_{f\perp} > 0$ for $V_{b}^{\perp} = 0.88$, and $G_{f\perp} < 0$ for $V_{b}^{\perp} = 0.92$.

Finally, we comment on the effect of $V_{b}^{\perp}$ on the SDW state. Within the conventional treatment of RPA, the interference effect between the scattering at different transverse momenta is neglected. For example, in eq. (9b), which is relevant to the SDW state, the onsite-repulsion $U$ is retained but the effect of $V_{b}^{\perp}$ is strongly reduced due to the summation of $k_{1} = \pm \pi$ and $k_{2} = \pm \pi$. However, the present RG method shows a clear effect of $V_{b}^{\perp}$ on SDW as illustrated by the strength of density-wave correlations in the $V_{b}^{\perp} - U$ plane at fixed $T$ (Fig. 15). The SDW and CDW regions are defined by the corresponding response functions that become larger than the bare value $\chi_{0}$ at $T = 0$ by a factor greater than $10^{6}$. The domain that separates the two regions shows a much reduced amplitude of the density-wave response functions, while its area reduces by the decrease of temperature. The region for

![Fig. 13](https://example.com/fig13.png)  
(Color online) Scattering processes giving rise to the SCd state (a) and SCf state (b). The Fermi surface is given by the line connecting the Fermi points (closed circle).

![Fig. 14](https://example.com/fig14.png)  
(Color online) The $V_{b}^{f}$ dependence of the renormalized coupling constants at $T = 10^{-3}$ for the SCd (a) and SCf (b) states, and for $G_{\sigma\perp}$. Here $t_{f}^{2} = 0.001t_{f}$ and $h = 0.0$. The initial values for $G_{1\perp(0,0,0)}$, $G_{1\perp(\pi,0,\pi)}$, $G_{2\perp(0,0,0)}$, $G_{2\perp(\pi,0,\pi)}$, $G_{1\parallel(0,0,0)}$, and $G_{1\parallel(\pi,0,\pi)}$, are respectively given by 0.45, 0.45, 0.45, 0.45, 0.00 and 0.00 for $V_{b}^{\perp} = 0$ and 0.72, 0.18, 0.45, 0.45, -0.27 and 0.27 for $V_{b}^{\perp} = 1.2$. The arrow represents $V_{b}^{\perp}$.
SDW is suppressed with increasing $V_{b}^\perp$ due to the increase of the charge fluctuations.

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Appendix: Two-loop level renormalization group

The renormalization of the interchain hopping $t_1$ is given by

$$\frac{d}{dt}t_1(l) = t_1(l) - \frac{1}{2N_\perp} \sum_{\mathbf{q},\mathbf{k},\mathbf{k}'\perp} G_{\Sigma_n(q,k,k')} J_0(q,k,k'),$$  

(A-1)

where the second term of the r.h.s. comes from interactions. Such an effect is negligibly small for the quarter-filled band although the strong effect is expected due to the Umklapp scattering for the half-filled band, e.g., the confinement of the interchain hopping.26,27

We show the results at the two-loop level in eq. (30). Applying the calculations already obtained at perfect nesting and half-filling24 to the case of the nesting deviation at quarter-filling, the self-energy and vertex corrections are

$$\Xi^{(2)}_{\Sigma_n(q,k,k')} = \sum_{\mathbf{q},\mathbf{k},\mathbf{k}'\perp} G^{(2)}_{\Sigma_n(q,k,k')} J_0(q,k,k'),$$  

(A-2a)

$$\Xi^{(2)}_{\Sigma_n(q,k,k')} = \sum_{\mathbf{q},\mathbf{k},\mathbf{k}'\perp} G^{(2)}_{\Sigma_n(q,k,k')} J_0(q,k,k'),$$  

(A-2a)

where $G^{(2)}_{\Sigma_n(q,k,k')}$ is given by

$$G^{(2)}_{\Sigma_n(q,k,k')} = G^2_{\Sigma_n(q,k,k')} = \sum_{v=1,2,\perp} G^2_{\Sigma_n(q,k,k')},$$  

(A-3)

and $J_0(q,k,k')$, $J_1(q,k,k')$ are given as follows. For $|\nu^p_{q,k,k',0}(l)| < E$,

$$J_0(q,k,k') = 2E \ln \left[ \frac{4E + \nu^p_{q,k,k',0}(l)}{4E - \nu^p_{q,k,k',0}(l)} \right],$$  

(A-4a)

$$J_1(q,k,k') = \frac{16E^2}{16E^2 - (\nu^p_{q,k,k',0}(l))^2},$$  

(A-4b)

For $|\nu^p_{q,k,k',0}(l)| > E$,

$$J_0(q,k,k') = 2E \ln \left[ \frac{4E + \nu^p_{q,k,k',0}(l)}{4E + \nu^p_{q,k,k',0}(l)} \right] \text{sgn}(\nu^p_{q,k,k',0}(l)),$$  

(A-5a)

$$J_1(q,k,k') = \frac{2E}{4E + |\nu^p_{q,k,k',0}(l)|} + \frac{2E}{2 + |\nu^p_{q,k,k',0}(l)|},$$  

(A-5b)

The quantity $J_2(q,k,k',k''\perp)$ is also given by

$$J_2(q,k,k',k''\perp) = \frac{1}{2} \left[ J_1(q,k,-k'',k''\perp) + J_1(q,k''-k',k''\perp) \right].$$  

(A-6)

In the present calculations carried out at the two-loop level, we treated nesting deviations as the dominant effect. The influence of magnetic field at that level remains to be examined. This will be the subject of a separate publication.
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