Time-reversal symmetry breaking superconductivity in the coexistence phase with magnetism in Fe-pnictides

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We argue that superconductivity in the coexistence region with spin-density-wave (SDW) order in weakly doped Fe-pnictides differs qualitatively from the ordinary $s^+$ state outside the coexistence region, as it develops an additional gap component which is a mixture of intra-pocket singlet ($s^+$) and inter-pocket spin-triplet pairings ($t$-state). The coupling constant for the $t$-channel is proportional to the SDW order and involves interactions that do not contribute to superconductivity outside of the SDW region. We argue that the $s^{+-}$ and $t$-type superconducting orders coexist at low temperatures, and the relative phase between the two is in general different than 0 or $\pi$, manifesting explicitly the breaking of the time-reversal symmetry promoted by long-range SDW order. We show that this exotic state emerges already in the simplest model of Fe-pnictides, with one hole pocket and two symmetry-related electron pockets. We argue that in some parameter range time-reversal gets broken even before long-range superconducting order develops.

Introduction

Iron-based superconductors (FeSCs) have been the subject of intense study since 2008. Their rich phase diagram includes the regions of superconductivity (SC), spin density wave (SDW), nematic order, and a region where SDW, SC, and nematic order coexist. Outside the SDW/nematic region, SC develops in the spin-singlet channel and in most of Fe-based superconductors has $s$-wave symmetry with a $\pi$ phase shift between the SC order parameters on hole and on electron pockets ($s^+$ gap structure). It has been recently argued by several groups that the multiband structure of FeSCs allows for superconducting states with more exotic properties. Of particular interest are SC states that break time-reversal symmetry (TRS), such as states with a plethora of interesting properties like, e.g., novel collective modes. TRS-broken states emerge when the phase differences $\psi_i$ between SC order parameters on different Fermi surfaces (FS) are not multiples of $\pi$.

The two current proposals for TRS breaking in FeSCs are $s + i\sigma_5 s$ and $s + i s$. The first emerges when attractions in the $d$-wave and $s$-wave channels are of near-equal strength. The second emerges when there is a competition between different $s^+$ states favored by inter-pocket and intra-pocket interactions. Both of these proposals were, however, argued to be applicable only to strongly hole or electron-doped FeSCs. For weakly/moderately doped FeSCs the common belief is that $s^+$ superconductivity is robust.

In this communication we argue that an exotic state which breaks TRS can emerge already at low doping, in a range where SC is known to emerge from a pre-existing SDW state. Previous works on SC in the coexistence region focused on the SDW-induced modification of the form of $s^+$ gap. We argue that there is another effect – SDW order also induces attraction in another pairing channel, for which the order parameter is an admixture of spin-singlet and spin-triplet components (the two are mixed in the SDW state since spin rotational symmetry is broken). Because a triplet component is involved, we will be calling this state as $t$-state. The coupling in the $t$-channel is a combination of interactions that do not contribute to $s^+$ SC in the paramagnetic state. A real admixture between these singlet and triplet SC states, $s \pm t$, has been discussed in the SDW/SC coexistence region of organics, cuprates, and heavy fermions. Here, however, we found that the situation is different – $s \pm t$ state exists only near $T_c$, while at low $T$, the relative phase between the two SC components is different from 0 or $\pi$, i.e., the order parameter has $s + e^{i\theta} t$ form. This order parameter does not transform into itself under TRS, unlike $s \pm t$ order. As a result, the order parameter manifold contains an additional $Z_2$ Ising degree of freedom, which gets broken by selection of $+\theta$ or $-\theta$. The TRS broken state emerges via a phase transition inside a superconductor, which should have experimental manifestations. We note in this regard that that, although TRS of the system is formally broken already at the SDW transition temperature $T_N > T_c$, the TR operation transforms one magnetic state into another state from the same $O(3)$ manifold, i.e., there is no additional $Z_2$ degree of freedom which one could associate with TRS. The $s^{+-}$ state also does not contain this extra degree of freedom simply because it transforms into itself under TRS. Only when $\theta$ becomes different from 0 or $\pi$, does the order parameter manifold acquire an additional $Z_2$ degree of freedom associated with TRS.

We show that the $s + e^{i\theta} t$ state emerges already in the simplest three-band model of one circular hole pocket and two symmetry-related elliptical electron pockets. Since SDW order in most of the range where SC and SDW coexist is of stripe type, the associated FS reconstruction involves only one hole and one electron pocket separated by either $(0, \pi)$ or $(\pi, 0)$ in the 1-Fe Brillouin zone, reducing the model to a two-pocket model.

The pairing interaction in the $t$-channel emerges once the original 4-fermion interactions for the two pockets connected by the SDW ordering vector are...
dressed up by SDW coherent factors. When the pairing interactions are rewritten in terms of $a$ and $b$ fermions, which describe states near the reconstructed FSs, they yield conventional terms like $a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger a_{-\mathbf{p}} a_{\mathbf{p}}$ or $a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger b_{-\mathbf{p}} b_{\mathbf{p}}$, and also anomalous terms like $a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger a_{-\mathbf{p}} a_{\mathbf{p}}$. As a consequence, spin-singlet pairing between FSs of the same kind ($i \sigma_{\alpha \beta}^y \langle a_{\mathbf{k}0} a_{-\mathbf{k}0} \rangle$ and $i \sigma_{\alpha \beta}^y \langle b_{\mathbf{k}0} b_{-\mathbf{k}0} \rangle$) mixes with spin triplet pairing between FSs of opposite type ($\sigma_{\alpha \beta}^x \langle a_{\mathbf{k}0} b_{-\mathbf{k}0} \rangle$). We show below that this gives rise to the emergence of two different superconducting channels. One is the usual spin-singlet $s^+$ channel, for which the SC order parameter is $\Delta_{s^+} \sim \sum_\mathbf{k} \langle a_{\mathbf{k}0} a_{-\mathbf{k}0} \rangle - \langle b_{\mathbf{k}0} b_{-\mathbf{k}0} \rangle$. If only this SC develops, the gaps on the two FSs have a phase difference $\pi$ (we define SC order parameters such that $\langle \mathbf{a} \rangle \propto \langle \mathbf{b} \rangle$). The other pairing channel, with order parameter $\Delta_2$, has two contributions. One is a spin-triplet inter-pocket term $\sum_\mathbf{k} \sigma_{\alpha \beta}^x \langle a_{\mathbf{k}0} b_{-\mathbf{k}0} \rangle$ (hence the name $t$ state), and the other is a spin-singlet $s^+$ type term $\sum_\mathbf{k} i \sigma_{\alpha \beta}^y \langle a_{\mathbf{k}0} a_{-\mathbf{k}0} \rangle + \langle b_{\mathbf{k}0} b_{-\mathbf{k}0} \rangle$. The presence of the $s^+$ component in $\Delta_2$ is crucial as with it the kernel in the gap equation for $\Delta_2$ is logarithmical (as it is for $\Delta_1$), implying that even a weak attraction in this channel gives rise to superconductivity. A similar situation emerges in Fe-pnictides with only electron pockets – the analog of $\langle ab \rangle$ term there is induced by hybridization.\(^{45}\)

The structure of $\Delta_1$ and $\Delta_2$ is shown in Figs. 1a and 1b. Our analysis of the non-linear gap equations for $\Delta_1$ and $\Delta_2$ shows that the two SC orders coexist in some parameter range, and the relative phase between the two is different than $0$ or $\pi$, in the general case when the two orders are linearly coupled in the Ginzburg-Landau (GL) functional, and equals to $\pm \pi/2$ for the special case when linear coupling is absent (Fig. 1b).

![Figure 1: The structure of gap functions in different SC states: (a) pure $s^+$ state, (b) pure $t^-$ state, (c) $s^+ + it^-$ state with $\pm \pi/2$ phase difference between the phases of $s^+$ and $t^-$ gaps. Operators $a$ and $b$ describe fermions near the reconstructed FSs.](image)

The model. We consider a three band model with $c$ fermions with momenta near the hole pocket at $(0, 0)$ and $f$ fermions near the electron pockets centered at $(0, \pi)$ and $(\pi, 0)$ in the 1-Fe Brillouin zone (Fig. 2).\(^{48, 49}\). The $c$ and $f$ fermions form circular and elliptical FSs, respectively, with dispersions given by $\xi_{\mathbf{k}c} = \mu_c - \frac{k^2}{2m_c}$ and $\xi_{\mathbf{k}f} = \mu_f + \frac{k^2}{2m_f} - \frac{k^2}{2m_e}$. Since the SDW state picks an ordering vector $\mathbf{Q}$, which is either $(0, \pi)$ or $(\pi, 0)$, one of the electron pockets does not participate in this order. We choose $\mathbf{Q} = (0, \pi)$ without loss of generality and effectively reduce the model to two bands. We follow earlier works\(^{50, 51}\) and consider five possible repulsive interactions in the band basis: inter-pocket, density-density, exchange, pair hopping, and intra-pocket interactions. The corresponding couplings are $U_1, U_2, U_3,$ and $U_4$, respectively. We present the interaction Hamiltonian in the Supplementary material (SM). All couplings are assumed to be already renormalized from their bare values by fermions with energies larger than the upper energy cutoff $\Lambda$. Without SDW, SC in this model arises only in the $s^+$ channel. The corresponding coupling is $U_3 - U_4$, and we assume that it is positive (attractive). The couplings $U_1$ and $U_2$ do not participate in SC pairing, but $U_1$ contributes to the coupling in the SDW channel $U_1 + U_3 > 0$, which for $U_1 > 0$ is larger than in SC channels, i.e., the system first develops SDW order upon lowering $T$, and superconductivity emerges from a pre-existing SDW state. RG studies found that the SC interaction gets larger as energy decreases in the RG flow.\(^{46, 47, 50, 51}\). Yet, at low dopings, the SDW order comes first and SC develops in the coexistence region with magnetism.

The self-consistent equation for the SDW order parameter $M$ and the reconstructed fermionic dispersions in the SDW state have been obtained before\(^{52}\). The quadratic Hamiltonian in terms of the new quasiparticles $a$ and $b$ is

$$H_0 = \sum_{\mathbf{k}} \left[ \xi_{\mathbf{k}c} a_{\mathbf{k}c}^\dagger a_{\mathbf{k}c} + \xi_{\mathbf{k}f} b_{\mathbf{k}f}^\dagger b_{\mathbf{k}f} \right],$$ (1)
where
\[ \xi_k^\pm = \delta_k - \sqrt{\xi_k^2 + M^2}, \]
\[ \xi_k^0 = \delta_k + \sqrt{\xi_k^2 + M^2}, \]
and we have expressed the original dispersions in terms of the linear combinations \( \delta_k = \frac{\xi_k^+ + \xi_k^-}{2} \) and \( \xi_k = \frac{\xi_k^+ - \xi_k^-}{2} \).

In general \( \delta_k = \delta_0 + \delta_2 \cos 2\theta \), where the first term measures the doping (\( \delta_0 = 0.5v_F(k_F^x - k_F^y) \)) and the second one accounts for the (weak) ellipticity of the electron pocket (Ref. [22]). The coherence factors \( u_k \) and \( v_k \) are expressed in terms of these parameters as \( u_k = \sqrt{\frac{1}{2} \left( 1 + \frac{\delta_k}{\sqrt{\xi_k^2 + M^2}} \right)} \). (See SM.) The FSs for \( a \) and \( b \) fermions are shown in Fig. 2.

**Superconductivity.** We now consider the pairing interactions leading to SC inside the SDW state. As a first step, we rewrite the interactions in terms of the new fermions. We then find conventional pairing terms like \( a_{k1}^\dagger a_{-k1}^\dagger a_{p1} b_{p1} \) or \( a_{k1}^\dagger a_{-k1}^\dagger a_{-p1} b_{p1} \), and anomalous terms like \( a_{k1}^\dagger a_{k1} a_{p1} b_{p1} \) and \( a_{-k1}^\dagger a_{-p1} b_{p1} \). To solve for the SC order parameter, we then need to introduce both spin-singlet pairings \( i^{\alpha} \bar{\sigma}_{\alpha\beta} a_{k\alpha} b_{-k\beta} \) and \( i^{\alpha} \bar{\sigma}_{\alpha\beta} b_{k\alpha} a_{-k\beta} \) between fermions belonging to the same pocket, and spin triplet pairing \( \sigma_{\alpha\beta}^{\alpha} a_{k\alpha} b_{-k\beta} \) between fermions belonging to different pockets.

The full pairing Hamiltonian in the BCS approximation has the form
\[ \mathcal{H}_\Delta = \frac{1}{2} \sum_p \Delta_{aa}(p) i^{\alpha} \bar{\sigma}_{\alpha\beta} a_{p\alpha}^\dagger a_{-p\beta} \]
\[ + \frac{1}{2} \sum_p \Delta_{bb}(p) i^{\alpha} \bar{\sigma}_{\alpha\beta} b_{p\alpha}^\dagger b_{-p\beta} \]
\[ + \frac{1}{2} \sum_p \Delta_{ab}(p) \sigma_{\alpha\beta}^{\alpha} a_{p\alpha}^\dagger b_{-p\beta} - \bar{\sigma}_{\alpha\beta}^\dagger b_{p\alpha}^\dagger a_{-p\beta} - \text{H.c.} \]

Because there are three different anomalous terms, the diagonalization of the pairing Hamiltonian leads to a set of three coupled equations for \( \Delta_{aa}, \Delta_{bb}, \) and \( \Delta_{ab} \). Parameterizing \( \Delta_{ij} \) as
\[ \Delta_{aa,bb}(p) = \pm \Delta_1 + \Delta_2 (2u_p^2 v_p^2) + \Delta_3 (u_p^2 - v_p^2), \]
\[ \Delta_{ab}(p) = \Delta_2 (2u_p^2 - v_p^2) - \Delta_3 (2u_p^2 v_p^2), \]
we express the equations for SC order parameters as
\[ \Delta_1 = \frac{U_3 - U_4}{2} \sum_k [\langle aa \rangle_k - \langle bb \rangle_k], \]
\[ \Delta_2 = (U_2 - U_1) \sum_k [u_k v_k (\langle aa \rangle_k + \langle bb \rangle_k) + (u_k^2 - v_k^2) \langle ab \rangle_k], \]
\[ \Delta_3 = -\frac{U_3 + U_4}{2} \sum_k [(u_k^2 - v_k^2) (\langle aa \rangle_k + \langle bb \rangle_k) - 4u_k v_k \langle ab \rangle_k]. \]

where \( \langle aa \rangle_k \pm \langle bb \rangle_k = \frac{\Delta_{aa}(k)}{2\xi_k^0} \tanh \frac{\xi_k^0}{2T} \pm \frac{\Delta_{bb}(k)}{2\xi_k^0} \tanh \frac{\xi_k^0}{2T} \]
\[ \langle ab \rangle_k = \frac{\Delta_{ab}(k)}{2(\xi_k^0 + \xi_k^0)} \left( \tanh \frac{\xi_k^0}{2T} + \tanh \frac{\xi_k^0}{2T} \right). \]

where \( \Delta_{ij} \) are expressed via \( \Delta_i \) by Eq. [10]. Substituting [11] into the r.h.s. of [7] we obtain the set of three coupled linearized Eqs. on \( \Delta_i \) which can be easily solved.

To understand the physics, we first focus on the case of “maximally-nested” FSs, where \( \delta_0 = 0 \) but \( \delta_2 \neq 0 \),

Figure 3: Schematic phase diagram of a superconductor in coexistence with SDW. (a) The special case when \( s \) and \( t \) order parameters do not couple linearly (nested FSs), (b) The general case when \( s \) and \( t \) superconducting components couple linearly (non-nested FSs). While in the \( s \)-phase superconductivity has only a singlet component, in the \( s+t \) phase both singlet and triplet components are present but TRS is not broken. In the \( s + e^{i\theta} t \) and \( s + it \) phases (\( \theta = \pi/2 \)), the relative phase between the \( s \) and \( t \) components is frozen at \( 0 < \theta < \pi \) and TRS is broken, together with the U(1) symmetry of the global phase. In the TRSB phase, only TRS is broken. This phase is likely present in the generic case but its boundaries are not known and we do not show it.
i.e. $\xi_k^b$ becomes $-\xi_k^a$ under a rotation by 90 degrees. We found that this symmetry decouples the three linearized gap equations for $\Delta_1$, which become

$$\Delta_1 \left[ 1 - \frac{U_3 - U_4}{2} N_F \int X_k \right] = 0 \quad (11)$$

$$\Delta_2 \left[ 1 - (U_2 - U_1) N_F \int \left( (u_k^a v_k^a) X_k + (u_k^b - v_k^b)^2 Y_k \right) \right] = 0$$

$$\Delta_3 \left[ 1 + \frac{U_3 + U_4}{2} N_F \int \left( (u_k^a - v_k^a)^2 X_k + 8 u_k^b v_k^b Y_k \right) \right] = 0$$

where $N_F$ is the density of states at the FS, $f = \int d\xi \frac{\xi}{2\pi}$, and $u_k^a v_k^a = M/(2\sqrt{M^2 + \xi_k^a})$ and $u_k^b - v_k^b = \xi_k/\sqrt{M^2 + \xi_k}$, and

$$X_k = \frac{\tanh \xi_k^a}{\xi_k^a} \ , \quad Y_k = \frac{\tanh \xi_k^a + \tanh \xi_k^b}{2(\xi_k^a + \xi_k^b)} \quad (12)$$

The first and the last Eqs. (11) have familiar forms for $s^+$ and $s^+$ superconductivity, respectively\cite{footnote}. For positive $U_1$, the $s^+$ channel is repulsive, but $s^+$ superconductivity develops at $T = T_{c1}$ if $U_3 - U_4$ is positive. The momentum integral $\int X_k$ is logaritmically singular, as expected in BCS theory, hence $T_{c1}$ is non-zero already at weak coupling. The second Eq. in (11) is the gap equation in the new pairing channel. In the presence of SDW the kernel in this channel is also logaritmically singular due to the contribution from $(aa)_k + (bb)_k$. Hence, if $U_2 - U_1$ is positive, the $t$-channel becomes unstable towards pairing at a non-zero $T_{c2}$. Once $\Delta_2$ becomes non-zero, it induces a non-zero inter-packet pairing component $(ab)_k$, which, due to the folding of the Brillouin zone imposed by SDW order, $k + Q \rightarrow k$, has zero center-of-mass momentum.

$s + i t$ state with broken time-reversal symmetry

As it is customary for competing SC orders, the order which develops first tends to suppress the competitor by providing negative feedback to the gap equation for the competing order\cite{footnote}. Yet, if the repulsion between the competing SC orders is not too strong, the two orders coexist at low enough temperatures. The issue then is what is the relative phase between the two $U(1)$ order parameters $\Delta_1$ and $\Delta_2$. To address this issue we derived by standard means\cite{footnote} the GL Free energy, $F(\Delta_1, \Delta_2)$ (see SM). To fourth order in $\Delta_1, 2$ we obtained

$$F(\Delta_1, \Delta_2) = \alpha_1 |\Delta_1|^2 + \alpha_2 |\Delta_2|^2 + \beta_1 |\Delta_1|^4 + \beta_2 |\Delta_2|^4$$

$$+ 2\gamma_1 |\Delta_1|^2 |\Delta_2|^2 + \gamma_2 (\Delta_1^2 (\Delta_2^*)^2 + (\Delta_1^*)^2 \Delta_2^2)$$

(13)

where $\beta_1$ and $\beta_2$ are positive. The two orders coexist when $\beta_1 \beta_2 > (\gamma_1 - \gamma_2)^2$. This condition can be satisfied in the presence of disorder\cite{footnote,footnote}. The relative phase $\theta$ between $\Delta_1 = |\Delta_1|e^{i\psi + \theta/2}$ and $\Delta_2 = |\Delta_2|e^{i\psi - \theta/2}$ is determined by the sign of the $\gamma_2$ term in (13). We found that $\gamma_2$ is positive:

$$\gamma_2 = \sum_{k} (2u_k v_k)^2 \left[ \frac{1}{\xi_k^b} \right]^3 \left[ 1 + \frac{1}{\xi_k^b} \right]^3$$

(14)

Minimization of Eq. (13) then shows that $\theta = \pm \pi/2$. Because $\theta = \pi/2$ and $\theta = -\pi/2$ are different states, the system spontaneously breaks the $Z_2$ TRS. In the TRS-broken state, the phases of the order parameters $(aa)_k$ and $(bb)_k$ are $\phi$ and $-\phi$, where $0 < \phi < \pi/2$. The third gap, which is generally required to satisfy the set of complex gap equations in TRS-broken state is provided by $(ab)_k$, whose phase in this situation is $-\pi/2$. We show the gap structure schematically in Fig. 1 where we associated $(ij)_k$ with vectors, whose directions are set by the phases. We also performed Hubbard-Stratonovich analysis beyond mean-field level\cite{footnote}, by allowing the phases of $\Delta_1, 2$ to fluctuate, and found (see SM) that when $T_{c2} \approx T_{c_1} \approx T_c$, the system breaks TRS and sets the relative phase $\theta = \pi/2$ at a temperature $T > T_c$. In between $T^*$ and $T_c$, TRS is broken, but the $U(1)$ symmetry associated with the global phase of $\Delta_1$ and $\Delta_2$ remains intact. At $T_c$, the global phase is broken and both SC orders develop simultaneously. A schematic phase diagram is shown in Fig. 3b.

$s + e^{i\theta} t$ state

So far we considered the “maximally-” nested case, with $\delta_0 = 0$. For the more generic case $\delta_0 \neq 0$ we find that the GL functional (13) contains a bilinear coupling between the two SC states, i.e. a term $\alpha_3 (\Delta_1^2 + \Delta_2^2)$ with $\alpha_3 < 0$ (details in the SM). In this situation, the onset of the $s^+$ state at $T_{c1}$ necessarily triggers the emergence of a $t$ state. The relative phase between the two order parameters at $T \leq T_{c1}$ is $\theta = 0$, i.e., the state is $s + t$. Yet, the SC state still breaks TRS at a lower temperature $T_{c3} < T_{c1}$. Indeed, comparing the $\alpha_3 (\Delta_1^2 + \Delta_2^2)$ and $\gamma_2 (\Delta_1^2 (\Delta_2^*)^2 + (\Delta_1^*)^2 \Delta_2^2)$ terms in the GL functional we immediately see that $\theta = 0$ only as long as $\Delta_1^2 + \alpha_3 < \Delta_2^2$ once the temperature is reduced and $\Delta_1, 2$ grow, this condition breaks down at $T = T_{c3}$, and at lower $T$ the minimum of the GL functional shifts to $\theta \neq 0$. Once this happens, the SC state becomes $s + e^{i\theta} t$ and TRS gets broken. A schematic phase diagram is shown in Fig. 3b.

Conclusions

In this paper we argued that a SC state, which explicitly breaks TRS, appears when SC emerges from a pre-existing SDW-ordered state. We found that in the presence of SDW, the spin-triplet channel with inter-packet pairing couples to spin-singlet intra-pocket pairings on the reconstructed FSs. This leads to the emergence of a new pairing channel, which we labeled as $t$-pairing to emphasize that it involves spin-triplet. We analyzed the interplay between $s^+$ and $t$- SC orders and showed that they coexist at low $T$ with a relative phase $0 < \theta < \pi$. As a result, the phases of the gaps on different FSs differ by less than a multiple of $\pi$. Such a state breaks time-reversal symmetry and has been long studied in the studies of FeSCs. We argued that in a generic case TRS gets broken in the SC manifold at temperatures lower than $T_{c}$. This should give rise to features in experimentally probed thermodynamic quantities.

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I. SUPPLEMENTARY MATERIAL

In the Supplementary Material we discuss some technical details of the analysis presented in the main text.

A. Interaction Hamiltonian

We include all five possible repulsive interactions in the band basis

\[ \mathcal{H}_{\text{int}} = U_1 \sum c_{p_1 \sigma} \hat{c}_{p_1 \sigma}^\dagger \hat{f}_{p_2 \sigma'} c_{p_2 \sigma'} + U_2 \sum f_{p_3 \sigma} c_{p_3 \sigma}^\dagger \hat{f}_{p_3 \sigma'} c_{p_3 \sigma'} + \frac{U_3}{2} \sum f_{p_3 \sigma}^\dagger \hat{f}_{p_3 \sigma'}^\dagger c_{p_3 \sigma} c_{p_3 \sigma'} + H.c. \],

(15)

The momentum conservation is implicit and \( \sigma \neq \sigma' \) in all sums. The first three are inter-pocket density-density, exchange, and pair hopping, interactions, respectively (all positive), while the last two are intra-pocket repulsions. For simplicity, we set \( U_4 = U_5 \) below. All couplings are assumed to be already renormalized from their bare values by fermions with energies larger than the upper energy cutoff \( \Lambda \).

B. SDW state

In order to introduce the SDW order starting from the paramagnetic state we first write the quadratic part of the Hamiltonian in the mean-field approximation, where the order parameter \( M \) is defined as

\[ M = -\frac{U_1 + U_3}{2} \sum p \sigma \sigma' \langle \hat{c}_{p \sigma}^\dagger \hat{f}_{p \sigma} \rangle , \]

(16)

Then we perform the following Bogoliubov transformation to bring it to diagonal form:

\[ \hat{c}_{k \sigma} = u_k a_{k \sigma} + v_k \sigma \hat{c}_{k \sigma}^\dagger b_{k \sigma} , \]

(17)

\[ \hat{f}_{k \sigma} = u_k b_{k \sigma} - v_k \sigma \hat{c}_{k \sigma}^\dagger a_{k \sigma} . \]

(18)

C. Gap equations

In order to carry out the diagonalization of the mean-field Hamiltonian (12) we apply the following Bogoliubov transformation, introducing new quasiparticle operators \( \alpha \) and \( \beta \):

\[ a_{k \mu} = u_k^\alpha a_{k \mu} + v_k^\alpha \sigma \hat{c}_{k \mu}^\dagger \beta_{k \mu} + g_k^\alpha \sigma \hat{c}_{k \mu}^\dagger \beta_{k \mu} + h_k^\alpha \sigma \hat{c}_{k \mu}^\dagger \beta_{k \mu} , \]

(19)

\[ b_{k \mu} = u_k^\beta \sigma a_{k \mu} + v_k^\beta \sigma \hat{c}_{k \mu}^\dagger \beta_{k \mu} + g_k^\beta \sigma \hat{c}_{k \mu}^\dagger \beta_{k \mu} + h_k^\beta \sigma \hat{c}_{k \mu}^\dagger \beta_{k \mu} . \]

(20)

As a result, we obtain a quadratic Hamiltonian

\[ \mathcal{H} = \sum_{k, \mu} \left[ E_k^\alpha \alpha_{k \mu} a_{k \mu} + E_k^\beta \beta_{k \mu} a_{k \mu} \right] \]

(21)

and new quasiparticle dispersions

\[ E_k^{\alpha, \beta} = \sqrt{A_k \pm \sqrt{B_k}} , \]

(22)

where

\[ A_k = \frac{(\xi_k^\alpha)^2 + (\xi_k^\beta)^2}{2} + |\Delta_1|^2 + |\Delta_2|^2 + |\Delta_3|^2 , \]

(23)

\[ B_k = \left[ (\xi_k^\alpha)^2 - (\xi_k^\beta)^2 \right]^2 + \left[ (\xi_k^\alpha)^2 - (\xi_k^\beta)^2 \right] \left[ t((\Delta_1 \Delta_3^* + \Delta_2^* \Delta_3) + s(\Delta_1 \Delta_2^* + \Delta_3^* \Delta_3)) \right] + \left[ (\xi_k^\alpha - \xi_k^\beta)^2 \right] \left( t\Delta_2 - s\Delta_3 \right) \left( t\Delta_2^* - s\Delta_3^* \right) + (\Delta_1 \Delta_2^* + \Delta_2 \Delta_3^*)^2 + (\Delta_1 \Delta_3^* + \Delta_3 \Delta_2^*)^2 - (\Delta_2 \Delta_3^* - \Delta_3 \Delta_2)^2 , \]

(24)

and we have defined \( s = \frac{M}{\sqrt{M^2 + \xi_k^2}} \) and \( t = \frac{\xi_k}{\sqrt{M^2 + \xi_k^2}} \).
The gap equations can be found by starting with the expressions for the order parameters,

\[ \Delta_1 = \frac{U_3 - U_4}{2} \sum_k \left[ (aa)_k - (bb)_k \right], \]

(25)

\[ \Delta_2 = (U_2 - U_1) \sum_k \left[ u_k v_k (aa)_k + (bb)_k \right] - u_k^2 v_k (ab)_k, \]

(26)

\[ \Delta_3 = -\frac{U_3 + U_4}{2} \sum_k \left[ (v_k^2 - u_k^2) (aa)_k + (bb)_k \right] - 4u_k v_k (ab)_k, \]

(27)

and substituting the following expressions for the averages \((ij)\):

\[ (aa)_k - (bb)_k = -(u_k^2 v_k^2 + g_k^0 h_k^0) (1 - 2n_F(E_k^0)) \]

\[ + \left( u_k^2 v_k^2 + g_k^0 h_k^0 \right) (1 - 2n_F(E_k^0)), \]

\[ (aa)_k + (bb)_k = -u_k v_k (1 - n_F(E_k^0)) - v_k^2 g_k^0 n_F(E_k^0) \]

\[ + u_k^2 h_k^0 n_F(E_k^0) - v_k^2 g_k^0 (1 - n_F(E_k^0)^2), \]

\[ (ab)_k = u_k v_k (1 - n_F(E_k^0)) - v_k^2 g_k^0 n_F(E_k^0) \]

\[ + u_k^2 h_k^0 n_F(E_k^0) - v_k^2 g_k^0 (1 - n_F(E_k^0)^2), \]

(30)

where \(n_F\) is the Fermi distribution function.

The coherence factors are given by

\[ \left( u_k^a, v_k^a, g_k^a, h_k^a \right) = \frac{(U_k^a, V_k^a, G_k^a, H_k^a)}{\sqrt{[U_k^a]^2 + [V_k^a]^2 + [G_k^a]^2 + [H_k^a]^2}}, \]

(31)

\[ \left( u_k^b, v_k^b, g_k^b, h_k^b \right) = \frac{(U_k^b, V_k^b, G_k^b, H_k^b)}{\sqrt{[U_k^b]^2 + [V_k^b]^2 + [G_k^b]^2 + [H_k^b]^2}}, \]

(32)

where

\[ U_k^a = [E_k^a + \xi_k^a] \left[ -\Delta_1^2 - \Delta_2^2 + s(\Delta_1 \Delta_2 + \Delta_1^2 \Delta_2) \right] \]

\[ + t(\Delta_1 \Delta_3^2 + \Delta_2 \Delta_3) \]

\[ + t(\xi_k^a - \xi_k^b) [t|\Delta_2|^2 - t|\Delta_3|^2 + s(\Delta_2 \Delta_3^2 + \Delta_2^2 \Delta_3)] \]

\[ + [E_k^a + \xi_k^b] [E_k^a + \xi_k^b] [E_k^a - \xi_k^a] - |\Delta_3|^2 \]

(33)

\[ U_k^b = [E_k^b + \xi_k^b] \left[ -\Delta_1^2 - \Delta_2^2 - s(\Delta_1 \Delta_2 + \Delta_1^2 \Delta_2) \right] \]

\[ - t(\Delta_1 \Delta_3^2 + \Delta_2 \Delta_3) \]

\[ + t(\xi_k^b - \xi_k^a) [t|\Delta_2|^2 - t|\Delta_3|^2 + s(\Delta_2 \Delta_3^2 + \Delta_2^2 \Delta_3)] \]

\[ + [E_k^b + \xi_k^a] [E_k^b + \xi_k^b] [E_k^b - \xi_k^b] - |\Delta_3|^2 \]

(34)

\[ V_k^a = [-E_k^a]^2 + (\xi_k^a)^2] [-\Delta_1 + s \Delta_2 + t \Delta_3] \]

\[ + [\Delta_1^2 - \Delta_2^2 - \Delta_3^2] [-\Delta_1^* - s \Delta_2 - t \Delta_3^*] \]

(35)

\[ V_k^b = [-E_k^b]^2 + (\xi_k^b)^2] [-\Delta_1 + s \Delta_2 + t \Delta_3] \]

\[ + [\Delta_1^2 - \Delta_2^2 - \Delta_3^2] [-\Delta_1^* - s \Delta_2 - t \Delta_3^*] \]

(36)

\[ G_k^a = [E_k^a + \xi_k^a] [t \Delta_1 \Delta_2^* - \Delta_1 \Delta_3^* + \Delta_2 \Delta_3^*] \]

\[ + [E_k^a + \xi_k^a] [t \Delta_1^* \Delta_2 - \Delta_1 \Delta_3^* - \Delta_2^* \Delta_3] \]

\[ + t(\xi_k^a - \xi_k^b) [s(-|\Delta_2|^2 + |\Delta_3|^2) - t(\Delta_2 \Delta_3^* + \Delta_2^* \Delta_3)] \]

(37)

\[ G_k^b = [E_k^b + \xi_k^b] [E_k^a - \xi_k^b] [t \Delta_1 - s \Delta_2 + t \Delta_3] \]

\[ + [E_k^b + \xi_k^b] [t \Delta_1^* \Delta_2 - s \Delta_1 \Delta_3 - \Delta_2^* \Delta_3] \]

\[ + t(\xi_k^b - \xi_k^a) [s(-|\Delta_2|^2 + |\Delta_3|^2) - t(\Delta_2 \Delta_3^* + \Delta_2^* \Delta_3)] \]

(38)

\[ H_k^a = [E_k^a + \xi_k^a] [E_k^a - \xi_k^a] [t \Delta_2 - s \Delta_3] \]

\[ + [\Delta_1^2 - \Delta_2^2 - \Delta_3^2] [t \Delta_2^* - s \Delta_3^*] \]

(39)

\[ H_k^b = [E_k^b + \xi_k^b] [E_k^b - \xi_k^b] [-t \Delta_2 + s \Delta_3] \]

\[ + [\Delta_1^2 - \Delta_2^2 - \Delta_3^2] [-t \Delta_2^* + s \Delta_3^*] \]

(40)

The expansion of the gap equations to linear order in \(\Delta_i\) yields

\[ \Delta_1 = \frac{U_3 - U_4}{2} \sum_k \left\{ \Delta_1 \left[ \frac{\tanh(\xi_k^a/(2T))}{2\xi_k^a} \right] + (a \to b) \right\} \]

(41)

\[ + \Delta_2 \left[ \frac{\tanh(\xi_k^a/(2T)) + \tanh(\xi_k^b/(2T))}{2(\xi_k^a + \xi_k^b)} \right] \]

\[ + \Delta_3 \left[ \frac{\tanh(\xi_k^a/(2T))}{2\xi_k^a} \right] \]

(42)

\[ \Delta_2 = (U_2 - U_1) \sum_k \left\{ \Delta_2 \left[ \frac{s^2}{2} \frac{\tanh(\xi_k^a/(2T))}{2\xi_k^a} \right] + (a \to b) \right\} \]

\[ + \Delta_2 t^2 \left[ \frac{\tanh(\xi_k^a/(2T)) + \tanh(\xi_k^b/(2T))}{2(\xi_k^a + \xi_k^b)} \right] \]

\[ + \Delta_3 \left[ \frac{\tanh(\xi_k^a/(2T))}{2\xi_k^a} \right] \]

(43)
D. Coexistence of superconducting orders

We present the conditions that are necessary for the coexistence of the $\Delta_1$ and $\Delta_2$ orders. We begin by listing the full expressions for all the coefficients of the free energy.

$$F(\Delta_1, \Delta_2) = \alpha_1|\Delta_1|^2 + \alpha_2|\Delta_2|^2 + \alpha_3(\Delta_1^2 + \Delta_1^2\Delta_2) + \beta_1|\Delta_1|^4 + \beta_2|\Delta_2|^4 + 2\gamma_1|\Delta_1|^2|\Delta_2|^2 + \gamma_2[(\Delta_1^2)^2 + (\Delta_1^2\Delta_2^2)]$$

(44)

$$\alpha_1 = -\frac{1}{2} \sum_k \left[ \frac{1}{|\xi_k^a|^2} + \frac{1}{|\xi_k^b|^2} \right] + \frac{2}{U_3 - U_4},$$

(45)

$$\alpha_2 = -\frac{1}{2} \sum_k s^2 \left[ \frac{1}{|\xi_k^a|^2} + \frac{1}{|\xi_k^b|^2} \right] - \sum_k t^2 \text{sgn} \xi_k^a + \text{sgn} \xi_k^b + \frac{2}{U_2 - U_1},$$

(46)

$$\alpha_3 = -\frac{1}{2} \sum_k s \left[ \frac{1}{|\xi_k^a|^3} - \frac{1}{|\xi_k^b|^3} \right],$$

(47)

$$\beta_1 = \frac{1}{8} \sum_k \left[ \frac{1}{|\xi_k^a|^3} + \frac{1}{|\xi_k^b|^3} \right],$$

(48)

$$\beta_2 = \frac{1}{8} \sum_k s^4 \left[ \frac{1}{|\xi_k^a|^3} + \frac{1}{|\xi_k^b|^3} \right] + \sum_k t^4 \left[ \text{sgn} \xi_k^a + \text{sgn} \xi_k^b \right],$$

(49)

$$\gamma_1 = \gamma_2 + \frac{1}{4} \sum_k s^2 \left[ \frac{1}{|\xi_k^a|^3} + \frac{1}{|\xi_k^b|^3} \right] + \frac{1}{4} \sum_k t^2 \left[ \frac{\text{sgn} \xi_k^a}{(\xi_k^a)^2(\xi_k^a + \xi_k^b)} + \frac{\text{sgn} \xi_k^b}{(\xi_k^b)^2(\xi_k^a + \xi_k^b)} \right],$$

(50)

$$\gamma_2 = \frac{1}{8} \sum_k s^2 \left[ \frac{1}{|\xi_k^a|^3} + \frac{1}{|\xi_k^b|^3} \right] + \frac{1}{8} \sum_k (\xi_k^a)^2 - (\xi_k^b)^2 \left[ \frac{1}{|\xi_k^a|^3} + \frac{1}{|\xi_k^b|^3} \right].$$

(51)

The largest contribution to these integrals comes from the regions around $\xi_k^a = 0$ and $\xi_k^b = 0$ (the SDW FSs), where the denominators become zero. This singularity is caused by calculating the coefficients at $T = 0$ and is removed by including a small cutoff at those points. One may think that the regions where $\xi_k^a + \xi_k^b = 0$ are also singular but in each case the integrand is actually finite. Thus the main contributions to the coefficients $\beta_i$ and $\gamma_i$ are the integrals with $|\xi_k^{a,b}|^{-3}$. All of these are positive definite so $\beta_i > 0$ and $\gamma_i > 0$.

In the case of $\delta_0 = 0$ the coefficient $\alpha_3$ vanishes, so the order parameters decouple at linear order. To determine whether coexistence occurs we search for minima of the free energy where both parameters are non-zero. First note that the remaining terms depend only on $|\Delta_1|^2$ and $|\Delta_2|^2$, except for the term with coefficient $\gamma_2$. Since $\gamma_2 > 0$, the minimum value of this term is $-2\gamma_2|\Delta_1|^2|\Delta_2|^2$, which corresponds to a phase difference between $\Delta_1$ and $\Delta_2$ of $\pm \pi/2$. After we fix this phase, partial differentiation with respect to $|\Delta_1|^2$ and $|\Delta_2|^2$ yields the following critical points:

$$|\Delta_1|^2 = \frac{\alpha_2(\gamma_1 - \gamma_2) - \alpha_1\beta_2}{2(\beta_1\beta_2 - (\gamma_1 - \gamma_2)^2)},$$

(52)

$$|\Delta_2|^2 = \frac{\alpha_1(\gamma_1 - \gamma_2) - \alpha_2\beta_1}{2(\beta_1\beta_2 - (\gamma_1 - \gamma_2)^2)}.$$  

(53)

We then perform the second partial derivative test to find a necessary condition for the existence of local minima. This condition is

$$\beta_1\beta_2 > (\gamma_1 - \gamma_2)^2.$$  

(54)

In addition, we require that the expressions for $|\Delta_1|^2$ and $|\Delta_2|^2$ be positive, which implies

$$\alpha_2(\gamma_1 - \gamma_2) - \alpha_1\beta_2 > 0,$$

(55)

$$\alpha_1(\gamma_1 - \gamma_2) - \alpha_2\beta_1 > 0.$$  

(56)

Coexistence will occur if and only if all three inequalities are satisfied.

E. Preemptive TRS breaking above $T_c$

In this section we show our Hubbard-Stratonovich analysis beyond mean-field level. We take the Ginzburg-Landau free energy as an effective action and study the case where $\delta_0 = 0$ and the critical temperatures $T_{c1} \approx T_{c2}$. We consider an action of the form

$$S(\Delta_1, \Delta_2) = \alpha(|\Delta_1|^2 + |\Delta_2|^2) + \beta_1(|\Delta_1|^2 + |\Delta_2|^2) - \beta(|\Delta_1|^2 - |\Delta_2|^2)^2$$

$$+ \gamma (\Delta_1^2 - \Delta_1^2\Delta_2^2)$$

(57)

where $\alpha = \alpha(T - T_c)$ and $\alpha, \beta_1, \beta_2$, and $\gamma$ are positive. Then we apply a Hubbard-Stratonovich transformation to this action by introducing collective variables $\Phi, \Psi, \Upsilon,$ and $\Gamma$, which are conjugate to $(|\Delta_1|^2 + |\Delta_2|^2)^2$, $(|\Delta_1|^2 - |\Delta_2|^2)^2$, and $(\Delta_1\Delta_2^* - \Delta_1^*\Delta_2)^2$, respectively. By integrating out the fields $\Delta_1$ and $\Delta_2$ we obtain an effective action

$$S(\Phi, \Psi, \Gamma) = \frac{\tilde{\alpha}^2}{4\beta_1} + \frac{\Psi^2}{4\beta} + \frac{\Gamma^2}{4\gamma} + \int \frac{d^2q}{(2\pi)^2} \log \left[ (\alpha - i\Phi + q^2)^2 - \Psi^2 - \Gamma^2 \right],$$

(58)

where we included the usual $q^2$ dispersion in the quadratic term by replacing $\alpha$ by $\alpha + q^2$. 
Now we search for local minima of this action by differentiating with respect to the three fields, obtaining a set of coupled equations. The solution requires \( \Phi \) to be purely imaginary, that is \( \Phi = i\Phi \). The set of equations becomes

\[
\Phi = 4\beta_1 \int \frac{d^2 q}{(2\pi)^2} \frac{\alpha + \Phi + q^2}{(\alpha + \Phi + q^2)^2 - \Upsilon^2 - \Gamma^2},
\]

\[
\Upsilon = 4\beta \int \frac{d^2 q}{(2\pi)^2} \frac{\Upsilon}{(\alpha + \Phi + q^2)^2 - \Upsilon^2 - \Gamma^2},
\]

\[
\Gamma = 4\gamma \int \frac{d^2 q}{(2\pi)^2} \frac{\Gamma}{(\alpha + \Phi + q^2)^2 - \Upsilon^2 - \Gamma^2}.
\]

Note that \( \Gamma \) and \( \Upsilon \) cannot simultaneously be nonzero as a solution to these equations except in the special case of \( \beta = \gamma \).

We first consider the solution with \( \Gamma = \Upsilon = 0 \), which yields

\[
\Phi = \frac{\beta_1}{\pi} \log \frac{\Lambda}{|\alpha + \Phi|},
\]

where \( \Lambda \) is an upper cutoff for the momentum integral. By expanding the action about this solution we find that it is stable as long as \( \alpha > \max(\alpha_{cr1}, \alpha_{cr2}) \), where

\[
\alpha_{cr1} = \frac{\gamma}{\pi} - \frac{\beta_1}{\pi} \log \frac{\pi \Lambda}{\gamma},
\]

\[
\alpha_{cr2} = \frac{\beta}{\pi} - \frac{\beta_1}{\pi} \log \frac{\pi \Lambda}{\beta}.
\]

This condition is equivalent to \( T > T^* \) where \( T^* = T_c + \max(\alpha_{cr1}, \alpha_{cr2})/a \). Whichever is greater between \( \gamma \) and \( \beta \) determines this critical temperature. Then if \( \gamma > \beta \) (\( \gamma < \beta \)) the field \( \Gamma (\Upsilon) \) will develop a nonzero solution and the other one will remain zero. When we calculate \( \beta \) and \( \gamma \) in terms of the original coefficients of the Ginzburg-Landau free energy we find that indeed \( \gamma > \beta \). This means that a preemptive order forms at a temperature above the critical temperature, where time-reversal symmetry is broken before the gaps acquire nonzero mean-field values.

This can be verified by solving the set of equations for \( \Gamma \neq 0 \). Expanding at small \( \Gamma \) we find that

\[
\Gamma^2 \left( \frac{\beta_1}{\gamma} - 2 \right) \propto (T^* - T),
\]

which means that if \( \beta_1 > 2\gamma \) (which is satisfied in our case) then \( \Gamma \) gradually increases as \( T \) becomes smaller than \( T^* \), as expected for a second-order transition.