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# Inter-pocket pairing and gap symmetry in Fe-based superconductors with only electron pockets

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We analyze the pairing symmetry in Fe-based superconductors  $\text{AFe}_2\text{Se}_2$  ( $A = \text{K, Rb, Cs}$ ) which contain only electron pockets. We argue that the pairing condensate in such systems contains not only intra-pocket component, but also inter-pocket component, made of fermions belonging to different electron pockets. We analyze the interplay between intra-pocket and inter-pocket pairing depending on the ellipticity of electron pockets and the strength of their hybridization. We show that with increasing hybridization the system undergoes a transition from a  $d$ -wave state to an  $s^{+-}$  state, in which the gap changes sign between hybridized pockets. This  $s^{+-}$  state has the full gap and at the same time supports spin resonance, in agreement with the data. Near the boundary between  $d$  and  $s^{+-}$  states we found a long-sought  $s + id$  state which breaks time-reversal symmetry.

**Introduction:** High-temperature superconductivity in Fe-based superconductors (FeSCs) is at the top of the list of the most relevant issues for the physics community [1–4]. Superconductivity in weakly/moderately doped FeSCs is generally believed to be the consequence of the complex geometry of the Fermi surface (FS), which consists of hole and electron pockets located in separate regions of the Brillouin zone. The prevailing scenario is that the gap has an  $s$ -wave symmetry, changes sign between hole and electron pockets [5, 6] and may even have accidental nodes [1, 7].

This scenario has been challenged recently by the observation of high-temperature superconductivity [8, 9] in  $\text{A}_x\text{Fe}_{2-y}\text{Se}_2$  ( $\text{AFe}_2\text{Se}_2$ ) with  $A = \text{K, Rb, Cs}$ , which have only electron pockets, according to photoemission [10]. Several groups argued [11–14] that interaction between electron pockets in  $\text{AFe}_2\text{Se}_2$  plays the same role as intra-pocket hole-electron interaction in weakly doped FeSCs, and the gap must change sign between two electron pockets. Such a "plus-minus" gap has no nodes, but it is antisymmetric with respect to the interchange of  $X$  and  $Y$  directions (along which the two pockets are located), and hence has  $d$ -wave symmetry. A no-nodal  $d$ -wave gap is, however, rather fragile and was argued [15] to acquire symmetry-related nodes once one includes the hybridization between the electron pockets due to an additional hopping via a chalcogen (Se). The data on  $\text{AFe}_2\text{Se}_2$ , however, show that the gap has no nodes [16–18], what led other groups to argue [19–21] that the gap in  $\text{AFe}_2\text{Se}_2$  must be a sign-preserving  $s$ -wave. Such gap, however, is also problematic as it is inconsistent with recent observation of the spin resonance below  $T_c$  in  $\text{Rb}_x\text{Fe}_{2-y}\text{Se}_2$  (Ref. [22]).

In this letter we show that a nodeless superconductivity, consistent with the spin resonance, in fact appears quite naturally in a situation when only electron pockets are present. We argue that complete theory of superconductivity in such geometry should include on equal footing a pairing condensate made out of fermions

on the same pocket (intra-pocket pairing) and a pairing condensate made out of fermions on different pockets (inter-pocket pairing). Inter-pocket pairing has been discussed in early days of Fe-pnictides regarding a possible spin-triplet, even-parity pairing in weakly doped FeSCs [23, 24], and in the context of pairing in orbital representation [25], but was not considered in previous works on the pairing in FeSCs with only electron pockets [26]. For  $\text{AFe}_2\text{Se}_2$  inter-pocket pairing is particularly important because both hybridization *and* ellipticity are small [15]. We show that the interplay between intra- and inter-pocket pairing leads to a competition between  $d$ -wave and  $s$ -wave states. We find three phases merging at the tetra-critical point – an  $s$ -wave, a  $s + id$  state which breaks time-reversal symmetry, and a  $d$ -wave state (Fig. 1). In  $s$ -wave and  $s + id$  states, all states are gapped. In a  $d$ -wave state, there are vertical loop nodes centered  $k_z = \pi/2$ . In some range of parameters, loops collapse and a  $d$ -wave state also becomes nodeless ( $d'$  phase in Fig. 1). The  $s$ -wave is of plus-minus type – the gaps on hybridized FSs have opposite signs. Such state has been earlier proposed phenomenologically by Mazin [15]. Our study provides the microscopic mechanism of such  $s^{+-}$  superconductivity.

**The model** We consider the low-energy physics of FeSCs with only electron pockets within a 2D model of interacting fermions near  $(0, \pi)$  and  $(\pi, 0)$ . The hopping via a pnictogen/chalcogen hybridizes the two electron pockets and also gives rise to additional 4-fermion interactions with excess momentum  $\mathbf{Q} = (\pi, \pi)$  taken by pnictogen/chalcogen. The hybridization in  $\text{AFe}_2\text{Se}_2$  actually involves momentum  $(\pi, \pi, \pi)$  because of body-centered tetragonal structure of these materials, i.e., hybridized fermions belong to different planes separated by  $k_z = \pi$  [15, 27]. To simplify the presentation, we first consider hybridization for a simple tetragonal structure, for which hybridized fermions have the same  $k_z$ , and then extend the analysis to body-centered tetragonal structure.

Let  $c_{\mathbf{k}}^\dagger$  be a creation operator for electrons at  $(0, \pi)$ , and

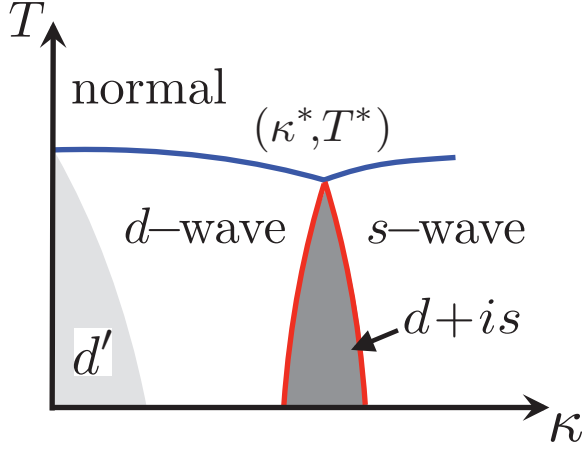


FIG. 1: The phase diagram in  $(\kappa, T)$ -plane for Fe-based superconductors with only electron pockets ( $\kappa$  is the ratio of the hybridization and the degree of ellipticity of the electron pockets). The  $s + id$  phase with broken time reversal symmetry is shown by the dark (grey) shaded area. The two neighboring superconducting phases at  $\kappa < (>)\kappa^*$  have  $d(s)$ -wave symmetry, respectively. In the  $d'$  region the excitation spectrum is fully gapped even though the symmetry is  $d$ -wave.

$f_{\mathbf{k}}^\dagger = c_{\mathbf{k}+\mathbf{Q}}^\dagger$  is a creation operator of electrons at  $(\pi, 0)$ . The quadratic part of the Hamiltonian  $H = H_2 + H_{int}$  is

$$H_2 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^c c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^f f_{\mathbf{k}}^\dagger f_{\mathbf{k}} + \sum_{\mathbf{k}} \lambda \left[ c_{\mathbf{k}}^\dagger f_{\mathbf{k}} + f_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right], \quad (1)$$

where the first two terms describe fermion dispersion, and the last term describes the hybridization. The two elliptical FSs are defined by  $\epsilon_{\mathbf{k}}^{c(f)} = \epsilon_F$ . We approximate fermion excitations near these FSs by  $\epsilon_{\mathbf{k}}^c = v_F(\phi)(k - k_F(\phi))$ ,  $\epsilon_{\mathbf{k}}^f = v_F(\phi + \pi/2)(k - k_F(\phi + \pi/2))$ , where  $\phi$  is the angle along each of the FSs counted from the  $x$ -axis. By virtue of tetragonal symmetry,  $v_F(\phi) = v_F(1 + a \cos 2\phi)$  and  $k_F(\phi) = k_F(1 + b \cos 2\phi)$ . The anisotropy of the Fermi velocity does not play a major role in our analysis, but the eccentricity of the FS (the parameter  $b$ ) is overly relevant. Both  $b$  and  $\lambda/(v_F k_F)$  are small for  $\text{AFe}_2\text{Se}_2$  (Ref.[15]), but their ratio  $\kappa = \lambda/(v_F k_F |b|)$  can be arbitrary.

The interaction Hamiltonian involves direct, momentum-conserving, 4-fermion interactions, and interactions with excess momentum  $\mathbf{Q}$ . There are four direct interactions allowed by symmetry:

$$\begin{aligned} H_1 &= \frac{u_1}{2} \int d\mathbf{x} \left( c_{\sigma}^\dagger f_{\sigma'}^\dagger f_{\sigma'} c_{\sigma} + f_{\sigma}^\dagger c_{\sigma'}^\dagger c_{\sigma'} f_{\sigma} \right) \\ H_2 &= \frac{u_2}{2} \int d\mathbf{x} \left( c_{\sigma}^\dagger f_{\sigma'}^\dagger c_{\sigma'} f_{\sigma} + f_{\sigma}^\dagger c_{\sigma'}^\dagger f_{\sigma'} c_{\sigma} \right) \\ H_3 &= \frac{u_3}{2} \int d\mathbf{x} \left( c_{\sigma}^\dagger c_{\sigma'}^\dagger f_{\sigma'} f_{\sigma} + f_{\sigma}^\dagger f_{\sigma'}^\dagger c_{\sigma'} c_{\sigma} \right) \\ H_4 &= \frac{u_4}{2} \int d\mathbf{x} \left( c_{\sigma}^\dagger c_{\sigma'}^\dagger c_{\sigma'} c_{\sigma} + f_{\sigma}^\dagger f_{\sigma'}^\dagger f_{\sigma'} f_{\sigma} \right) \end{aligned} \quad (2)$$

$H_1$  and  $H_2$  are inter-band density-density and exchange interactions,  $H_4$  is the intra-band density-density interaction, and  $H_3$  describes the umklapp pair-hopping processes. For circular pockets, the couplings  $u_i$  are related as there are only three combinations invariant under  $O(2)$  rotational symmetry in  $(c, f)$  space and  $SU(2)$  spin symmetry -  $n^2$ ,  $\mathbf{S}^2$ , and  $\tilde{n}^2$ , where  $n = c_{\alpha}^\dagger c_{\alpha} + f_{\alpha}^\dagger f_{\alpha}$  is the total charge density,  $\mathbf{S} = (1/2)(c_{\alpha}^\dagger c_{\beta} + f_{\alpha}^\dagger f_{\beta})\sigma_{\alpha\beta}$ , is the total spin, and  $\tilde{n} = c_{\alpha}^\dagger f_{\alpha} - f_{\alpha}^\dagger c_{\alpha}$ . Hence  $H = Un^2/2 + J'\tilde{n}^2/2 + 2J\mathbf{S}^2$ , and the interactions  $u_i$  are  $u_1 = U - J, u_2 = -2J - J', u_3 = J', u_4 = U - 3J$ . Then  $u_4 - u_3 = u_1 + u_2 = U - 3J - J'$ . For weak ellipticity,  $u_1 + u_2$  and  $u_4 - u_3$  do not have to be identical, but remain close and we will keep them equal for simplicity. We will need  $u$  to be positive for superconductivity. This is the case when Hund interaction is the dominant one. If  $u$  is negative, the system likely develops a magnetic order instead of superconductivity. The interaction with excess momentum  $\mathbf{Q}$  is

$$H_{\mathbf{Q}} = w_1 \int d\mathbf{x} (c_{\sigma}^\dagger f_{\sigma} + f_{\sigma}^\dagger c_{\sigma})(c_{\sigma'}^\dagger c_{\sigma'} + f_{\sigma'}^\dagger f_{\sigma'}). \quad (3)$$

Other interactions with  $\mathbf{Q}$  vanish without time-reversal symmetry breaking.

The quadratic Hamiltonian can be diagonalized by unitary transformation to new operators  $a_{\mathbf{k}} = c_{\mathbf{k}} \cos \theta_{\mathbf{k}} + f_{\mathbf{k}} \sin \theta_{\mathbf{k}}$ ,  $b_{\mathbf{k}} = -c_{\mathbf{k}} \sin \theta_{\mathbf{k}} + f_{\mathbf{k}} \cos \theta_{\mathbf{k}}$  with  $\sin 2\theta_{\mathbf{k}} = \lambda/\sqrt{\lambda^2 + (\epsilon_{\mathbf{k}}^c - \epsilon_{\mathbf{k}}^f)^2/4}$ ,  $\cos 2\theta_{\mathbf{k}} = (\epsilon_{\mathbf{k}}^c - \epsilon_{\mathbf{k}}^f)/(2\sqrt{\lambda^2 + (\epsilon_{\mathbf{k}}^c - \epsilon_{\mathbf{k}}^f)^2/4})$ . In terms of new operators,

$$H_2 = \sum_{\mathbf{k}} E_{\mathbf{k}}^a a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}} E_{\mathbf{k}}^b b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \quad (4)$$

with

$$E_{\mathbf{k}}^{a,b} = \frac{1}{2} (\epsilon_{\mathbf{k}}^c + \epsilon_{\mathbf{k}}^f) \pm \left[ \lambda^2 + (\epsilon_{\mathbf{k}}^c - \epsilon_{\mathbf{k}}^f)^2/4 \right]^{1/2}. \quad (5)$$

In our notations,  $(\epsilon_{\mathbf{k}}^c + \epsilon_{\mathbf{k}}^f)/2 \approx \epsilon_F + v_F(k - k_F) = \epsilon_F + \xi$ , and  $(\epsilon_{\mathbf{k}}^c - \epsilon_{\mathbf{k}}^f)/2 \approx v_F k_F b \cos 2\phi$ , such that  $E_{\mathbf{k}}^{a,b} - \epsilon_F = \xi \pm \lambda(1 + \cos^2 2\phi/\kappa^2)^{1/2}$ ,  $\cos^2 2\theta = \cos^2 2\phi/(\kappa^2 + \cos^2 2\phi)$ , and  $\sin^2 2\theta = \kappa^2/(\kappa^2 + \cos^2 2\phi)$ .

The interplay between intra-pocket and inter-pocket pairing can be understood by considering the limits of small and large  $\kappa$  (Fig. 2). At  $\kappa \rightarrow 0$  the hybridization vanishes, and  $c$  and  $f$  are primary operators. For elliptical pockets, intra-pocket pairing susceptibility is larger than inter-pocket one, and when  $u_3 > u_4$ , the system develops a conventional pairing instability with  $\Delta_c = \langle c_{\uparrow}^\dagger c_{\downarrow}^\dagger \rangle$  and  $\Delta_f = \langle f_{\uparrow}^\dagger f_{\downarrow}^\dagger \rangle$  and  $\Delta_f = -\Delta_c$  (Fig. 2a). This solution is antisymmetric with respect to  $c \leftrightarrow f$  and hence is  $d$ -wave. In the opposite limit of large  $\kappa$ ,  $a$  and  $b$  are primary fermion operators, and the FSs of  $a$  and  $b$  fermions are well separated in the momentum space (Fig. 2b). The

leading pairing instability is again a conventional intra-pocket one, and the gaps  $\Delta_a = \langle a^\dagger_\uparrow a^\dagger_\downarrow \rangle$  and  $\Delta_b = \langle b^\dagger_\uparrow b^\dagger_\downarrow \rangle$  obey  $\Delta_a = -\Delta_b$ . This gap, however, is a sign-changing  $s$ -wave rather than  $d$ -wave. To see this, we note that at large  $\kappa$ ,  $a^\dagger_\uparrow a^\dagger_\downarrow - b^\dagger_\uparrow b^\dagger_\downarrow = c^\dagger_\uparrow f^\dagger_\downarrow + f^\dagger_\uparrow c^\dagger_\downarrow$ , i.e., the solution  $\Delta_a = -\Delta_b$  corresponds to non-zero  $\langle c^\dagger_\uparrow f^\dagger_\downarrow + f^\dagger_\uparrow c^\dagger_\downarrow \rangle$ . The latter combination is symmetric with respect to  $c \leftrightarrow f$  and hence is an  $s$ -wave, but it also shows that in terms of  $c$  and  $f$  fermions we now have inter-pocket pairing. What happened with the  $d$ -wave solution? At large  $\kappa$  we have  $c^\dagger_\uparrow c^\dagger_\downarrow - f^\dagger_\uparrow f^\dagger_\downarrow = -(a^\dagger_\uparrow b^\dagger_\downarrow + b^\dagger_\uparrow a^\dagger_\downarrow)$ . Hence, in terms of  $a$  and  $b$  operators,  $d$ -wave pairing now becomes inter-pocket pairing. We see therefore that intra-pocket pairing in terms of one set of fermions corresponds to inter-pocket pairing in terms of the other set. To describe the transformation from  $d$ - to  $s$ -wave symmetry we then have to include the two pairings on equal footing.

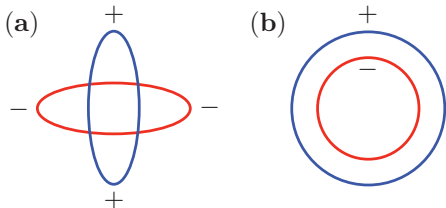


FIG. 2: The structure of superconducting gap at small and large  $\kappa$ . At the smallest  $\kappa$  (panel a), the gap has different sign on the original FS pockets and is  $d$ -wave because it is antisymmetric with respect to rotation by  $90^\circ$ . At large  $\kappa$  (panel b), the gap again changes sign, but now between hybridized FS pockets. This gap is symmetric with respect to  $90^\circ$  rotation and is an  $s$ -wave.

It is natural to analyze the pairing in terms of  $a$  and  $b$  fermions because the Hamiltonian, Eq. (1), is then quadratic at all values of  $\kappa$ . We introduce intra- and inter-band pair creation operators,

$$J_\pm^\dagger = \frac{1}{2} (a^\dagger a^\dagger \pm b^\dagger b^\dagger), \quad \tilde{J}_\pm^\dagger = \frac{1}{2} (a^\dagger b^\dagger \pm b^\dagger a^\dagger). \quad (6)$$

The combinations  $J_\pm^\dagger$  and  $\tilde{J}_\pm^\dagger$  describe an ordinary, "plus-plus"  $s$ -wave pairing and spin-triplet, even parity inter-band pairing, respectively (the triplet channel is identical to the one considered in [23]). In our case, these two pairing channels are strongly repulsive, and we can safely omit them. The linear combinations of the other two components  $J_-^\dagger$  and  $\tilde{J}_+^\dagger$  describe  $s$ -wave pair creation operators

$$\frac{1}{2} (c^\dagger_\sigma f^\dagger_{\sigma'} + f^\dagger_\sigma c^\dagger_{\sigma'}) = [\cos 2\theta \tilde{J}_+^\dagger + \sin 2\theta J_-^\dagger]_{\sigma\sigma'}, \quad (7)$$

and  $d$ -wave pair creation operators

$$\frac{1}{2} (c^\dagger_\sigma c^\dagger_{\sigma'} - f^\dagger_\sigma f^\dagger_{\sigma'}) = [\cos 2\theta J_-^\dagger - \sin 2\theta \tilde{J}_+^\dagger]_{\sigma\sigma'}, \quad (8)$$

The interaction, Eq. (2), can then be decomposed into an  $s$ -wave and  $d$ -wave channels,  $H_{int} = H_s + H_d$  with

$$H_s = -2u[s' J_-^\dagger + c' \tilde{J}_+^\dagger]_{\sigma\sigma'} [s J_- + c \tilde{J}_+]_{\sigma'\sigma}, \quad (9)$$

$$H_d = -2u[c' J_-^\dagger - s' \tilde{J}_+^\dagger]_{\sigma\sigma'} [c J_- - s \tilde{J}_+]_{\sigma'\sigma}, \quad (10)$$

where  $c \equiv \cos 2\theta$ ,  $c' \equiv \cos 2\theta'$ ,  $s \equiv \sin 2\theta$ ,  $s' \equiv \sin 2\theta'$ . We emphasize that the intra- and inter- band pairings enter Eqs. (9), (10) on equal footing. The interaction  $H_Q$  couples these two channels with plus-plus  $s$ -wave channel and spin-triplet channels which we already neglected, and does not play a role in our analysis.

**Ginzburg-Landau Functional:** To map a phase diagram in  $(\kappa, T)$ -plane we derive the Ginzburg-Landau Functional (GLF). We introduce order parameters  $\Delta_s$  and  $\Delta_d$  to decouple the interaction in two Cooper channels using the Hubbard-Stratonovitch identity, integrate over fermion fields and expand the effective action in powers of  $\Delta_s$  and  $\Delta_d$ . Carrying out the calculations (see [28]) we obtain

$$F_{GL} = A_s |\Delta_s|^2 + A_d |\Delta_d|^2 + \frac{B_s}{2} |\Delta_s|^4 + \frac{B_d}{2} |\Delta_d|^4 + C |\Delta_s|^2 |\Delta_d|^2 + \frac{E}{2} ((\Delta_s \Delta_d^*)^2 + (\Delta_s^* \Delta_d)^2). \quad (11)$$

The transition to either  $s$ -wave or  $d$ -wave state is de-

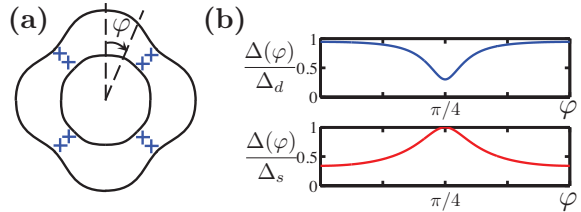


FIG. 3: a) Location of the nodal points in the  $d$ -wave phase (crosses). Upon approaching the boundary of  $d'$  phase in Fig.1, nodal points come closer and eventually collapse, leading to a nodeless  $d$ -wave state. b) The modulation of the gap magnitude along the FSs for  $d$ -wave and  $s$ -wave states.

termined by  $A_s = 0$  or  $A_d = 0$ , whichever comes first. The lines  $A_s = 0$  and  $A_d = 0$  cross at some critical  $\kappa^*$ , at which  $T_c = T_c^*$ . For  $\lambda \gg T_c^*$  (the case of  $\text{AFe}_2\text{Se}_2$ , Ref.[15]), we obtain  $\kappa^* = 1/\sqrt{3}$  (in the other limit  $\lambda \ll T_c^*$   $\kappa^* = 1/\sqrt{2}$  (Ref. [28])). Near the critical  $\kappa$ , the first instability occurs at  $T_{c,s} = T_c^* (1 + \alpha(\kappa - \kappa^*))$  for  $\kappa > \kappa^*$  and at  $T_{c,d} = T_c^* (1 + \alpha(\kappa^* - \kappa))$  for  $\kappa < \kappa^*$ , where  $\alpha = 3\sqrt{3}/(2uN_F)$  (see Fig. 1).

The type of the transition from a  $d$ -wave order at  $\kappa < \kappa^*$  to an  $s$ -wave order at  $\kappa > \kappa^*$  is determined by the the interplay between fourth-order terms in Eq. (11). The transition can be either first order or continuous, via an intermediate phase where both orders are present. At

$T = T_c^*$  we obtained  $B_s = B_d = B = \frac{5}{8}I_0$ ,  $C = \frac{3}{8}I_0$ , and  $E = C/2$ , where  $I_0 = 7\zeta(3)/8\pi^2(T_c^*)^2$ . We see that  $E > 0$  and  $B + E > C$ . An elementary analysis then shows that the transition from  $d$  to  $s$  involves an intermediate phase in which the two orders mix with relative phase  $\pm\pi/2$ . This is long-sought  $s \pm id$  state [29,30]. The system chooses either  $s + id$  or  $s - id$  state and by doing this breaks time-reversal symmetry. An  $s + id$  state contains orbital currents and should be detectable in, e.g., neutron scattering [31] and Josephson junction experiments. [32] The boundaries of this intermediate phase are set by  $T_{s+id} = T_c^*(1 - \beta|\kappa - \kappa^*|)$ , where  $\beta = 6\sqrt{3}/(uN_F)$ . We emphasize again that both the transition from  $s$  to  $d$  and the existence of the intermediate phase are due to the competition between intra-pocket and inter-pocket pairing.

*Fermion excitations* In the  $s$ -wave state and in the intermediate  $s \pm id$  state excitations are fully gapped. In the  $d$ -wave state, the excitation spectrum is given [28]:

$$\omega_{\pm}^2 = |\Delta_d|^2 \cos^2 2\theta + \left( \sqrt{\xi^2 + |\Delta_d|^2 \sin^2 2\theta} \pm \frac{\lambda}{\sin 2\theta} \right)^2, \quad (12)$$

where, we remind,  $\xi \approx v_F(k - k_F)$ . The dispersion  $\omega_-$  has nodes along the diagonal directions where  $\cos 2\theta = 0$ , as it should be for a  $d$ -wave superconductor. However the nodal points are located in between  $a$  and  $b$  FSs, as shown in Fig. 3a. This is another consequence of inter-pocket pairing. We plot the dispersions in  $s$ - and  $d$ -wave states in Fig. 3b. We furthermore see from (12) that nodes in the  $d$ -wave state exist only if  $|\Delta_d| < \lambda$ , otherwise the second term in the r.h.s of (12) does not vanish even when  $\xi = 0$ . The condition  $|\Delta_d| = \lambda$  then sets the boundary of the *nodeless*  $d$ -wave state ( $d'$  state on Fig. 1).

*Application to  $AFe_2Se_2$ :* The hybridization of electron pockets in  $AFe_2Se_2$  is more involved because of the body-centered tetragonal structure of these materials [8]. The two hybridized electron FSs differ by  $k_z = \pi$  and are rotated by  $\pi/2$  (see Fig. 4a-c and Refs.[15, 27]). For  $k_z = 0$  and  $k_z = \pi$ , the FS in the folded zone consists of co-aligned ellipses (Fig. 4d-f), the pair near  $(\pi, \pi)$  at  $k_z = 0$  is identical to the one near  $(-\pi, \pi)$  at  $k_z = \pi$ . At  $k_z = \pm\pi/2$ , the pockets are  $C_4$  symmetric already before hybridization, and the hybridization leads to identical pairs at  $(\pi, \pi)$  and  $(-\pi, \pi)$ .  $s$ -wave and  $d$ -wave gaps differ in whether the gap on the larger ellipsis retains sign or changes sign between  $k_z = 0$  and  $k_z = \pi$  (Fig. 4g-h). Near  $k_z = \pi/2$ , the hybridization instantly favors  $s$ -wave, if we approximate  $C_4$ -symmetric pockets as circles, but overall which of the two states is realized depends on  $\kappa$  averaged along  $k_z$  and on the strength of  $k_z$  dependence of the interaction  $u$ . Note that in a  $d$ -wave state nodes exist near  $k_z = \pi/2$ , but not near  $k_z = 0$  and  $k_z = \pi$ , where the two FSs in the same corner in the folded zone are separated – they are co-axial ellipses of different sizes, and hybridization only causes minor vari-

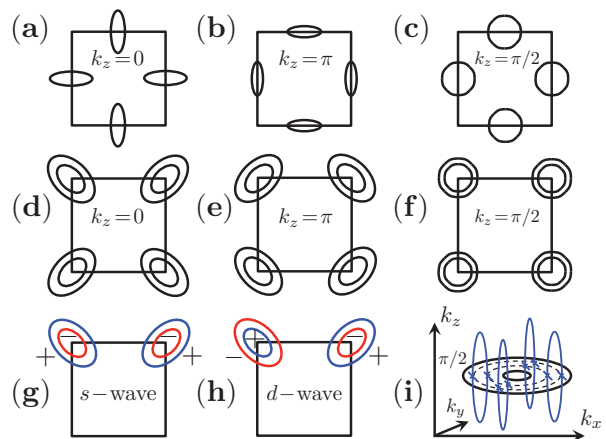


FIG. 4: The structure of electronic states and the superconducting gap in  $AFe_2Se_2$  which have body-centered tetragonal structure. Panels a-c – electron pockets in the unfolded Brillouin zone for different  $k_z$ . Panels d-f – same in the folded zone. The two ellipses at each corner remain co-axial and rotate by  $90^\circ$  between  $k_z = 0$  and  $k_z = \pi$ . Panels g-h –  $s$ -wave and  $d$ -wave gap structure near  $k_z = 0$  and  $k_z = \pi$ . Panel i – the location of the nodes at  $k_z \approx \pi/2$ . The nodal points form vertical loops (only two are shown for clarity). If hybridized FSs at  $\pi/2$  are two circles, the crosses extend and form lines in  $(k_x, k_y)$  plane (dashed lines in the Figure).

ations of originally angle-independent gap (this behavior is the same as in  $d'$  region in Fig. 1). Because of this, the nodes in the  $d$ -wave state form vertical loops centered at  $k_z = \pi/2$  (Fig. 4i). Vertical loop nodes have been earlier suggested on phenomenological grounds [33,34], but have not been obtained microscopically earlier.

To conclude, in this work we argued that the pairing in Fe-based superconductors with only electron pockets must necessarily include inter-band condensate made of fermions belonging to different pockets. We demonstrated that the interplay between intra-pocket and inter-pocket pairing leads to a transition from  $d$ -wave pairing at small degree of hybridization to an  $s^{+-}$ -wave pairing at larger hybridization. In between there is an intermediate  $s \pm id$  state with broken time reversal symmetry.

Fermionic excitations in  $s^{+-}$  and  $s + id$  states are fully gapped, yet in both states there is the spin resonance below  $T_c$  [15, 35, 36]. The absence of the nodes and the existence of the spin resonance are consistent with the data on  $AFe_2Se_2$  [8, 22], what makes  $s^{+-}$  state, and, potentially,  $s + id$  state the likely candidates.

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