

# Coexistence of superconductivity and a spin density wave in pnictides: Gap symmetry and nodal lines

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We investigate the effect of a spin-density wave (SDW) on  $s_{\pm}$  superconductivity in Fe-based superconductors. We show that, contrary to the common wisdom, no nodes open at the new, reconnected Fermi surfaces when the hole and electron pockets fold down in the SDW state, despite the fact that the  $s_{\pm}$  gap changes sign between the two pockets. Instead, the order parameter preserves its sign along the newly formed Fermi surfaces. The familiar experimental signatures of an  $s_{\pm}$  symmetry are still preserved, although they appear in a mathematically different way. For a regular  $s$  case ( $s_{++}$ ) the nodes do appear in the SDW state. This distinction suggests a novel simple way to experimentally separate an  $s_{\pm}$  state from a regular  $s$  in the pnictides. We argue that recently published thermal conductivity data in the coexisting state are consistent with the  $s_{\pm}$ , but not the  $s_{++}$  state.

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The superconducting pnictides continue to attract great interest over a year after the original discovery. Despite more than a thousand preprints and publications, the most basic questions about pairing symmetries and mechanisms remain controversial. Early on the  $s_{\pm}$  pairing symmetry was proposed<sup>1,2</sup>, in which the superconducting gap function changes sign from the hole to the electron pockets, but is roughly constant on each surface. A possibility of an accidentally nodal  $s_{\pm}$  state, or a d-wave state, depending upon parameter values, was also proposed<sup>2</sup>, and investigated in many details recently<sup>3</sup>.

As of now, significant experimental evidence has been accumulated in favor of the  $s_{\pm}$  proposal, and substantial theoretical effort has been devoted to the study of various properties of such a state (see Refs. 4,5 for reviews). So far, however, no one has addressed the possible modification of an  $s_{\pm}$  state due to a static spin density wave (SDW) coexisting with superconductivity. At the same time the emerging consensus among experimentalists (see Refs. 6,7,8,9,10,11) is that in most systems, most notably in both electron and hole doped 122 materials, there is a range of coexistence of SDW and superconductivity, probably up to the optimal doping level (some, however, have argued for mesoscopic phase separation on the hole-doping side<sup>11,12</sup>). It was recently estimated that the magnetic moment at the Co concentration of 7% is 0.1  $\mu_B$  per Fe, corresponding, roughly, to an antiferromagnetic field of the order of 50–100 meV<sup>10</sup>.

The subject of an SDW coexisting with superconductivity has a long history, dating back to Bulaevskii et al in 1980<sup>13</sup> and numerous work since then. It was shown<sup>13,14</sup> that in a one-band BCS superconductor a spiral SDW induces a gap anisotropy that leads to gap nodes, while a collinear SDW still leads to a finite energy gap<sup>14</sup>. The case of the  $s_{\pm}$  superconductivity in Fe-based superconductors (FBS), on the first glance, seems quite simple: first, the SDW wave we are dealing with here is simply a collinear double-cell antiferromagnetic (AF) order, so one need not be bothered by the difference between a spiral and collinear SDW; second, the doubling of the unit cell in real space leads to the folding down of the Brillouin zone in momentum space, which projects the elec-

tron Fermi surfaces (FS) with the negative order parameter ( $\Delta_e < 0$ ) onto the hole Fermi surface with the positive order parameter ( $\Delta_h > 0$ ). Whenever the two FSs intersect, an SDW gap opens up. It seems obvious that, when that happens,  $\Delta$  on the newly formed FSs should change sign, that is, develop nodes.

However, not everything that seems obvious is true. We will show below that, instead, a curious novel state is formed, which is fully gapped and, formally, has an order parameter (OP) of the same sign everywhere. This should not be confused though with the conventional BCS-like  $s$  state: when the SDW amplitude is vanishingly small, this state *has the same observable properties as the original  $s_{\pm}$  state, despite having a single-sign OP*. This bizarre property, which, incidentally, is also relevant to the coexistence of d-wave superconductivity and AF order in electron-doped cuprates<sup>15</sup>, can be traced down to two facts, well known but often not appreciated: (1) not only the overall sign of the OP in a superconductor, but also the *relative* sign of  $\Delta_{\mathbf{k}}$  and  $\Delta_{\mathbf{k}'}$  is not uniquely defined, but depends on the convention for the wave function phases and (2) as opposed to a nonmagnetic material, in an AF metal it is not possible to fix the phases of the wave functions in such a way that the wave functions for both spin projections are identical at any  $\mathbf{k}$ -point.

With these considerations in mind, let us now outline the derivation. We will follow the approach of Ref. 14, and for illustrative purposes will use a simple semimetallic model bandstructure with a hole band centered at the  $\Gamma$  point and an electron band around  $\mathbf{Q} = (\pi, 0)$  and related points in the unfolded Brillouin zone which we will be using. We assume the Fermi energies to be, respectively,  $\varepsilon_h$  and  $\varepsilon_e$ , and take an isotropic effective mass  $m$  for the hole band. To account for the fact that nesting is always imperfect (and if it were perfect, the SDW would open a gap on the entire FS, thus preventing any coexisting superconductivity), we take  $m_e$  to be anisotropic, with  $m_x \neq m_y$ . This reflects the fact that the actual calculated and measured anisotropy of the electron pockets is larger than that of the hole ones. The Hamiltonian for this

system is given by<sup>13</sup>

$$\hat{H} = \sum_{k,i} \epsilon_{k,i} \phi_{k,i}^\dagger \phi_{k,i} + \mathbf{h}_{Q,i} \cdot \mathbf{S}_k \quad (1)$$

with an effective field  $h \propto \cos(\mathbf{Q}\mathbf{r})$ , which interacts with the electron spin  $\mathbf{S}$  and leads to the SDW. The index  $i = e, h$  refers to the hole or electron Fermi surface bands, with the dispersions

$$\begin{aligned} \epsilon_{k,e} &= \hbar^2(k_x - \pi)^2/2m_x + \hbar^2k_y^2/2m_y - \epsilon_e, \\ \epsilon_{k,h} &= -\hbar^2k^2/2m + \epsilon_h. \end{aligned} \quad (2)$$

For the purpose of this work – demonstrating the effect of AF – we will take  $\epsilon_h$  and  $\epsilon_e$  equal. In real life, of course, they will depend on the relative location of  $E_F$  which will change with doping. We take  $m_y < m < m_x$  to ensure intersections between the hole and electron Fermi surfaces upon translating by the SDW vector. We take  $m_x m_y \sim m^2$  so that the electron and hole densities of states (DOS) are comparable.<sup>16</sup>

In the following we will work in the downfolded Brillouin zone corresponding to the antiferromagnetic unit cell. Let  $G$  be the matrix element (assumed to be  $k$ -independent) of the SDW potential mixing the hole and electron wave functions,  $\phi_h$  and  $\phi_e$ . Then the dispersion in the SDW state is

$$E_k^\pm = \frac{\epsilon_{\mathbf{k},h} + \epsilon_{\mathbf{k},e} \pm \sqrt{(\epsilon_{\mathbf{k},h} - \epsilon_{\mathbf{k},e})^2 + 4G^2}}{2} \quad (3)$$

with the new wave functions

$$\psi_{k\uparrow}^+ = \cos\theta_k \phi_{k,h} + \sin\theta_k \phi_{k,e}; \quad \psi_{k\uparrow}^- = \sin\theta_k \phi_{k,h} - \cos\theta_k \phi_{k,e} \quad (4)$$

$$\psi_{k\downarrow}^+ = \cos\theta_k \phi_{k,h} - \sin\theta_k \phi_{k,e}; \quad \psi_{k\downarrow}^- = \sin\theta_k \phi_{k,h} + \cos\theta_k \phi_{k,e} \quad (5)$$

where  $\tan\theta_k = G/(E_k^- - \epsilon_{\mathbf{k},e})$ . In Figure 1 we plot the separate hole and electron Fermi surfaces above the SDW ordering temperature (main panel), as well as the Fermi surface for two values of  $G$ . Of course, we are most interested in the limit in which the SDW-created reconstruction of the Fermi surface is relatively minor. In practical terms the SDW gap may be (albeit not necessary for retaining superconductivity!) smaller than the SC gap, but the concept is easier to illustrate for an SDW gap comparable to the superconducting one. Figure 2 shows the behavior of  $\theta_k$  along the SDW-state Fermi surfaces. Note that while the energy spectrum (3) is double degenerate, the wave functions (4) are not equal to the wave functions (5). If we now create a singlet anomalous average (the superconducting OP), it will look like

$$\begin{aligned} \Delta^+(\mathbf{k}) &= \langle \psi_{k\uparrow}^+ \psi_{-k\downarrow}^+ \rangle = \cos^2\theta_k \langle \phi_{k,h} \phi_{k,h} \rangle \\ &\quad - \sin^2\theta_k \langle \phi_{k,e} \phi_{k,e} \rangle + 2 \sin\theta_k \cos\theta_k \langle \phi_{k,e} \phi_{k,h} \rangle, \end{aligned} \quad (6)$$

and a similar expression for  $\Delta^-(\mathbf{k})$ . At  $G \rightarrow 0$ , on the new “+” FS pockets  $\theta_k$  takes the value of 0 or  $\pi/2$  depending on whether the point on the FS originated from holes or from

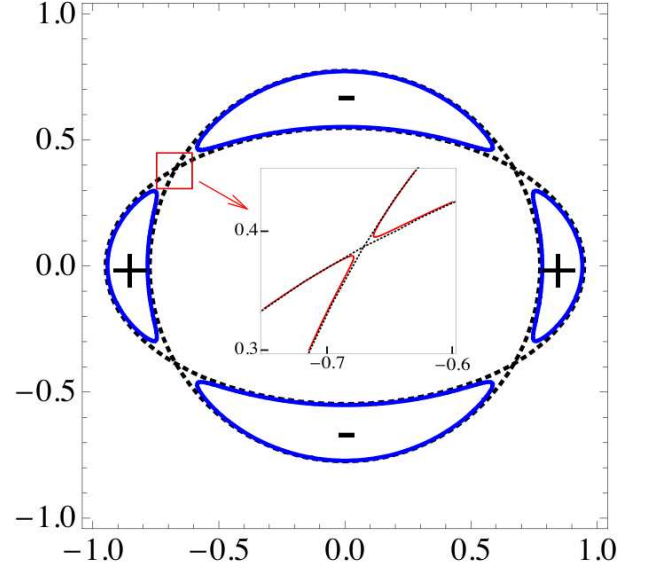


FIG. 1: (Color online) Main figure: heavy line, the Fermi surface in the SDW state for  $G = E_F/12$ ; dashed line, the Fermi surface above the SDW ordering temperature. The “+” and “-” Fermi surfaces are indicated. Inset: the Fermi surfaces for  $G = E_F/120$ .

electrons (and the reverse holds for the “-” pockets). Recalling the original  $s_\pm$  assumption,  $\Delta^h = -\Delta^e$  with  $\Delta^i = \langle \phi_i \phi_i \rangle$ ,  $\langle \phi_h \phi_e \rangle = 0$  we immediately observe that  $\Delta^+$ , as opposed to  $\Delta^{h,e}$ , never changes sign!

However, the system remembers all too well that part of the new FS has come from electrons and part from holes, and that these used to have the OPs of the opposite sign. If we try to calculate any observable quantity (the OP *per se* is not observable), such as pair scattering from one part of the FS to another, we will have to take into account the fact that the new wave functions for the up spin (4) are approximately equal to the old wave functions (e- or h-, depending on what part of the pocket we consider), but for the down spin (5) the same holds for the hole-type part of the FS, while for the electron-type parts the sign of the wave function is flipped. That is to say, any observable matrix elements include a product of the OPs *and* of the one-particle wave function; in the original, unfolded bands, we were able to choose signs of the wave functions to be spin-invariant, so that the scattering from the hole to the electron FS involved a sign change ( $s_\pm$ ). However, in the new, AF zone, no sign change is generated by the OPs, but the same sign change necessarily appears from the normal part of the matrix elements.

We see that we cannot describe the system even with infinitesimally weak SDW in terms of the same wave functions we used for the nonmagnetic parent system. Yet one can restore the conceptual continuity by describing the *parent* system differently. Let us select the wave function phases in the nonmagnetic system so that  $\phi_{k,h\downarrow}(\mathbf{r}) = \phi_{k,h\uparrow}(\mathbf{r})$ , but  $\phi_{k,e,\downarrow}(\mathbf{r}) = -\phi_{k,e,\uparrow}(\mathbf{r})$ . This is a very inconvenient, but legitimate gauge. In this gauge, the OP in the  $s_\pm$  state will have the same sign on the both FSs, but any physical observable involving pair scattering will have to account for a sign flip

for electrons, but not holes, and thus the overall result will be unchanged — the same physical situation that we find (and in that case cannot avoid) in the SDW state.

Let us move on to an arbitrary strength SDW and evaluate<sup>17</sup> the pairing matrix involved in a superconducting state below the SDW ordering temperature,  $\Lambda_{kk'}^{\alpha\beta} = -\langle \psi_{k\uparrow}^\alpha | U | \psi_{k'\uparrow}^\beta \rangle \langle \psi_{k'\downarrow}^\beta | U | \psi_{k,\downarrow}^\alpha \rangle$ , where  $U$  is the pairing interaction, with all relevant factors included and  $\alpha, \beta = \pm 1$  are new band indices. We assume that only hole-electron matrix elements  $\langle \phi_{k,h} | U | \phi_{k',e} \rangle$  are nonzero, and the minus in front accounts for the fact that the pairing interaction is assumed to be generated by spin fluctuations. We furthermore assume that this matrix element does not depend on  $k, k'$ .<sup>18</sup>

After some trigonometric manipulations, we get the answer:

$$\Lambda_{kk'}^{\alpha\beta} = \frac{V}{2} (1 - \alpha\beta \cos 2\theta_k \cos 2\theta_{k'} + \alpha\beta \sin 2\theta_k \sin 2\theta_{k'})$$

The factor 1/2 was selected so that (as we will show later) the effective coupling constant in the  $G = 0$  limit will be equal to  $V\sqrt{N_e N_h}$ . Now we can write the BCS equation at  $T = T_c$  as (with  $\omega$  being the BCS cutoff energy in temperature units)

$$\ln(1.13\omega/T_c)\Delta_k^\alpha = \frac{V}{2} \sum_{k'\beta} \delta(E_{k'}^\beta) \Delta_{k'\beta} \quad (7)$$

$$\begin{aligned} & - \frac{V}{2} \alpha \cos 2\theta_k \sum_{k'\beta} \beta \delta(E_{k'}^\beta) \cos 2\theta_{k'} \Delta_{k'\beta} \\ & + \frac{V}{2} \alpha \sin 2\theta_k \sum_{k'\beta} \beta \delta(E_{k'}^\beta) \sin 2\theta_{k'} \Delta_{k'\beta} \end{aligned} \quad (8)$$

We seek the solution of this equation in the following form

$$\Delta_k^\alpha / \Delta_0 = c + \alpha a \cos 2\theta_k + \alpha b \sin 2\theta_k, \quad (9)$$

and

$$\begin{aligned} \ln(1.13\omega/T_c)c &= \frac{V}{2} (aN_c + bN_s + cN) \\ \ln(1.13\omega/T_c)a &= -\frac{V}{2} (aN_{c2} + bN_s + cN_c) \\ \ln(1.13\omega/T_c)b &= \frac{V}{2} (aN_{cs} + bN_{s2} + cN_s) \end{aligned} \quad (10)$$

where we introduced the weighted DOSs:  $N = \sum \delta(E_k^\alpha)$ ,  $N_c = \sum \alpha \delta(E_k^\alpha) \cos 2\theta_k$ ,  $N_s = \sum \alpha \delta(E_k^\alpha) \sin 2\theta_k$ ,  $N_{c2} = \sum \delta(E_k^\alpha) \cos^2 2\theta_k$ ,  $N_{s2} = N - N_{c2} = \sum \delta(E_k^\alpha) \sin^2 2\theta_k$ ,  $N_{cs} = \sum \delta(E_k^\alpha) \cos 2\theta_k \sin 2\theta_k$ . All summations are over  $k$  and  $\alpha$ , and  $\delta$  represents the Dirac delta function.

The maximal eigenvalue of the matrix

$$\lambda = \frac{V}{2} \begin{pmatrix} N & N_c & N_s \\ -N_c & -N_{c2} & -N_{cs} \\ N_s & N_{cs} & N_{s2} \end{pmatrix}, \quad (11)$$

as usual, defines the BCS transition temperature  $T_c$ , and the corresponding eigenvector gives the distribution of the order parameter over the Fermi surfaces.

In the limit  $G \rightarrow 0$ ,  $\cos 2\theta_k \rightarrow \pm 1$ ,  $N_c \rightarrow N_e - N_h$ ,  $N_{c2} \rightarrow N$ , and all other DOSs vanish. Here  $N_{e(h)}$  is the density of states on the electron (hole) Fermi surface without the SDW. The effective coupling constant  $\lambda_{eff} = V\sqrt{N^2 - N_c^2}/2 = V\sqrt{N_e N_h}$ , which is the well-known result for the  $s_\pm$  pairing. The ratio of the two gaps at  $G \rightarrow 0$  is  $\sqrt{N_h/N_e}$  as it should be in a weak-coupling  $s_\pm$  superconductor<sup>19</sup>.

At a finite  $G$ , the gap does become angle-dependent, via  $\theta_k$ , but it is easy to prove<sup>20</sup> that the eigenvector for maximal  $\lambda$  in (7) gives  $c > a \gg b$ , so that the gap has the same sign everywhere, in agreement with general discussion after Eq. (6). The gap is depicted in Figure 2, where we note that the gap

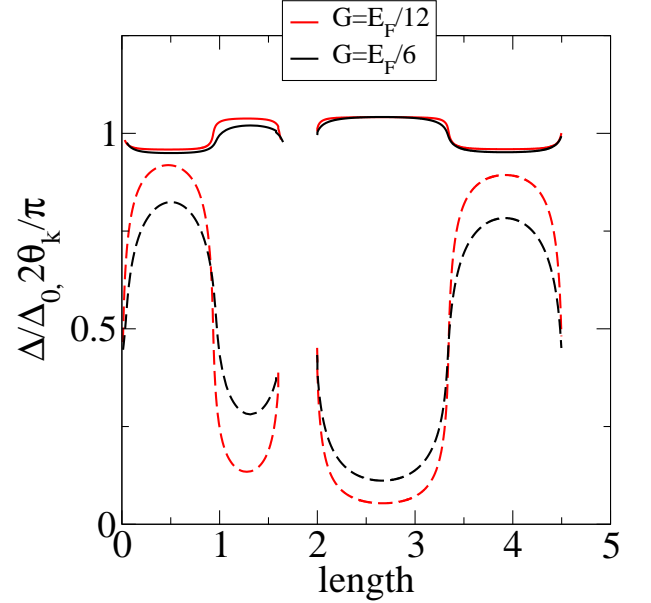


FIG. 2: (Color online) Depicted is the variation of  $\Delta(\mathbf{k})$  (solid lines) and  $\theta_k$  (dashed lines) along the Fermi surfaces for the indicated values of  $G$ . Note that the angle  $\theta_k$  will approach a step function, with regions where  $\theta_k = 0$  or  $\theta_k = \pi/2$ , as  $G \rightarrow 0$ . Here “length” refers to the  $k$ -space arc-length around the Fermi surface; note that the actual arc-length depends on  $G$ . To facilitate comparison we have scaled the arclengths for these two cases lengths to be equal; actual  $G = E_F/6$  arclengths are  $\sim 20$  percent smaller than for  $G = E_F/12$ .

changes rapidly within a finite area where the SDW gap opens; the length of this region scales with  $G$ .

We have also found that the effective coupling constant is reduced slightly at a finite  $G$  compared to its value at  $G = 0$ , i.e., superconducting  $T_c$  drops in the presence of an SDW order. At small  $G$ , we found  $\delta\lambda_{eff} \approx -(VN_{s2}/8)(\sqrt{N_e} - \sqrt{N_h})^2/\sqrt{N_e N_h}$  and<sup>20</sup>  $N_{s2} \propto |G|/|N_e - N_h|$ . Note that the dependence on  $G$  is non-analytic.

The calculations above can be easily generalized to three other cases: an  $s_\pm$  with a charge density wave (CDW), a regular  $s$  with a SDW, and a regular  $s$  with a CDW. The last case is mathematically equivalent to the one considered above. The first two cases are equivalent to each other and constitute a different set. Indeed, in that case the  $V$  in Eqs. 7, 10, 11 should have the opposite sign, and the solution will always have eight node lines at the tips of the banana-shaped FSs of Fig. 1. The

eigenvector for the largest eigenvalue will have, for  $N_e \sim N_c$ , the largest weight on  $a$ , not  $c$ , and the OP will have one sign for the parts of the FS that originated from the electrons and the opposite sign for those originating from the holes.

To summarize, we have shown that, surprisingly, the SDW observed in underdoped pnictide compounds, does not have any considerable destructive effect on the  $s_{\pm}$  superconductivity, besides the obvious competition between the two instabilities for the density of states at the Fermi level. As opposed to a hypothetical CDW, which would have created nodes on the FS and additionally weakened superconductivity, an SDW wave retains the gapped nature of the  $s_{\pm}$  superconductivity. Nevertheless, this constant-sign state has the same observable physical properties as the sign-changing  $s_{\pm}$  state without an SDW. In particular, the penetration depth  $\lambda(T) \propto 1/\sqrt{\rho_s(T)}$  is still exponential at the lowest  $T$  and crosses over to roughly  $T^2$  at higher  $T$ <sup>21</sup>. The slope of  $\delta\lambda(T) \propto \delta\rho_s(T)/(\rho_s(T=0))^{3/2}$  however increases with increasing SDW order simply because  $\rho_s(T=0)$  decreases together with the area of the Fermi surface. This slope increase upon approaching the SDW state was observed in Ref. 22. If, however, the pairing state were

a conventional  $s$ -wave, an SDW order would give rise to gap nodes, and  $\delta\lambda$  would be linear in  $T$  at the smallest  $T$  (we have explicitly verified that the SDW coherence factors do not affect this behavior). Similarly, the reduced thermal conductivity  $\kappa/T$  should still vanish at  $T \rightarrow 0$  if the gap is  $s_{\pm}$  but should become finite below the onset of the SDW order if the gap is a conventional  $s$ -wave, and the more we go into the underdoped regime, the larger the residual  $\kappa/T$  should be because its value does not depend on impurity concentration, but only on the inverse of the slope of  $\Delta_{\mathbf{k}}$  near the nodes. Indeed, a recent study of the low- $T$  thermal conductivity in the underdoped  $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ , where microscopic coexistence of SDW and superconductivity has been well documented, shows<sup>23</sup> that  $\kappa/T$  vanishes at  $T \rightarrow 0$  indicating absence of any gap nodes. This is consistent, according to our results, with an  $s_{\pm}$  state.

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  - 17 We note that the approach we follow here, in which we pair the electrons from SDW eigenstates, suggests that  $T_{SDW} \gg T_c$ , or more precisely, that  $G \gg \Delta(\mathbf{k})$ . In Ref. 13 the problem of explicit coexistence of SDW and SC was considered, which results in a minor change to the dispersion relation of order  $A \frac{\Delta(\mathbf{k})^2 G^2}{E_F^2 (\Delta(\mathbf{k})^2 + G^2)}$  in the coexistence state, where A is a constant factor dependent on the mass anisotropy. This complicates the derivations but does not alter the qualitative conclusions. Given that our model is oversimplified compared to the actual multiband material, we feel it sufficient to present an analysis in the  $G \gg \Delta(\mathbf{k})$  regime.
  - 18 This is equivalent to the assumption that the interaction depends only on the transversed momentum but not on the total incoming momentum. In “g-ology” models<sup>5</sup> this implies that the pair-hopping and the backscattering interaction are taken equal. We verified that the conclusions do not change if the two interactions split under RG flow. The only difference in this situation is a reduction of the  $\sin 2\theta_k$  term in Eq. 9.
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