Doping-dependent pairing symmetry in the Iron-Pnictides

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Introduction—The discovery of high-temperature superconductivity in iron arsenide and related compounds at the beginning of 2008 [2] has triggered an enormous interest in condensed matter physics. This new class of materials exhibits transition temperatures Tc beyond the conventional BCS regime upon electron doping [3] and hole doping [4] of a collinear antiferromagnetic parent state, with Tc’s extending up to 56 K [5, 6], thereby breaking the cuprate monopoly on high-temperature superconductivity [7]. Present experimental evidence accompanied by theoretical modelling suggest that the pairing in the iron-pnictides is different from the d-wave in cuprates. This could be due to both the different strength of the electron-electron interactions in the two materials, which results in an itinerant antiferromagnet in the parent pnictide compounds, and to the topology of the Fermi surfaces (FS) with complex multi-band character [8, 9]. However, very similar to the cuprates is the belief that the magnetism of the parent state crucially influences the pairing symmetry of the doped system.

Various approaches have been pursued to investigate the pairing symmetry in the iron-pnictides. By now, after a short period of analysis providing a wide-spread range of possible pairings [10, 11, 12], the general theoretical view started to converge to an extended s-wave order parameter (denoted s± or s2z2-r2) that takes opposite signs on the electron and hole pockets along the multi-band FS, which is consistent with some experimental data and also has broad theoretical support [8, 13, 14, 15, 16, 17, 18]. However, experimentally, there is still no broad consensus about the nature of the order parameter. While most experiments can be explained in the framework of an s± gap [13], several facts, such as the T3 dependence of the NMR penetration depth over a significant temperature range, as well as the linear penetration depth in LaOFeP remain unsettled. Other experiments such as penetration depth on the 1111 and 122 compounds, as well as thermal conductivity can be explained by an s± order parameter but with large gap anisotropy. Gaps with significant momentum dependence, but no nodes, are reported experimentally in [13]. In contrast, ARPES data reveals very isotropic nodeless gaps on the hole Fermi surfaces [20, 21, 22], of magnitudes matching a strong-coupling form Δ(k) = Δ0 cos(kx) · cos(ky) [13] in the unfolded Brillouin zone. Non-nodal gaps have been found in several analytical and numerical theoretical approaches to the pnictides [16, 23, 24, 25, 26]. Functional renormalization group (FRG) studies [16] with orbital interactions reveal the presence of largely anisotropic, almost nodal, gaps. A recent RPA analysis suggests the existence of a nodal extended s-wave state within the 5-orbital Hubbard model [27]. It was also recently predicted that the momentum dependence of the interaction along the electron pockets may result in the development of gap anisotropy and possibly nodes on top of the constant s± signal [28, 29]. In the strong coupling mean-field picture [15, 16], the gap anisotropy is doping dependent: the gap has a form cos(kx) · cos(ky) which becomes more anisotropic as the doping is increased. In a weak coupling expansion of FS interactions, the gap anisotropy can arise from the presence of an A1g term cos(kx) + cos(ky) (which does not break the crystal symmetry but can create nodes on the (π, 0) and (0, π) electron surfaces) in the band interactions [28].

In this Letter, we study the influence of interaction anisotropy on the superconducting instability by (FRG) [20, 31, 32] methods. Our aim is to investigate the possibility that details of the material and the theoretical model might play a decisive role in determining the pairing symmetry. In order to have a simple control and...
pockets situated at the legs are on hole- or electron-pockets. To these we add a minimal model of the interaction anisotropy that allows the hole pockets situated at the Γ point.

The patches 1, … , 3, … , 96 to 49, 48 and 73, … , 96 to the hole pockets situated at the Γ point.

minimal model of the interaction anisotropy that allows to generate gap nodes, we do not consider interactions defined in an orbital representation, but use constant band interactions that only depend on whether the external legs are on hole- or electron-pockets. To these we add an $A_{1g}$ momentum dependence in the inter-band pair hopping interactions $g_4$ with zero total momentum, as suggested recently in [28]. For the electron doped regime, we mostly find non-nodal $s^\pm$, where the scale of the gap anisotropy increases with enhanced intra-band repulsion $g_4$. For highly dominant $g_4$, we indeed find a small parameter regime of nodal $s^\pm$. On the hole-doped side, we first find a rather isotropic $s^\pm$ signal where the scale of anisotropy does not decisively depend on $g_4$. Upon further increasing $g_4$ and hole doping, a phase transition occurs, where both the electron and the hole pockets become nodal: the hole pockets develop a $d$-wave intra-band cooper pairing. This clearly demonstrates the possibility of a doping-dependent gap function. Furthermore, we find that dominant momentum dependence of $g_3$ can increase $T_c$ of $s^\pm$-wave pairing at half filling such that it even exceeds SDW as the previously leading instability. Recent experimental evidence for a superconducting parent compound leaves open the possibility to have a leading superconducting instability even at half filling [33].

4-band model—As a tight-binding model, we constrain ourselves to the 4-band model given by Korshunov and Eremin [24] containing the decisive weight of the density of states in the vicinity of the FS’s (see Fig 1). In the folded BZ with two Fe ions per unit cell, the kinetic Hamiltonian reads:

$$H_0 = -\sum_{k,i,\sigma} \epsilon_i n_{k\sigma} - \sum_{k,i,\sigma} t_i^\alpha d_{k\alpha}^\dagger d_{k\sigma},$$ (1)

where $i$ denotes the band index $i = \alpha_1, \alpha_2, \beta_1, \beta_2$, and the $\epsilon_i$’s are the on-site energies. The hopping dispersion parameters for the $\alpha$ bands around the Γ point are given by $t_i^\alpha = t_i^\alpha (\cos k_x + \cos k_y) + t_i^\alpha \cos k_x \cos k_y$, whereas parameters for the $\beta$ bands around the M point are given by $t_i^\beta = t_i^\beta (\cos k_x + \cos k_y) + t_i^\beta \cos k_x/2 \cos k_y/2$. In units of eV and grouped by $(\epsilon_i, t_i^\alpha, t_i^\beta)$, the parameters take on the values $(-0.60, 0.30, 0.24)$ for $\alpha_1$, $(-0.40, 0.20, 0.24)$ for $\alpha_2$, $(1.70, 1.14, 0.74)$ for $\beta_1$, and $(1.70, 1.14, -0.64)$ for $\beta_2$. The chemical potential can be adjusted such that two hole pockets emerge at the Γ point, whereas two electron pockets emerge at the M point. At half filling, i.e., $\mu = 0$, hole and electron pockets are almost perfectly nested.

Band interactions—We distinguish four types of band interactions. First, there are two types of inter-band interaction vertices depending on whether momentum from ingoing and outgoing propagators is transferred within the same band or between the bands:

$$H_{\text{i}}^\text{inter} = \sum_{k,k',q} g_1 (d_{k+q\sigma}^\dagger d_{k'\alpha\sigma} - q\beta\sigma d_{k'\alpha\sigma}^\dagger d_{k\beta\sigma} + \text{h.c.})$$

$$+ g_2 (d_{k+q\sigma}^\dagger d_{k'\alpha\sigma} - q\beta\sigma d_{k'\alpha\sigma}^\dagger d_{k\beta\sigma} + \text{h.c.}),$$ (2)

with implicit sums over $\sigma, \sigma'$, and the band indices $\alpha$ and $\beta$ extending over $\alpha_1,2$ and $\beta_1,2$, respectively (this convention is kept throughout the article). While $g_1$ turns out to be rather unimportant with respect to the analysis of the leading instabilities driven by band interactions, $g_2$ is necessary (but not sufficient) to drive the SDW instability in the $(\pi, \pi)$ channel between electron and hole pockets in the folded BZ. Furthermore, we consider the inter-band pair hopping interaction $g_3$:

$$H_{\text{i}}^\text{pair} = \sum_{k,k',q} g_3^b (d_{k+q\sigma}^\dagger d_{k'\alpha\sigma}^\dagger - q\alpha\sigma d_{k'\beta\sigma}^\dagger d_{k\beta\sigma} + \text{h.c.}),$$ (3)

where, as one central point of our analysis, we include a momentum dependence of the $A_{1g}$-projected pair hopping amplitude for the zero momentum cooper channel [1]:

$$g_3^b|_{k'=-k} = g_3 (1 + b(\cos k_x + \cos k_y)) \cdot (1 + b(\cos k_x + q_x) + \cos(k_y + q_y)),$$ (4)

and constant $g_3$ otherwise. $b$, the anisotropy scale, gives the relative scale of momentum dependence. To make connection to [1], $g_3$ defined in [1] is given in terms of the unfolded $(u)$ momenta, which relate to the folded

FIG. 1: (Color online) (a) The band structure of the four band model. Electron pocket bands are denoted by $\beta_{1,2}$ and hole pocket bands by $\alpha_{1,2}$. The dashed line shows the Fermi level at half filling. (b) Change of Fermi surfaces upon doping. Bold lines are FS’s at half filling. Upon electron (hole) doping ($x = -0.15$ and $x = 0.15$ shown as dashed lines), the electron (hole) pockets grow while the hole (electron) pockets shrink. (c) Illustration of the patching segments in the Brillouin zone. The patches 1, … , 24 and 49, … , 72 belong to the electron pockets situated at the $M$ point, 25, … , 48 and 73, … , 96 to the hole pockets situated at the $\Gamma$ point.
points (and band index $k$) on the momenta along the electron FS, but gives only a constant value $g_3 \approx 1 + 2b$ on the hole pockets.

$f\text{RG} \text{ method}$— We use the fRG method to study the flow of the two-particle coupling function $V^\Lambda(k_1, a, k_2, b, k_3, c, k_4, d)$, where $k_{1,2}$ ($k_{3,4}$) denote the ingoing (outgoing) particles, $a, \ldots, d$ are the different band indices, and $\Lambda$ is the energy cutoff above which the high energy contributions are integrated out and incorporated into the effective coupling function. Details on the implementation for the multi-band case of pnictides can be reviewed in [16, 23]. While $k_1$ is implicitly given by momentum conservation, the spin convention is chosen such that $k_1$ ($k_2$) and $k_3$ ($k_4$) have the same spin. As usual, we omit the frequency dependence of the vertex, and assume that the relevant processes are located in the close vicinity of the FS. This, together with the neglect of self-energy corrections, is tantamount to a weak-coupling approach initially, although interactions strengths grow large under RG flow. To solve the RG equations numerically, the momenta in the BZ are discretized as shown in Fig. 1. Each momentum is confined within two neighboring dotted lines running from $(\pi, \pi)$ to one of the corner points $(\pi \pm \pi, \pi \pm \pi)$. For a given continuous momentum $k$ and band index $i$, its value is effectively projected onto the Fermi momentum value of the $i$th band in the angle section where $k$ is situated. Testing discretizations of 48, 64, 96, 128, and 256 patches, we find that $N = 96$ both provides sufficient resolution and suitable computation time performance for our studies. Essentially, the RG flow in terms of the cutoff parameter $\Lambda$ starts at cutoff energy scales of the order of the bandwidth, and successively decreases towards the FS. In each differential step, both particle-particle and particle-hole contributions influence the evolution of the coupling function. Quite generically, these flows lead to strong coupling, i.e. one or more channels in the coupling function flow to large absolute values at a critical scale $\Lambda_c$. Comparing the growth of the various pairing and density-wave channels allows one to compare between leading and subleading instabilities. For standard cases, the critical scale $\Lambda_c$ provides a reasonable estimate of the actual critical temperature $T_c$ for phase transitions when long-range ordering is possible.

Electron doping— First we want to specify the parameter window where nodal and non-nodal $s^\pm$ appears for electron doping ($x = 0.2$). We consider the case of $g_1 = 0.1$ and $g_2 = 0.25$, and choose $g_3 = 0.3$ to be of the order of $g_2$ (throughout the article, the interaction couplings are given in units of eV where the total bandwidth is $\sim 6eV$). The $g_3$ anisotropy scale $b$ and $\gamma = g_4/g_3$ span the relevant parameter space of interactions and allow for nodal gaps according to Ref. [1]. For electron doping, the pockets nesting is lifted and the SDW instability is suppressed. For $b \ll 1$, one finds a constant $s^\pm$ instability, as observed in [23], whose critical divergence scale $T_c$ decreases with increasing $\gamma$. The $s^\pm$ instability manifests itself as a Cooper instability corresponding to divergent vertex couplings for $k_1 = -k_2$, with a sign change of the vertex going from electron to hole pockets, as it can be seen both in the vertex plot and the form factors as shown in Fig. 2. Upon increasing $b$, the critical divergence scale increases considerably and helps to counteract the intra-band repulsion $g_4$. In addition, a gap variation starts to emerge on the electron pockets, while the hole pockets remain unchanged. In particular, the gap anisotropy increases upon increasing $\gamma$, which shows that the system favors a nodal variation to compensate the increasing intra-band repulsion $g_4$, as predicted in [3]. However, for $\gamma \lesssim 3$, this anisotropy never becomes comparable to the constant gap scale on the electron pockets, i.e. the nodes do not completely develop. Upon increasing $\gamma$, the gap variation on the electron pockets gets more pronounced, to finally yield a nodal extended s-wave instability (Fig. 2c). However, for increasing $b$ even further at constant $\gamma$, the value of $g_3 \approx 1 + 2b$ on the hole pockets is considerably enhanced and leads to a reduction of gap anisotropy developing on the electron pockets. Hence, while the trends pointed out in Ref. [1] are

![Fig. 2](image_url)
where $\delta$ hole doped scenario still favors a constant system likewise develops a rather constant $\gamma$ and the ratio along the diagonals of the BZ correspond to the $d$-wave function $\Gamma_k$ lines building the rhombohedron centered around the $\Gamma$ point sating from a

In (c1), we observe a leading signal on the hole pockets originating from a $d$-wave pairing, where the nodes can be seen in the form factor $e^{i\mathbf{G} \cdot \mathbf{r}}$, (c3) gives a visualization of the extended $d$-wave state in the unfolded Brillouin zone. The bold dashed lines building the rhombohedron centered around the $\Gamma$ points correspond to $\cos k_x + \cos k_y$ yielding the sign change on the electron pockets around $(\pm \pi, 0)$ and $(0, \pm \pi)$. The dashed lines along the diagonals of the BZ correspond to the $d$-wave function $\cos k_x - \cos k_y$ labelling the nodal points on the hole pockets. Upon folding, we observe that the gaps on the line $\Gamma \rightarrow M$ have opposite signs.

Clearly visible, we only observe a clean nodal $s^\pm$ instability with sign-changes around the electron pockets in a comparably narrow window of intermediate $b$ and high $\gamma$ (see Fig. 2 and Fig. 3). In our understanding, this difference occurs due to the renormalization of the interactions at higher energy scales before the pairing instability sets in. This effect is mentioned but not explicitly taken into account in [1], and hence the parameter ranges for the nodal state differ. Concluding this part, we note that on the electron-doped side, the fully-gapped $s^\pm$-state is rather stable. It is well possible that fine-tuning of the band structure like a strengthening of the scattering between the electron pockets can enhance the anisotropy again, but primary instability favors an isotropic gap.

**Hole Doping**—We now consider hole doping to the system, and choose the same interaction parameters $g_1 = 0.1$, $g_2 = 0.25$, $g_3 = 0.3$. For small anisotropy $b$, the system likewise develops a rather constant $s^\pm$ instability, where $\Delta_c$ decreases with $\gamma$. For considerable values of $b$ and the ratio $\gamma$ as for electron doping, we find that the hole doped scenario still favors a constant $s^\pm$ instability (Fig. 3). Unlike in the electron-doped case, increasing $\gamma$ does not immediately induce gap anisotropy on the electron pockets: the only result (mostly) is a decreasing gap on the hole Fermi surfaces. This behavior can be explained due to the small electron FS size: for hole-doping, the hole FS’s dominate the behavior of the system. The $A_{1g}$ term induces anisotropy mostly on the electron FS’s, which at hole doping are rather small. On the hole pockets, the $A_{1g}$ term increases the size of the constant part of the interaction $g_3$, which favors an $s^\pm$. This, coupled to the fact that the electron FS’s play a rather secondary role with respect to their hole counterparts, renders the symmetry to be $s^\pm$ for moderate $\gamma$. Increased $\gamma$ has the effect of reducing the scale of the superconducting instability. Regarding the gap anisotropy, while in the electron doped-case, increasing $\gamma$ resulted in nodal electron FS’s (while keeping the hole FS’s isotropic nodeless), for hole doping, the situation is completely different. Beyond a critical $\gamma$, when the $s^\pm$ gaps have vanished, the system exhibits a phase transition with nodal superconductivity on both hole and electron FS’s. For $\gamma \gtrsim 2.4$, at comparably low transition temperature, we find that the leading instability becomes a $d$-wave intra-band Cooper pairing on the hole pockets. This is plausible from the FS topology upon doping as shown in Fig. 1: The hole FS’s around $\Gamma$ grow significantly upon hole doping. For dominant intra-band repulsion $g_4$, the favorable ordering becomes a $d$-wave Cooper pairing on the hole pockets, as shown in Fig. 3 In terms of the hole FS only, this is a situation similar to the cuprate superconductors. We also find a subdominant $d$-wave type signal on the electron pockets, which relates to the $d$-wave signal on the hole pockets shifted by $\pi$ so that there is still an overall sign change in the gaps going from the hole pocket to the electron pocket in the unfolded BZ; in this way, the system minimizes both intra and inter-band repulsion: this is the $d$-wave equivalent of the $s^\pm$ instability, which one may denote extended $d^{\pm}$-wave (Fig. 3). This gap symmetry represents another, time-reversal symmetric way to cope with the frustration pointed out in Ref. [34].

While interesting in its own right, the phase diagram on the hole-doped side does not allow for a nodal electron FS while keeping the hole FS fully gapped. If this latter
gap structure turns out to be experimentally correct, we conclude that an $A_1g$ symmetry term alone is not sufficient to make the electron FS nodal while keeping the hole FS fully gapped at both electron and hole doping.

Interplay of SDW and $s^\pm$ at half filling—For all parameter settings discussed in the previous sections, we always find a leading SDW instability as we approach half filling. This is because the SDW instability benefits enormously from the increased nesting of hole and electron pockets. However, we observe that upon further increasing $b$, the $s^\pm$ instability can overcome SDW and becomes the leading instability even at half filling. This is illustrated in Fig. 4. There, we find that upon changing $b$ from 1.5 to 1.8, the $s^\pm$ instability becomes dominant. The $b_c$, where this occurs increases with $\gamma$. Interestingly, the critical scale is not suppressed between the two regimes which in a less approximate treatment would be most likely separated by a first-order transition. This means that a slight change of the system parameters can turn the system from a high-scale SDW into a $s^\pm$ state with comparable pairing scale - another possibility for a marked material-dependence of the phase diagrams of different pnictides, which may relate to recent measurements reported on in [33].

Full Phase Diagram—For various interactions settings, we computed the complete phase diagram for different fillings and anisotropy $b$, four representatives of which are shown with increasing $\gamma$ in Fig. 5 and Fig. 6. We observe that for comparably small $\gamma$, the phase diagram looks rather uniform and only contains SDW and $s^\pm$ with moderate gap variation as leading instabilities. For larger $\gamma$ and generally reduced $T_c$ due to strong intra-band repulsion, the phase diagram shows a more complex structure including the extended d-wave instability on the hole doped side and the increasingly pronounced $s^\pm$ gap variation for the electron doped side, which finally yields a small parameter window of nodal $s^\pm$ for very large $\gamma$ (Fig. 6b). Thus, we find smoothly connected instabilities at comparable scales, pointing to competing orders. This, however, suggests a potentially high sensitivity to material-specific parameters.

Conclusion—We studied the effect of certain momentum dependence of band interactions for a 4-band model of the pnictides by adding an $A_{1g}$-symmetric term to the pair-hopping interactions, while keeping all other band interactions constant. While most of our data shows, in agreement with previous results, an $s^\pm$ wave superconducting instability, on the electron doped side, we find that increasing intra-band repulsion enhances the gap anisotropy on the electron pockets, which may ultimately, but not readily, lead to a true nodal electron FS gap. For the hole-doped regime, however, the gap anisotropy remains rather small even on the electron FS upon increasing the interaction anisotropy, until a critical value of the intra-band repulsion beyond which the system favors an interesting state with intra-band d-wave Cooper pairing on the hole pockets and a reminiscent extended and sign-reversed d-wave signal on the electron pockets. This represents a novel way to reduce the repulsion within and between the Fermi surface pockets. However, in the range of our model, we are unable to find a regime which satisfies the conditions of having gapped hole FS and nodal electron FS for both electron and hole doping.
feature fully-gapped $s^\pm$ superconducting states. Alternatively, if the experiments confirm gap nodes, this would indicate a strong anisotropy of the bare interaction and a stronger role of other repulsive interaction, e.g., between the electron pockets. In this case, electron- and hole-doping may well lead to different pairing states, and even undoped superconductivity could be obtained for relatively mild parameter changes. One can ask how much these findings depend on the type of anisotropy of the bare interaction. In our understanding any pronounced wave vector-dependence of the interaction will very likely cause differences between electron and hole doping, as the relevant hole- or electron Fermi surfaces are located in different regions of the Brillouin zone. Likewise, for the undoped system, a strong interaction anisotropy generally enhances pairing states competing with the SDW order such that material-specific parameter differences might lead to observable consequences even in the undoped state. The trends observed in our study should hold for any specific choice of anisotropy in general.

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