Gap symmetry and stability analysis in the multi-orbital Fe-based superconductors

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Abstract. The iron-based superconductors allow for a zoo of possible order parameters due to their orbital degrees of freedom. These order parameters are often written in an orbital basis for a microscopic analysis and a comprehensive symmetry classification. Unlike in standard single-band superconductors, where electrons of the same band—and hence, energy—are paired, a general order parameter in such a multi-orbital system also contains pairing of electrons belonging to different bands. As this corresponds to pairing of electrons of different energy, such order parameters are energetically less stable. Here, we present a simple criterion for a stability analysis of the orbital part of the gap function based on the basic principle that electrons of equal energy are paired in the superconducting state. This not only allows us to find the most stable states, but also to identify the terms in a (tight-binding) Hamiltonian suppressing any given superconducting state. Our approach thus allows us to identify the minimal Hamiltonian necessary to compare competing instabilities.
1. Introduction

The symmetry classification of superconducting order parameters has proven to be a powerful tool in the context of unconventional superconductivity [1]. In single-band superconductors, one distinguishes various gap functions $\Delta(k)$ according to their behavior under all the symmetry transformations of the generating point group of the crystal, i.e. the irreducible representation they belong to. While the interactions are the dominant factor for determining the pairing channel, many interactions allow for instabilities of different symmetry. With only gap functions belonging to the same irreducible representation mixing, this allows one to find each class’ critical temperature and thus the dominant pairing channel. An interaction with dominant nearest-neighbor character on a square lattice, such as antiferromagnetic spin fluctuations, for example, allows for extended-$s$-, or $d$-wave (singlet) order parameters, which can be analyzed independently for the leading instability [2].

In the Fe-based superconductors, several bands are involved in the low-energy physics. According to bandstructure calculations, the main contribution to the density of states at the Fermi level stems from Fe d orbitals hybridizing with As p orbitals [3, 4]. In most compounds, the bands crossing the Fermi energy have mainly $d_{xz}$ and $d_{yz}$ orbital character and thus, minimal tight-binding models consider only these two orbitals [5–7]. After back-folding of the Brillouin zone due to the out-of-plane positions of the As ions leading to a two-Fe unit cell, these models indeed yield an overall agreement with the experimentally found Fermi surfaces. However, at least the three $t_{2g}$ orbitals have to be considered in order to find an agreement in the Fermi velocities as well [8, 9].

This multi-orbital nature of the Fe-pnictides complicates any order parameter analysis. The additional orbital degrees of freedom lead to an abundance of gap functions, which are
now matrices in orbital space\(^1\). A symmetry classification of all possible gap functions with respect to the generating point group \(D_{4h}\) of the Fe–As layer has been done for two-, as well as three-orbital models for example in \([11, 12]\) and \([13]\), respectively. One difficulty arising with such an analysis is that the order parameter has to be written in orbital space, whereas the pairing of electrons in the standard theory of Bardeen, Cooper and Schrieffer (BCS) is best described in band space. Indeed, only pairing of electrons with the same energy, hence belonging to the same band, leads to a superconducting instability. While the analytical transformation into the band basis to analyze the stability of an order parameter is straightforward in a two-orbital description \([11, 12, 14]\), the generalization to three or even more orbitals is not possible. Alternatively, the loss of condensation energy due to nodes can be used as a criterion for the stability of the various gap functions. This requires knowledge of all the nodes of a given gap function and also only allows for an even cruder first estimate.

In this work, we build on the aforementioned pairing of equal-energy electrons and present a simple criterion to analyze the stability of a gap with a given orbital structure. Simply speaking, we analyze whether a gap structure corresponds to a pure intra-band pairing, or whether electrons belonging to different bands are paired. For a systematic analysis, a comprehensive symmetry analysis of the free Hamiltonian and the order parameter, both matrices in orbital space, is necessary first. Our approach then also allows us to identify the terms in the Hamiltonian that (partially) suppress the other gap structures. This has an important application in determining the minimal Hamiltonian needed to (numerically) compare different superconducting instabilities on equal footing. Note that such an analysis is unlike comparing extended-s- and d-wave paring in the single-band case, where always electrons belonging to the same band are paired. Here, the suppression is due to inter-band pairing, more comparable to the suppression of spin-singlet superconductivity due to a magnetic field.

After introducing the general scheme in the next section, we apply it to the case of the iron-based superconductors. In order to construct the general tight-binding models, we start in section 3 with a few comments on the symmetry of the Fe–As layer and its generating point group \(D_{4h}\). We then focus our discussion in section 4 on a two-orbital description of the Fe–As layer and, with experiments strongly supporting spin-singlet pairing, we restrict our analysis on this pairing channel \([15, 16]\). The two-orbital model carries the advantage that we can gain additional analytical insight from the linearized gap equation. Finally, we also comment on the three-orbital model in section 5. As a starting point for both models, we present a comprehensive symmetry analysis of the Hamiltonian and the gap structures including the two-Fe unit cell. As an interesting result, we find that the extended-s and \(d_{x^2-y^2}\)-wave pairing in the (two-Fe unit cell) three-orbital model is (partially) suppressed by the hybridization of the \(d_{xz}/d_{yz}\) with the \(d_{xy}\) orbitals, whereas this suppression is missing in general two-orbital models or when working with a one-Fe unit cell.

2. Symmetry and stability in multi-orbital systems

2.1. Single-band systems

Before discussing the multi-orbital case, we give a brief overview over some symmetry aspects and notation for a superconductor in a single-band system. Only considering spin-singlet superconductivity, the mean-field Hamiltonian is a \(2 \times 2\) matrix in Nambu space,

\(^1\) This is similar to the spin-space matrices used when describing spin-triplet pairing \([10]\).
\[ \Psi_k = (c_{k\uparrow}, c_{-k\downarrow}^\dagger), \] given by

\[ H_{MF}(k) = \begin{pmatrix} \mathcal{H}_0^+(k) & \Delta(k) \\ \Delta^*(k) & -\mathcal{H}_0^+( -k) \end{pmatrix}, \tag{1} \]

\[ \mathcal{H}_0^+(k) = \mathcal{H}_0^+( -k) = \xi_k(= \xi_{-k}) \] is the free hopping Hamiltonian and \( \Delta(k) = \Delta \psi(k) \) is the superconducting order parameter or gap function. Since \( \xi_k \) describes the non-interacting system, it has to transform trivially under time reversal and all the symmetry operations of the generating point group \( G \) of the crystal. From the transformation behavior of the single-particle operator under \( g \in G \), \( g c_k = c_{gR_k} \) and \( R_g \) the corresponding rotation matrix in momentum space, we find \( \xi_{gR_k} = \xi_k \) for all \( g \in G \). In a similar way, the pair-wave functions \( \psi(k) \) are symmetry classified in terms of the irreducible representations of \( G \), i.e. their behavior under \( \psi(k) \mapsto \psi(R_gk) \). Note that the Pauli principle requires the full gap function to change sign under the exchange of the two electrons, leading to the well-known requirement that an even wave function \( \psi(k) \) is combined with spin-singlet pairing. Within BCS theory, the mechanism of superconductivity requires the pairing of electrons of equal energy. In the above Hamiltonian, the gap function always connects two electrons with the same energy, thus allowing for a superconducting instability for arbitrary small (attractive) interactions.

### 2.2. Multi-orbital systems

In a system with \( n \) orbitals, the Hamiltonian and the (spin-singlet) gap function are \( n \times n \) matrices in orbital space, leading to a mean-field Hamiltonian analogous to equation (1) that is a \( 2n \times 2n \) matrix

\[ H_{MF}(k) = \begin{pmatrix} \hat{H}_0(k) & \hat{\Delta}(k) \\ \hat{\Delta}^*(k) & -\hat{H}_0(k) \end{pmatrix}, \tag{2} \]

where we have again assumed time-reversal and inversion symmetry and for simplicity omitted any spin–orbit coupling. The Hamiltonian in orbital space is of the general form:

\[ \hat{H}_0(k) = \sum_a \hat{\Lambda}^a h_a(k), \tag{3} \]

where \( \{ \hat{\Lambda}^a \} \) is a basis for the \( n \times n \) matrices. The Hamiltonian equation (2) still has to transform trivially under all the symmetry operations of the generating point group \( G \). Since the symmetry transformations now act on the basis functions as \( g \tilde{c}_k = \hat{U}_g \tilde{c}_{R_gk} \), the individual elements of the Hamiltonian (3) transform as

\[ g[\hat{\Lambda}^a h_a(k)] = (\hat{U}_g \hat{\Lambda}^a \hat{U}_g^\dagger) h_a(R_gk). \tag{4} \]

For matrices and functions that transform as one-dimensional representations, simply the product of them has to transform trivially. For higher-dimensional representations, multiple matrices and momentum functions can be combined (such an example is shown in section 5). It is thus helpful to write the Hamiltonian as

\[ \hat{H}_0(k) = \hat{H}_0^0(k) + \sum_a \hat{H}_0^a(k), \tag{5} \]

For simplicity, we only consider time-reversal and inversion symmetric systems.
where $\mathcal{H}_0^0(k)$ is proportional to the $n \times n$ identity matrix and $\hat{\mathcal{H}}_0^\alpha(k)$ are all the other smallest parts transforming trivially.

The (spin-singlet) superconducting order parameter $\hat{\Delta}(k)$ can similarly be written as

$$\hat{\Delta}(k) = \sum_a \hat{\lambda}^a \psi_a(k).$$

This order parameter can now describe the pairing of electrons of all possible orbitals. As for

$$g[\hat{\Delta}(k)] = \sum_a (\hat{U}_g \hat{\lambda}^a \hat{U}_g^\dagger) \psi_a(R_g k).$$

The multi-orbital structure leads to a plethora of different gaps due to the additional degree of freedom. Most of these gaps will, however, lead to inter-band pairing and are thus less (or not at all) stable. After a brief discussion of the stability of general gap structures, we will see in section 4 for the two-orbital model and in section 5 for the three-band model an explicit symmetry classification and stability analysis of such order parameters.

### 2.3. Stability of the gap structures

In this section, we discuss a simple qualitative argument for the stability of gap structures and show that only the ones with $[\hat{\mathcal{H}}_0(k), \hat{\Delta}(k)] = 0$ are fully supported by the Hamiltonian. For a quantitative stability analysis of the terms in the Hamiltonian harming the superconducting state, one can for example resort to the linearized gap equation as done analytically for a two-band model in section 4.3. The superconducting instability requires to pair electrons of equal and opposite momentum, and most importantly, equal energy. For a gap structure that commutes with the orbital structure of the Hamiltonian, i.e. $[\hat{\mathcal{H}}_0(k), \hat{\Delta}(k)] = 0$, $\hat{\mathcal{H}}_0(k)$ and $\hat{\Delta}(k)$ can both be simultaneously diagonalized by the same $n \times n$ matrix $\hat{U}_k$. The block-diagonal matrix with the two blocks $\hat{U}_k$ thus leads to a diagonal form of the mean-field equation (2) with the gap only connecting states with equal energy, i.e. the gap function describes intra-band pairing only. If $[\hat{\mathcal{H}}_0(k), \hat{\Delta}(k)] \neq 0$, we define the set $L = \{\alpha | [\hat{\mathcal{H}}^\alpha, \hat{\Delta}(k)] = 0\}$ and write the Hamiltonian as

$$\hat{\mathcal{H}}_0(k) = \hat{\mathcal{H}}_0^0(k) + \sum_{\alpha \in L} \hat{\mathcal{H}}_0^\alpha(k) + \sum_{\beta \notin L} \hat{\mathcal{H}}_0^\beta(k)$$

with the first sum commuting with $\hat{\Delta}(k)$, while the second sum does not. If the Hamiltonian consisted of only the first two terms, the gap structure would describe intra-band pairing only and would be fully supported. The last sum, however, leads to inter-band contributions. The fact that there are terms in this last sum does, however, not necessarily lead to a full suppression of the instability. As we will see explicitly for the two-band model, the stability instead depends on the respective energy scales of the two groups of terms. This scheme thus allows for a first estimate of the stability of all possible gap functions and also provides an insight into what terms in the non-interacting Hamiltonian harm a specific superconducting gap function.

### 3. Symmetry of the Fe–As layer

In order to apply the above scheme, we first recapitulate the symmetry properties of a single Fe–As plane [8, 13]. Figure 1(a) shows the structure of the Fe–As layer with its two-sublattice
Figure 1. (a) Crystal structure of the Fe–As layer with the two Fe sublattices A (dark circles) and B (white circles). The small crosses (dots) in the middle of the Fe squares are the As sites above (below) the plane. Also, the symmetry operations belonging to $D_{2d}$ are depicted with $C_2$ and $S_4$ being around the square on one of the Fe sites. Finally, the star between two iron sites denotes a center of inversion. (b) Orbital basis for the two-Fe unit cell.

structure due to the out-of-plane positions of the As ions. The individual (two-Fe) unit cell is invariant under the following symmetry operations. The identity $E$, a two-fold rotation $C_2$ and two improper rotation $S_4$, both around the $z$-axis, two two-fold rotations $C_{2}^\prime$ around the $x$ ($y$) axis, as well as two mirror planes $\sigma_d$ along the diagonals of the $xy$-plane, together building the point group $D_{2d} = \{E, C_2, 2C_{2}^\prime, 2S_4, 2\sigma_d\}$. Note that the generating point group of the layer is isomorphic to $D_{4h}$, where all the elements $D_{4h}\backslash D_{2d}$ have to be combined with a lattice translation interchanging the two sublattices. Taking this into account ensures having the inversion as a symmetry element of the layer, though not the unit cell. This is crucial for both, the construction of the Hamiltonian as well as the classification and analysis of the superconducting order parameter.

4. Two-orbital model

4.1. Hopping Hamiltonian

In this section, we discuss the symmetry allowed terms of the multi-orbital hopping Hamiltonian based on the $d_{xz}$ and $d_{yz}$ orbitals with real-space operators $d_{is}^{(xz)}$ and $d_{is}^{(yz)}$, respectively. We work with the two-Fe unit cell, and hence, additionally introduce the states $\tilde{d}_{is}^{(xz)}$ and $\tilde{d}_{is}^{(yz)}$, where the orbitals on the B sublattice are multiplied by $-1$ (see figure 1(b)). In momentum space, this translates to having two operators $d_{k}\tilde{c}_{k}^{(xz)} / d_{k}^{(xz)}$ and $d_{k}\tilde{c}_{k}^{(yz)} / d_{k}^{(yz)}$, respectively, with $Q = (\pi, \pi)$. It is thus convenient to work in a tensor space of the $(d_{xz}, d_{yz})$ orbital space and the $(k, k + Q)$ momentum space. The Hamiltonian can then be factorized in analogy to equation (3) as

$$H_0 = \sum_{k, s} \tilde{c}_{k}^{\dagger} \left[ \sum_{a, b} \tilde{S}_{ab} h_{ab}(k) \right] \tilde{c}_{k}$$  (9)

$^3$ A crystal with this property is called non-symmorphic.
summarizes all the hopping factors. Table 1 shows the classification of all the matrices to be combined with the trivial representation \( \hat{\tau}^0 \) to third-nearest-neighbor hopping together with the symmetries under inversion \((u/g)\), while the behavior under the symmetry transformations of the unit cell \((D_{2h})\) is given by the orbital part \( \hat{\rho}^a \) (see appendix A).

| IR(\(D_{2h}\)) | \( A_{1g} \) | \( A_{2g} \) | \( B_{1g} \) | \( B_{2g} \) | \( A_{1u} \) | \( A_{2u} \) | \( B_{1u} \) | \( B_{2u} \) |
|----------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| \( \hat{\Sigma}^{ab} \) | \( \hat{\Sigma}^{00} \), \( \hat{\Sigma}^{03} \) | \( \hat{\Sigma}^{20} \), \( \hat{\Sigma}^{23} \) | \( \hat{\Sigma}^{10} \), \( \hat{\Sigma}^{13} \) | \( \hat{\Sigma}^{31} \), \( \hat{\Sigma}^{32} \) | \( \hat{\Sigma}^{11} \), \( \hat{\Sigma}^{12} \) | \( \hat{\Sigma}^{01} \), \( \hat{\Sigma}^{02} \) | \( \hat{\Sigma}^{21} \), \( \hat{\Sigma}^{22} \) |

Table 2. The basis functions for hopping terms \( h_{ab}(\mathbf{k}) \) up to third-nearest neighbors classified in terms of irreducible representations of \( D_{4h} \). The functions are divided into the ones that change sign for \( \tau_3 (\hat{\tau}^3) \) in the Hamiltonian, and those that do not, thus allowing for combinations with \( \hat{\tau}^0 (\hat{\tau}^1) \).

| IR | \( \hat{\tau}^0 \) | \( \hat{\tau}^3 \) |
|----------------|-------------|-------------|
| \( A_{1g} \) | 1, \( \cos k_x \cos k_y \), \( \cos 2k_x + \cos 2k_y \), \( \cos k_x + \cos k_y \) | \( \cos k_x - \cos k_y \) |
| \( B_{1g} \) | \( \cos 2k_x - \cos 2k_y \) | \( \cos k_x - \cos k_y \) |
| \( B_{2g} \) | \( \sin k_x \sin k_y \) | \( - \) |
| \( \hat{\tau}^1 \) | \( \hat{\tau}^2 \) |
| \( E_u \) | \( \{ \sin k_x \cos k_y, \sin k_x \cos k_y \} \) | \( \{ \sin k_x \sin k_y \} \) |

The Hamiltonian reads

\[
\mathcal{H}_0 = \sum_{k,s} \hat{\Sigma}^{00}_{ks} h_{00}(\mathbf{k}) + \hat{\Sigma}^{03}_{ks} h_{03}(\mathbf{k}) + \hat{\Sigma}^{30}_{ks} h_{30}(\mathbf{k}) + \hat{\Sigma}^{33}_{ks} h_{33}(\mathbf{k}) + \hat{\Sigma}^{10}_{ks} h_{10}(\mathbf{k}) |\tilde{\rho}_{ks}^{(x)}| \tag{10}
\]
Figure 2. Sketch of the possible spin-singlet gap structures in momentum space with the full $A_{1g}$ symmetry. Panel (a) shows the standard s- and panel (b) extended-s- and (c) $s_{\pm}$-wave gap functions. Panels (d) and (e) are possible fully symmetric gap functions with band and momentum structure belonging to $B_{1g}$ and $B_{2g}$, respectively. The two colors depict the sign change of the gap and the dashed (dotted) lines the nodes of the momentum (orbital) part of the gap.

with $h_{00}(\mathbf{k}) = 4t_{2g} \cos k_x \cos k_y + 2t_{3g}(\cos 2k_x + \cos 2k_y) - \mu$, $h_{03}(\mathbf{k}) = 2t_{1g}(\cos k_x + \cos k_y)$, $h_{30}(\mathbf{k}) = 2t_{3d}(\cos 2k_x - \cos 2k_y)$, $h_{33}(\mathbf{k}) = 2t_{1d}(\cos k_x - \cos k_y)$ and $h_{10}(\mathbf{k}) = 4t_{2d} \sin k_x \sin k_y$. Note that these hopping terms correspond to isotropic hopping along the $x$- and $y$-axis ($h_{00}(\mathbf{k})$ and $h_{03}(\mathbf{k})$), anisotropic hopping with respect to the axes ($h_{30}(\mathbf{k})$ and $h_{33}(\mathbf{k})$), as well as inter-orbital hopping ($h_{10}(\mathbf{k})$). The Hamiltonian (10) has four bands with dispersions

$$\xi^{(a)}_{\pm}(\mathbf{k}) = \epsilon^{(a)}_{\pm}(\mathbf{k}) \pm \sqrt{[\epsilon^{(a)}_{-}(\mathbf{k})]^2 + [h_{10}(\mathbf{k})]^2}$$

(11)

with $\epsilon^{(1/2)}_{+}(\mathbf{k}) = h_{00}(\mathbf{k}) \pm h_{03}(\mathbf{k})$, $\epsilon^{(1/2)}_{-}(\mathbf{k}) = h_{30}(\mathbf{k}) \pm h_{33}(\mathbf{k})$ and $a = (1, 2)$ for the subspace of $(\mathbf{k}, \mathbf{k} + \mathbf{Q})$. Note that no terms transforming trivially can be constructed containing the matrices $\hat{\tau}^1$ or $\hat{\tau}^2$ and thus, there is no allowed coupling terms between $\mathbf{k}$ and $\mathbf{k} + \mathbf{Q}$. The first Brillouin zone is thus only artificially folded down to the two-Fe zone. Terms that explicitly fold the Brillouin zone in such a two-orbital description necessarily involve spin–orbit coupling. When sketching the gap functions below, we thus consider only one of the two subspaces for simplicity.

4.2. Gap classification and stability

Only considering spin-singlet gap functions already allows for a large variety of different gap functions (see e.g. [11, 12]). The combination of all the matrices from table 1 with momentum functions from table 2 allows for 54 different order parameters and we thus discuss only some examples. Figure 2 sketches the $A_{1g}$ gap functions with momentum parts going up to next-nearest neighbors and only showing one of the momentum subspaces in the one-Fe Brillouin zone. In addition to the conventional s-wave, extended-s and $s_{\pm}$ gap functions, given by

$$\hat{\Delta}(\mathbf{k}) = \hat{\Sigma}^{00},$$

(12)

$$\hat{\Delta}(\mathbf{k}) = \hat{\Sigma}^{03}(\cos k_x + \cos k_y),$$

(13)

$$\hat{\Delta}(\mathbf{k}) = \hat{\Sigma}^{10} \cos k_x \cos k_y$$

(14)
Figure 3. Momentum space representations of the gap functions with \(B_{1g}\) (a)–(c) and \(B_{2g}\) (d and e) symmetry. Panel (a) is the standard \(d_{x^2-y^2}\)- and (d) the \(d_{xy}\) wave gap. Panels (b), (c) and (e) have an \(A_{1g}\) momentum dependence combined with a \(B_{1g}\) and \(B_{2g}\) band dependence, respectively. In addition to the nodes dictated by their momentum part (dashed lines), they thus also have nodes coming from their orbital structure (dotted lines).

also gap functions with gap nodes on the Fermi surface around the \(\Gamma\) point, namely
\[
\Delta(k) = \tilde{\Sigma}^{33}(\cos k_x - \cos k_y), \tag{15}
\]
\[
\Delta(k) = \tilde{\Sigma}^{10} \sin k_x \sin k_y \tag{16}
\]
are shown.

Figure 3 shows gap functions that transform as \(B_{1g}\) and \(B_{2g}\). These are, first, the so-called \(d_{x^2-y^2}\)-wave gap (figure 3(a))
\[
\tilde{\Delta}(k) = \tilde{\Sigma}^{03}(\cos k_x - \cos k_y) \tag{17}
\]
and \(d_{xy}\)-wave gap (figure 3(d))
\[
\tilde{\Delta}(k) = \tilde{\Sigma}^{00} \sin k_x \sin k_y. \tag{18}
\]
In addition, three gap structures are shown with a ‘trivial’ momentum part in combination with a \(B_{1g}\) (figures 3(b) and (c)) and \(B_{2g}\) (figure 3(e)) orbital part, respectively,
\[
\tilde{\Delta}(k) = \tilde{\Sigma}^{33}(\cos k_x + \cos k_y), \tag{19}
\]
\[
\tilde{\Delta}(k) = \tilde{\Sigma}^{30} \cos k_x \cos k_y, \tag{20}
\]
\[
\tilde{\Delta}(k) = \tilde{\Sigma}^{10} \cos k_x \cos k_y. \tag{21}
\]
The gap structures with non-trivial orbital part in equations (15) and (16), as well as (19)–(21) have not only gaps due to their momentum dependence (dashed lines), but also their orbital dependence (dotted lines). Note, however, that here the former ones are not protected by symmetry and thus any admixture of other gap structures belonging to the same irreducible representation can shift or open these nodes. Nevertheless, these gaps by themselves are not fully gapped and hence, in general less stable.

The fact that the gaps with non-trivial orbital structure have (additional) nodes and thus a reduced superconducting condensation energy already points toward less stable superconductivity. Even without the knowledge of these gap nodes, we can analyze the
stability of the above gap structures using the criterion introduced in section 2. All the gap structures that transform trivially in the two subspaces \((\mathbf{k}, \mathbf{k} + \mathbf{Q})\), namely the ones defined in equations (12)–(14), (17) and (18), commute with the free Hamiltonian (10). These gap structures are thus intra-band only and fully supported. However, the gap structures with non-trivial orbital parts do not commute with the Hamiltonian (10). The gap structures defined in equations (15), (19) and (20) do not commute with the term \(\tilde{\Sigma}^{10} h_{10}(\mathbf{k})\) in the Hamiltonian (10), while they commute with all the other terms. This means that these gap functions are suppressed by inter-orbital hopping. The gap structures in equations (16) and (21), on the other hand, do not commute with the terms \(\tilde{\Sigma}^{30} h_{30}(\mathbf{k})\) and \(\tilde{\Sigma}^{33} h_{33}(\mathbf{k})\), i.e. they are suppressed by the ‘one-dimensional nature’ of the \(d_{xz}\) and \(d_{yz}\) bands.

Finally, we comment on the peculiar gap structures that combine an odd momentum function with spin-singlet pairing. In order to obey the Pauli principle, either \(\hat{\rho}^2\) or \(\hat{\tau}^2\) has to appear in the decomposition of \(\tilde{\Sigma}^{ab}\). Examples are

\[
\hat{\Delta}(\mathbf{k}) = \hat{\Sigma}^{02} \sin k_x
\]

belonging to the two-dimensional representation \(E_g\), or

\[
\hat{\Delta}(\mathbf{k}) = \hat{\Sigma}^{23} \sin k_x
\]

belonging to \(E_u\). The former gap structure corresponds to finite-momentum pairing in the one-Fe zone and it is thus suppressed. The latter gap structure only commutes with the terms proportional to \(\hat{\Sigma}^{00}\) and \(\hat{\Sigma}^{03}\) in the Hamiltonian (10). From our discussion so far, we hence also expect this gap structure to be suppressed. Calculating the linearized self-consistency equation in the next section, we can explicitly analyze how the various terms influence the pairing instability for the above gap structures.

4.3. Linearized gap equation

In this section, we evaluate the linearized self-consistency equation for the gap structures to see explicitly how the criterion introduced in section 2 works out. For this purpose, we introduce a spin-singlet pairing interaction of the general form

\[
\mathcal{H}' = \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} V_{ab,\mu\nu}(\mathbf{k}, \mathbf{k}') \hat{C}_{\mathbf{k}k\uparrow}^\dagger \hat{C}_{\mathbf{k}' - \mathbf{k} \downarrow}^\dagger \hat{C}_{\mathbf{\nu}k\downarrow} \hat{C}_{\mathbf{\mu}k\uparrow}.
\]

(We use the convention of summing over repeated indices.) In the framework of the Gorkov equations, we find the linearized gap equation

\[
\Delta_{ab}(\mathbf{k}) = -T \sum_{\omega_n, \omega_{n'}} \sum_{\mathbf{k}'} V_{ab,\mu\nu}(\mathbf{k}, \mathbf{k}') \times \left[ \hat{G}_0(\mathbf{k}', \omega_n) \hat{\Delta}(\mathbf{k}') \hat{G}_0^\dagger (-\mathbf{k}', -\omega_n) \right]_{\mu\nu},
\]

where \(\hat{G}_0(\mathbf{k}, \omega_n) = [i\omega_n \hat{\Sigma}^{00} - \hat{\mathcal{H}}_0(\mathbf{k})]^{-1}\) is the non-interacting Green’s function with \(\omega_n = (2n + 1)\pi T\) the fermionic Matsubara frequencies. This equation determines the critical temperature \(T_c\) for a given gap structure, where the largest \(T_c\) belongs to the leading instability. Parameterizing the interaction similar to equation (6),

\[
V_{ab,\mu\nu}(\mathbf{k}, \mathbf{k}') = \sum_{a, b} \sum_{l} V_{ab}^{(l)} \left[ \hat{\Sigma}_{ab} \psi_{ab}^{(l)}(\mathbf{k}) \right]_{\mu\nu} \times \left[ \hat{\Sigma}_{ab} \psi_{ab}^{(l)}(\mathbf{k}') \right]_{\mu\nu}^\dagger
\]

with \(\psi_{ab}^{(l)}(\mathbf{k})\) the individual basis functions from table 2, we find the self-consistency equation for each individual gap structure.
We neglect here all possible gap mixing and only focus on the diagonal elements. We first consider gap structures that commute with the Hamiltonian, namely the ones with a ‘trivial’ structure $\Sigma^{00}$ and $\Sigma^{03}$, respectively, given in equations (12)–(14), (17) and (18). After summation over the Matsubara frequencies, the linearized gap equation for each gap reads

$$1 = -v^{(l)}_{ab} \sum_{\mathbf{k}} \sum_{a} \sum_{\alpha=\pm} \left[ \psi_{a}^{(l)}(\mathbf{k}') \right]^{2} \frac{\xi_{\alpha}^{a}(\mathbf{k}')}{2\xi_{\alpha}^{a}(\mathbf{k}')} \tanh \left( \frac{\xi_{\alpha}^{a}(\mathbf{k}')}{2T} \right),$$

where $ab = 00, 03$ and $\psi_{a}^{(l)}(\mathbf{k})$ is the momentum part of the respective gap. In this equation, every state with energy close to the Fermi energy adds to the instability due to the intra-band (equal-energy) character of the pairing with an instability even for an infinitesimal attractive interaction due to the divergence for $T \to 0$. As expected, these gap structures are thus fully supported by the hopping Hamiltonian.

The non-trivial gap structures from equations (15) and (19) (and analogously for equation (20)) yield a self-consistency equation of the form

$$1 = -v^{(l)}_{33} \sum_{\mathbf{k}',\alpha,a} \left\{ \frac{[\varepsilon_{\alpha}^{a}(\mathbf{k}')]^{2}}{[h_{10}(\mathbf{k}')]^{2} + [\varepsilon_{\alpha}^{a}(\mathbf{k}')]^{2}} \left[ \psi_{a}^{(l)}(\mathbf{k}') \right]^{2} \frac{\xi_{\alpha}^{a}(\mathbf{k}')}{2\xi_{\alpha}^{a}(\mathbf{k}')} \tanh \left( \frac{\xi_{\alpha}^{a}(\mathbf{k}')}{2T} \right) \right\}.$$  

Note that the first term on the right-hand side again corresponds to intra-band pairing with the $T \to 0$ divergence, whereas the second term comes from inter-band pairing and has no such divergence. Hence, this self-consistency equation still allows for a solution for an infinitesimal interaction, however, $T_{c}$ is suppressed. As expected from the discussion in the previous section, the ratio $h_{10}(\mathbf{k})/\varepsilon_{\alpha}^{a}(\mathbf{k})$ determines the strength of the instability. Analogously, we find that

$$1 = -v^{(l)}_{10} \sum_{\mathbf{k}',\alpha,a} \left\{ \frac{[h_{10}(\mathbf{k}')]^{2}}{[h_{10}(\mathbf{k}')]^{2} + [\varepsilon_{\alpha}^{a}(\mathbf{k}')]^{2}} \left[ \psi_{a}^{(l)}(\mathbf{k}') \right]^{2} \frac{\xi_{\alpha}^{a}(\mathbf{k}')}{2\xi_{\alpha}^{a}(\mathbf{k}')} \tanh \left( \frac{\xi_{\alpha}^{a}(\mathbf{k}')}{2T} \right) \right\}.$$  

for the gap functions from equations (16) and (21) with the same structure as equation (28). Finally, for the gap structure given in equation (23) we find that

$$1 = -v^{(l)}_{23} \sum_{\mathbf{k}'} \sum_{a} \sum_{\alpha=\pm} \left\{ \frac{\sin k_{x}'}{2\xi_{\alpha}^{a}(\mathbf{k}')} \tanh \left( \frac{\xi_{\alpha}^{a}(\mathbf{k}')}{2T} \right) \right\}.$$  

This gap function is only describing inter-band pairing and thus has no $T \to 0$ divergence and associated instability for an arbitrarily small interaction any more.

5. Three-orbital model

We now turn to the three-orbital model, where in addition to the $d_{xz}$ and $d_{yz}$ orbitals, also the $d_{xy}$ orbital is introduced. This is necessary for an accurate description of the low-energy electronic
Table 3. Classification of the Gell–Mann matrices in terms of irreducible representations of $D_{2d}$. The momentum part $\hat{\tau}^b$ then determines how the matrices $\hat{\lambda}^{ab} = \hat{\lambda}_a \otimes \hat{\tau}_b$ behave under inversion and thus what irreducible representation they belong to (see appendix A for details).

| IR($D_{2d}$) | $\hat{\lambda}^i$ |
|--------------|-------------------|
| $A_1$        | $\hat{\lambda}^0$, $\hat{\lambda}^8$ |
| $A_2$        | $\hat{\lambda}^2$ |
| $B_1$        | $\hat{\lambda}^3$ |
| $B_2$        | $\hat{\lambda}^1$ |
| $E$          | $\{\hat{\lambda}^4, \hat{\lambda}^6\}$, $\{\hat{\lambda}^5, \hat{\lambda}^7\}$ |

structure and we hence briefly repeat the analysis of the symmetry and stability of the gap functions. The Hamiltonian can again be factorized as

$$H_0 = \sum_{k,s} \vec{c}_{ks}^\dagger \left[ \sum_{a,b} \hat{\Lambda}^{ab} h_{ab}(\mathbf{k}) \right] \vec{c}_{ks},$$

where now

$$\vec{c}_{ks} = (d_{ks}^{(xz)}, d_{ks}^{(yz)}, d_{ks}^{(xy)}, q_{ks+Qx}^{(xz)}, q_{ks}^{(yz)}, q_{ks+Qy}^{(xy)}, d_{ks+Qz}^{(xz)}, d_{ks+Qz}^{(yz)})^T.$$  

We have introduced the matrices $\hat{\Lambda}^{ab} = \hat{\lambda}^a \otimes \hat{\tau}^b$, with $\hat{\tau}^b$ as before the matrices in $\{\mathbf{k}, \mathbf{k} + \mathbf{Q}\}$ space and the orbital basis is given in terms of the $(3 \times 3)$ Gell–Mann matrices $\hat{\lambda}^a$ (see appendix B). In analogy to section 4.1, we analyze the behavior of these matrices under the symmetry operations of the generating point group. For simplicity, table 3 only lists the classification of the Gell–Mann matrices. The full matrix $\hat{\lambda}^{ab} = \hat{\lambda}^a \otimes \hat{\tau}^b$ then transforms like $\hat{\lambda}^a$ under $D_{2d}$ and is even (odd) under inversion for $b = 0, 3$ ($b = 1, 2$), cf, table 1. All the matrix elements only connecting the $d_{xz}$ and $d_{yz}$ orbitals are (with the appropriate matrices) the same as for the two-orbital case. For the diagonal part of $d_{xy}$, we simply add the terms

$$\frac{1}{3}(\hat{\lambda}^{03} - \sqrt{3}\hat{\lambda}^{83})2t_{xy}(\cos k_x + \cos k_y)$$

$$+ \frac{1}{3}(\hat{\lambda}^{00} - \sqrt{3}\hat{\lambda}^{80})(4t'_{xy}\cos k_x \cos k_y - \mu_{xy})$$

including nearest- and next-nearest-neighbor hopping and the chemical potential $\mu_{xy}$. Due to the out-of-plane position of the As atoms, there is also an allowed hopping between the $d_{xz}$ / $d_{yz}$ and the $d_{xy}$ orbitals. This is a nearest-neighbor hopping of the form

$$\hat{\lambda}^{42} \sin k_x - \hat{\lambda}^{62} \sin k_y$$

and a next-nearest-neighbor hopping

$$\hat{\lambda}^{51} \sin k_x \cos k_y - \hat{\lambda}^{71} \sin k_y \cos k_x,$$

both odd under inversion. Note that these terms now are made from matrices/momentum functions that transform like the two-dimensional representation $E_u$ and can thus not be split further. To choose which $E_u$ matrices from table 3 have to be used, time-reversal symmetry
has to be considered, which requires $H_0^{ab}(k) = [H_0^{ab}(-k)]^*$. Further note that the Hamiltonian again separates into two blocks, with $(d_{kx}^{(xz)}, d_{ky}^{(yz)}, d_{kQ}^{(xy)})$ and vice versa.

With this hopping Hamiltonian, we can again analyze the stability of possible gap structures. Compared with the two-orbital case, there is one key difference: even without spin–orbit coupling the $k$ and $k + Q$ subspaces are connected through the hopping terms in equations (35) and (36). As a result, the only spin-singlet gap function that has no inter-band contributions and hence is fully supported by the Hamiltonian has the trivial orbital structure $\Lambda^{00}$. This has two important consequences. Firstly, the most stable gap structure has the same momentum dependence on all Fermi surfaces, i.e. there is a single gap function determining the gap everywhere in the Brillouin zone [13]. Secondly, the orbital structure $\Lambda^{00}$ only allows for functions $\psi(k)$ that transform trivially under $k \mapsto k + Q$. This means that a finite nearest-neighbor hopping between the $d_{xz}/d_{yz}$ and the $d_{xy}$ orbitals favors gap functions with $\psi(k + Q) = -\psi(k)$ over the gap function of extended-s and $d_{x^2-y^2}$ symmetry with $\psi(k) = \cos k_x \pm \cos k_y$.

6. Discussion and conclusion

In this work, we have introduced a simple criterion to analyze the stability of the orbital structure of superconducting order parameters in the context of multi-orbital systems: a vanishing commutator of the gap function with the free Hamiltonian. This argument is based on intra-band pairing, i.e. the equal-energy pairing of electrons in a weak-coupling approach. Depending on the structure of the interaction, the instability can therefore still occur in an orbital channel that is not fully supported by the Hamiltonian, especially with almost degenerate bands and within strong coupling. The analysis is thus only a first step and resembles the argument regarding the nodes in the superconducting gap due to non-trivial orbital structures and the associated loss of condensation energy. However, the introduced scheme additionally allows for the identification of the superconductivity-suppressing hopping terms. In the case of competing gap functions, this can help in finding a minimal model for an unbiased description.

We have applied our scheme to the case of spin-singlet pairing in the Fe-based superconductors. Looking at all symmetry-allowed hopping terms in a three-orbital model for the two-Fe unit cell, we have found that only the trivial orbital structure proportional to the identity is fully supported by the system, i.e. only describes intra-band pairing. In particular, the gap functions with $\psi(k + Q) = -\psi(k)$ are (partially) suppressed by the hopping terms connecting $k$ and $k + Q$. Moreover, the gap functions belonging to $B_{1g}$ in a two-dimensional model have additional gap nodes due to their orbital structure along the folded Brillouin zone, as this symmetry belongs to $B_{2g}$ in this reduced Brillouin zone [18]. The gap function shown in figure 3(c) then corresponds to a ‘$d_{x^2}$’ gap [19], to give an example. Both the (partial) suppression and the additional nodes are missed considering two-orbital or general one-Fe-unit-cell models. While the $d_{x^2-y^2}$ gap function is not necessarily fully suppressed in these systems, our analysis emphasizes the importance of using at least a (two-Fe) three-orbital description when studying the competition of such an order parameter with an s- or s±-wave gap. Particularly in the description of Fe-based superconductors with only electron pockets this could be relevant [20–22].

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4 This separation into two blocks can be understood from the behavior under a glide-plane transformation as noted by Lee and Wen [8].

5 Note that this effect does not depend on the hybridization of the electron pockets discussed in [17].
Finally, we comment on the generalization of the introduced scheme to spin-triplet superconductivity and the introduction of spin–orbit coupling. For simplicity, we have focused in this work on spin-singlet pairing and no spin–orbit coupling. For a generalization, the Nambu spinors have to be written in a way as to preserve the form of the mean-field Hamiltonian (1). The application of the commutation criterion is then again straightforward. In the case of a single-band system with time-reversal symmetry, for example, the appropriate basis is \( \hat{\Psi}(k) = (c_{kt}, c_k^\dagger, -c_{-kt}^\dagger, c_{-k}^\dagger)^T \). The lifting of the degeneracy of the spin-triplet gap functions in non-centrosymmetric superconductors [23] is for example easily obtained in this way.

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Appendix A. Transformation of the basis states

In this appendix, we explicitly analyze how the symmetry transformations of the generating point group of the Fe–As layer, \( D_{4h} \), act on the basis states

\[
\hat{\mathbf{c}}_k = (d_{k}^{(xz)}, d_{k}^{(yz)}, d_{k+Q_y}^{(xz)}, d_{k+Q_y}^{(xy)})^T
\]

of the two-orbital model introduced in section 4. For this purpose, we first analyze the behavior under all the symmetry operations of the unit cell \( D_{2d} \) and than add inversion, since \( D_{4h} = D_{2d} \otimes \mathbb{I} \). It is convenient to look at the respective states in real space, as depicted in figure 1(b). The two-fold rotation around the \( z \)-axis, \( C_2 \), amounts to multiplication of all the states by \(-1\), i.e. the transformation matrix is given by \( \hat{U}_{C_2} = -\hat{\Sigma}^{00} \). Therefore, all the basis matrices transform trivially under \( C_2 \), i.e. \( \hat{U}_{C_2} \Sigma^{ab} \hat{U}_{C_2}^\dagger = \hat{\Sigma}^{ab} \). This already means that all possible orbital matrices only belong to one-dimensional representations of \( D_{2d} \), as can be seen from the character table A.1. We continue with the two-fold rotation around the \( y \)-axis. Under such a rotation, \( d_{i}^{(xy)} \) \( (d_{i}^{(yz)}) \) stays the same, while \( d_{i}^{(yz)} \) \( (d_{i}^{(xy)}) \) is multiplied by \(-1\). The improper rotation \( S_4 \) is a combination of a \( C_4 \) rotation around \( z \), followed by a mirror operation \( \sigma_y \) at the \( xy \)-plane. This will take \( d_{i}^{(xz)} \) to \( d_{i}^{(yz)} \), \( d_{i}^{(yz)} \) to \(-d_{i}^{(xz)} \), as well as \( d_{i}^{(xz)} \) to \(-d_{i}^{(yz)} \) and \( d_{i}^{(yz)} \) to \(-d_{i}^{(xz)} \). Finally, the mirror operation can be obtained by combining \( C_2 \) and \( S_4 \). This then yields the following eight matrix representations:

\[
\hat{U}_{E} = \hat{\Sigma}^{00}, \quad \hat{U}_{C_2} = -\hat{\Sigma}^{00}, \quad \hat{U}_{C_2} = \pm\hat{\Sigma}^{30}, \quad \hat{U}_{S_4} = \pm i \hat{\Sigma}^{20}, \quad \hat{U}_{\sigma_y} = \pm \hat{\Sigma}^{10}.
\]

By calculating how the matrices \( \hat{\Sigma}^{ab} = \hat{\rho}_a \otimes \hat{\tau}_b \) transform under these transformations, we can thus analyze what irreducible representation of \( D_{2d} \) they belong to.

Finally, the Fe–As lattice possesses centers of inversion lying between neighboring Fe sites, which transform the basis as \( \hat{U}_i = \hat{\Sigma}^{03} \). The transformation properties of the individual basis matrices under \( D_{2d} \) and inversion leads to the classification shown in table 1. Note that \( \hat{\Sigma}^{ab} \) with \( b = 1, 2 \) are odd under inversion. As can be seen from table A.1, this means that

New Journal of Physics 15 (2013) 073006 (http://www.njp.org/)
Table A.1. Character table for $D_{4h} = D_{2d} \otimes I$. Note that the symmetry operations are ordered such that the first five columns belong to $D_{2d}$.

| IR  | E  | 2$C_4$ | $2C'_4$ | 2$\sigma_d$ | I  | 2$C_4$ | $\sigma_h$ | 2$\sigma_v$ | 2$C'_4$ |
|-----|----|--------|---------|-------------|----|---------|----------|------------|---------|
| $A_{1g}$ | 1  | 1      | 1       | 1           | 1  | 1       | 1        | 1          | 1       |
| $A_{2g}$ | 1  | 1      | -1      | -1          | 1  | 1       | 1        | -1         | -1      |
| $B_{1g}$ | 1  | -1     | 1       | -1          | 1  | 1       | 1        | 1          | -1      |
| $B_{2g}$ | 1  | -1     | 1       | -1          | 1  | 1       | 1        | -1         | 1       |
| $E_g$   | 2  | 0      | -1      | 0           | 2  | 0       | -1       | 0          | 0       |
| $A_{1u}$ | 1  | -1     | 1       | -1          | 1  | -1      | 1        | -1         | 1       |
| $A_{2u}$ | 1  | -1     | 1       | -1          | 1  | -1      | 1        | -1         | 1       |
| $B_{1u}$ | 1  | 1      | 1       | -1          | -1 | -1      | -1       | -1         | 1       |
| $B_{2u}$ | 1  | 1      | -1      | -1          | -1 | -1      | -1       | 1          | 1       |
| $E_u$   | 2  | 0      | -1      | 0           | 2  | 0       | 0        | 0          | 0       |

for example $\Sigma_{01}$, which belongs to $A_1$ in $D_{2d}$, belongs to $B_{1u}$ in $D_{4h}$. This can be understood from the transformation behavior of the $\hat{\tau}$ matrices \cite{24}. While $\hat{\tau}^0$ and $\hat{\tau}^3$ transform trivially ($A_{1g}$), the matrices $\hat{\tau}^1$ and $\hat{\tau}^2$ transform as $B_{1u}$ in $D_{4h}$. As shown in table A.1, this is the irreducible representation that transforms in the same way as $A_{1g}$ in $D_{2d}$. The total matrix $\hat{\Sigma}_{ab}$ then transforms as the product of the irreducible representation of the orbital part with $B_{1u}$.

Appendix B. Gell–Mann matrices

For the three-orbital model used in section 5, we introduce the Gell–Mann matrices:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad \lambda_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Note that the matrices $(2\lambda_0 + \sqrt{3}\lambda_8)/3, \lambda_1, \lambda_2$ and $\lambda_3$ correspond to the $(2 \times 2)$ identity and Pauli matrices of the two-band model and

$$\frac{1}{3}(\lambda_0 - \sqrt{3}\lambda_8) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$
References

[1] Sigrist M and Ueda K 1991 Phenomenological theory of unconventional superconductivity Rev. Mod. Phys. 63 239–311

[2] Moriya T and Ueda K 2000 Spin fluctuations and high temperature superconductivity Adv. Phys. 49 555–606

[3] Singh D J and Du M-H 2008 Density functional study of LaFeAsO$_{1-x}$F$_x$: a low carrier density superconductor near itinerant magnetism Phys. Rev. Lett. 100 237003

[4] Lebègue S 2007 Electronic structure and properties of the Fermi surface of the superconductor LaOFeP Phys. Rev. B 75 035110

[5] Li T 2008 Orbital degeneracy and the microscopic model of the FeAs plane in the iron-based superconductors J. Phys.: Condens. Matter 20 425203

[6] Han Q, Chen Y and Wang Z D 2008 A generic two-band model for unconventional superconductivity and spin-density-wave order in electron- and hole-doped iron-based superconductors Europhys. Lett. 82 37007

[7] Raghu S, Qi X-L, Liu C-X, Scalapino D J and Zhang S-C 2008 Minimal two-band model of the superconducting iron oxypnictides Phys. Rev. B 77 220503

[8] Yuan W and Qiang-Hua W 2009 Pairing symmetry and properties of iron-based high-temperature superconductors Phys. Rev. B 80 144517

[9] Khodas M and Chubukov A V 2012 Interpocket pairing and gap symmetry in Fe-based superconductors with only electron pockets Phys. Rev. Lett. 108 247003

[10] Mazin I I 2011 Symmetry analysis of possible superconducting states in K$_x$Fe$_2$Se$_2$ superconductors Phys. Rev. B 84 024529

[11] Johnston D C 2010 The puzzle of high temperature superconductivity in layered iron pnictides and chalcogenides Adv. Phys. 59 803–1061

[12] Hirschfeld P J, Korshunov M M and Mazin I I 2011 Gap symmetry and structure of Fe-based superconductors Rep. Prog. Phys. 74 124508

[13] Frigeri P A, Agterberg D F, Koga A and Sigrist M 2004 Superconductivity without inversion symmetry: MnSi versus CePt$_3$Si Phys. Rev. Lett. 92 097001

[14] Fischer M H, Loder F and Sigrist M 2011 Superconductivity and local noncentrosymmetry in crystal lattices Phys. Rev. B 84 184533

New Journal of Physics 15 (2013) 073006 (http://www.njp.org/)