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## Glide plane symmetry and gap structure in the iron-based superconductors

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We consider the effect of glide plane symmetry of the Fe-pnictogen/chalcogen layer in Fe-based superconductors on pairing in spin fluctuation models. Recent theories have proposed that so-called  $\eta$ -pairing states with nonzero total momentum can be realized and possess exotic properties such as odd parity spin singlet symmetry and time-reversal symmetry breaking. Here we show that  $\eta$ -pairing is inevitable when there is orbital weight at the Fermi level from orbitals with even and odd mirror reflection symmetry in z; however, by explicit calculation, we conclude that the gap function that appears in observable quantities is identical to that found in earlier, 1 Fe per unit cell pseudo-crystal momentum calculations.

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The common element in the crystal structure of all Fe-based superconductors is a two-dimensional plane of Fe atoms on a square lattice with pnictogen/chalcogen atoms sitting in alternating positions below or above the center of each square [1-4]. The alternating buckling of pnictogen/chalcogen atoms results in a unit cell with 2 inequivalent Fe atoms. A model that takes into account all Fe *d*-orbitals therefore has 10 orbitals (5 *d*-orbitals per Fe). In spite of this, most theoretical calculations (e.g., Refs. 5 and 6 and many others) have been carried out using a 5-orbital model for an "unfolded" Brillouin zone (BZ) of the 1-Fe unit cell, which appears to miss the effects of the out-of-plane pnictogen/chalcogen degrees of freedom on the bandstructure. In particular, an important question has been raised regarding whether these 5orbital calculations can correctly determine the superconducting properties such as the gap structure, given the large non-perturbative effects of the pnictogen/chalcogen potential that appear to be neglected in these studies. In addition there are questions regarding the possibility of odd parity spin singlet [7-9] and time reversal breaking [10] associated with the so called  $\eta$ -pairing [7–11].

To better understand this issue, we review the implications of the glide plane symmetry of a single Fepnictogen/chalcogen plane, as has been discussed before by various authors [12–17]: While the 1-Fe lattice does not have translational symmetry since the two sublattices A and B made up respectively of the two different Fe atoms are inequivalent, it is symmetric under the glide plane symmetry operation  $P_z = T_r \sigma_z$ , i.e., a 1 unit translation along the x- or y-direction  $T_r$  combined with a reflection  $\sigma_z$  along z. As a consequence, the diagonal intra-sub-lattice hopping between d orbitals that are even under  $P_z$   $(xy, x^2 - y^2, 3z^2 - r^2)$  and orbitals that are odd (xz, yz) changes sign between the A- and B-sublattice. When transformed to the physical 1-Fe crystal momentum **k**-space, this leads to a mixing between momenta **k** and **k** + **Q** with **Q** =  $(\pi, \pi)$ of the type  $\sum_{\mathbf{k},\sigma} \left[ t^{xz,xy}(\mathbf{k}) c^{\dagger}_{xz,\sigma,\mathbf{k}+\mathbf{Q}} c_{xy,\sigma,\mathbf{k}} + \text{h.c.} \right]$ , and other similar terms between even and odd (with respect to  $P_z$ ) orbitals. Because of this, there are off-diagonal propagators involving even and odd orbitals with momenta **k** and **k** + **Q**. This has important consequences with respect to the pairing: in addition to the standard zero center of mass momentum pairs  $\langle c_{\ell_1,\uparrow,\mathbf{k}}c_{\ell_2,\downarrow,-\mathbf{k}}\rangle$  for  $\ell_1, \ell_2$  either both even or both odd orbitals, there are also nonzero total momentum  $\eta$ -pairs  $\langle c_{\ell_1,\uparrow,\mathbf{k}}c_{\ell_2,\downarrow,-\mathbf{k}+\mathbf{Q}}\rangle$ for  $\ell_1$  even,  $\ell_2$  odd or vice versa [10].

However, this mixing is absent if one uses the eigenvalues of  $P_z$ , i.e., the pseudo-crystal momentum  $\tilde{\mathbf{k}}$  to classify the states [12–14]. This basically corresponds to shifting the momentum of either the even or the odd orbitals by  $\mathbf{Q}$ . Here we choose the shift in the even orbitals so that states defined in pseudo-crystal momentum  $\tilde{\mathbf{k}}$  are related to the states defined with physical crystal momentum  $\mathbf{k}$  through

$$\tilde{c}_{\ell,\sigma,\tilde{\mathbf{k}}} = \begin{cases} c_{\ell,\sigma,\mathbf{k}}, & \text{if } \ell \text{ odd,} \\ c_{\ell,\sigma,\mathbf{k}+\mathbf{Q}}, & \text{if } \ell \text{ even.} \end{cases}$$
(1)

The Hamiltonian is diagonal in  $\mathbf{k}$  and, as we will discuss, the usual 5-orbital calculations, when performed in this space, automatically take into account the additional terms stemming from the mixing between  $\mathbf{k}$  and  $\mathbf{k} + \mathbf{Q}$  in the physical 1-Fe crystal momentum  $\mathbf{k}$  space. Here  $\eta$ -pairing is implicitly included since pairs like  $\langle \tilde{c}_{xy,\uparrow,\mathbf{k}}\tilde{c}_{xz,\downarrow,-\mathbf{k}} \rangle$  in  $\mathbf{\tilde{k}}$ -space transform to  $\langle c_{xy,\uparrow,\mathbf{k}}c_{xz,\downarrow,-\mathbf{k}+\mathbf{Q}} \rangle$  in  $\mathbf{k}$ -space as indicated in Fig. 1(c). Here we study the parity properties of these terms, the way in which they combine with normal (zero center of mass momentum) pairing states, and their implications for the gap structure in the physical crystal momentum  $\mathbf{k}$ -space. We calculate the one-particle spectral function in the proper crystal momentum space and show that the energy gaps deduced from spectral function leading edges correspond to those calculated in the 1-Fe zone, although the quasiparticle weights are strongly renormalized. We conclude that, as usual, an even frequency gap for a singlet pair has even parity in the band basis and there is no time reversal symmetry breaking as a result of  $\eta$ -pairing.

To this end, we use the 2D 5-orbital tight-binding model for LaOFeAs introduced in Graser *et al.* [6]. This model was obtained from a Wannier transformation of an LDA bandstructure calculation of this compound with a 2-Fe 10-orbital model and performing a gauge transformation corresponding to a  $\pi$ -phase shift of the even orbitals on the B-sublattice, which in momentum space corresponds to a transformation to pseudo-crystal  $\mathbf{k}$  momentum. The Fermi surface of this model in the 1-Fe pseudo-crystal momentum **k** space is shown in Fig. 1(a)with the dominant orbital weights indicated by the coloring. The corresponding Fermi surface in physical crystal momentum **k**-space is plotted in Fig. 1(c). According to Eq. (1), it is obtained by shifting the even orbital contribution by  $\mathbf{Q}$ . The size of the points indicates the sum of the orbital weights.

This model is then supplemented with the usual Hubbard (intra-orbital U and inter-orbital U') and Hund (Hund's rule coupling J and pair-hopping J') interactions. Here we assume spin rotational invariance so that U' = U - 2J and J' = J, set U = 1.3 eV and J = 0.2 eV, and take  $\langle n \rangle = 5.95$ . We then use a randomphase approximation (RPA) to calculate the pairing interaction  $\Gamma_{\ell_1\ell_2\ell_3\ell_4}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}')$  which represents the particleparticle scattering of electrons in orbitals  $\ell_1, \ell_4$  with momenta  $(\tilde{\mathbf{k}}, -\tilde{\mathbf{k}})$  to electrons in orbitals  $\ell_2, \ell_3$  and momenta  $(\tilde{\mathbf{k}}', -\tilde{\mathbf{k}}')$ . The pairing strengths  $\lambda_{\alpha}$  for various pairing channels  $\alpha$  are then given as the eigenvalues of

$$-\sum_{j} \oint_{C_{j}} \frac{d\tilde{\mathbf{k}}_{\parallel}'}{(2\pi)^{2} v_{F}(\tilde{\mathbf{k}}_{\parallel}')} \Gamma_{ij}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}') g_{\alpha}(\tilde{\mathbf{k}}') = \lambda_{\alpha} g_{\alpha}(\tilde{\mathbf{k}}) .$$
(2)

Here,  $\Gamma_{ij}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}')$  represents the irreducible vertex for scattering of a pair of electrons  $(\tilde{\mathbf{k}} \uparrow, -\tilde{\mathbf{k}} \downarrow)$  on Fermi pocket  $C_i$  to  $(\tilde{\mathbf{k}}' \uparrow, -\tilde{\mathbf{k}}' \downarrow)$  on pocket  $C_j$ . It is obtained from  $\Gamma_{\ell_1 \ell_2 \ell_3 \ell_4}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}')$  as

$$\Gamma_{ij}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}') = \sum_{\ell_1, \ell_2, \ell_3, \ell_4} \tilde{a}^{\ell_1^*}_{\nu, \tilde{\mathbf{k}}} \tilde{a}^{\ell_4^*}_{\nu, -\tilde{\mathbf{k}}} \Gamma_{\ell_1 \ell_2 \ell_3 \ell_4}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}') \\ \times \tilde{a}^{\ell_2}_{\mu, \tilde{\mathbf{k}}'} \tilde{a}^{\ell_3}_{\mu, -\tilde{\mathbf{k}}'}, \qquad (3)$$

where the matrix-elements  $\tilde{a}_{\nu,\tilde{\mathbf{k}}}^{\ell} = \langle \ell \mathbf{k} | \nu \mathbf{k} \rangle$  transform the orbital basis to the band representation in pseudo-crystal momentum space. The momenta  $\tilde{\mathbf{k}}$  and  $\tilde{\mathbf{k}}'$  in Eq. (3) are restricted to the Fermi surface and  $v_F(\tilde{\mathbf{k}}_{\parallel}')$  is the Fermi velocity. The eigenfunction  $g_{\alpha}(\tilde{\mathbf{k}})$  for the largest eigenvalue determines the leading pairing instability and provides an approximate form for the superconducting gap  $\tilde{\Delta}(\tilde{\mathbf{k}}) \propto g_{\alpha}(\tilde{\mathbf{k}})$ . The structure of the leading gap function



FIG. 1. (Color online) (a) Fermi surfaces and (b) the leading gap function for the 5-orbital model in the zone of the pseudo-crystal momentum  $\tilde{\mathbf{k}}$ . The Fermi surface is colored to show the dominant orbital weight  $(d_{xz} \text{ red}, d_{yz} \text{ green}, d_{xy})$ blue). (c) The unfolded Fermi surface in the physical crystal momentum **k**-space. The size of the dots is proportional to the sum of the orbital weights of the spectral function and the color shows the dominant orbital weight. The red line denotes the boundary of the 2-Fe per unit cell Brillouin zone. An " $\eta$ " pair ( $\mathbf{k} \uparrow, -\mathbf{k} + \mathbf{Q} \downarrow$ ) is shown. (d) Comparison of the angle dependence of the leading gap function calculated from the 5-orbital model (orange line) and the 10-orbital model (blue dots) on the various Fermi pockets. Here we denote the two crossed electron pockets in the 10-orbital model at the X-point as  $\beta_1$  and  $\beta_1^{\hat{i}}$  and at the Y-point  $\beta_2$  and  $\beta_2^{\prime}$ . The gaps along the  $\beta_{1,2}^{\prime}$  pockets are not plotted since  $\beta_1^{\prime} = \beta_2$  and  $\beta'_2 = \beta_1$  by symmetry.

 $g_{\alpha}(\mathbf{k})$  with  $s_{\pm}$ -wave symmetry on the Fermi surface is shown Fig. 1(b).

We have also calculated the leading gap function and eigenvalue in the original 10-orbital model, from which the 5-orbital model was derived through a gauge transformation as discussed above. We obtain the same leading eigenvalue  $\lambda = 0.76$  in the 10-orbital as in the 5-orbital model, and Fig. 1(d) shows that the gap function obtained in the 10-orbital model is identical to what is obtained in the 5-orbital model. From this it is clear that calculations performed in the 1-Fe 5-orbital pseudo-crystal momentum space indeed contain all the information of the more complex 10-orbital calculation performed in the 2-Fe crystal momentum space.

As discussed above, this includes the information about  $\eta$ -pairing terms in the physical 1-Fe momentum **k**space. In order to analyze the structure of these terms, we transform the gap function  $\tilde{\Delta}_{\nu}(\tilde{\mathbf{k}})$  we obtained in pseudo-crystal momentum space to 1-Fe physical crystal momentum **k**-space. To this end, we first transform



FIG. 2. (Color online) Gap functions  $\Delta_{\ell_1\ell_2}(\mathbf{k})$  in the orbital basis plotted on the Fermi surface in the physical momentum BZ. When  $\ell_1$  and  $\ell_2$  have the same z-reflection symmetry one has normal  $(\mathbf{k}, -\mathbf{k})$  pairing and the gap function  $\Delta_{\ell_1\ell_2}^N(\mathbf{k})$  is real and has even parity. When  $\ell_1$  and  $\ell_2$  have different z-reflection symmetry, one has  $(\mathbf{k}, -\mathbf{k} + \mathbf{Q}) \eta$  pairing and  $\Delta_{\ell_1\ell_2}^{\eta}(\mathbf{k})$  is purely imaginary and has odd parity.

 $\tilde{\Delta}_{\nu}(\mathbf{\tilde{k}})$  from band to orbital space and then to **k**-space. This gives normal pairing terms with zero center of mass momentum,

$$\langle c_{\ell_1\uparrow,\mathbf{k}}c_{\ell_2\downarrow,-\mathbf{k}} - c_{\ell_1\downarrow,\mathbf{k}}c_{\ell_2\uparrow,-\mathbf{k}} \rangle \propto \Delta^N_{\ell_1\ell_2}(\mathbf{k}) =$$

$$\begin{cases} \tilde{a}^{\ell_1}_{\nu,\mathbf{k}}\tilde{a}^{\ell_2}_{\nu,-\mathbf{k}}\tilde{\Delta}_{\nu}(\mathbf{k}), & \ell_1,\ell_2 \text{ odd,} \\ \tilde{a}^{\ell_1}_{\nu,\mathbf{k}-\mathbf{Q}}\tilde{a}^{\ell_2}_{\nu,-\mathbf{k}+\mathbf{Q}}\tilde{\Delta}_{\nu}(\mathbf{k}-\mathbf{Q}), & \ell_1,\ell_2 \text{ even,} \\ 0, & \text{otherwise,} \end{cases}$$

$$\end{cases}$$

and  $\eta$ -pairing terms with center of mass momentum  $\mathbf{Q}$ ,

$$\langle c_{\ell_{1}\uparrow,\mathbf{k}}c_{\ell_{2}\downarrow,-\mathbf{k}+\mathbf{Q}} - c_{\ell_{1}\downarrow,\mathbf{k}}c_{\ell_{2}\uparrow,-\mathbf{k}+\mathbf{Q}} \rangle \propto \Delta_{\ell_{1}\ell_{2}}^{\eta}(\mathbf{k}) = (5)$$

$$\begin{cases} \tilde{a}_{\nu,\mathbf{k}}^{\ell_{1}}\tilde{a}_{\nu,-\mathbf{k}}^{\ell_{2}}\tilde{\Delta}_{\nu}(\mathbf{k}), & \ell_{1} \text{ odd, } \ell_{2} \text{ even,} \\ \tilde{a}_{\nu,\mathbf{k}-\mathbf{Q}}^{\ell_{1}}\tilde{a}_{\nu,-\mathbf{k}+\mathbf{Q}}^{\ell_{2}}\tilde{\Delta}_{\nu}(\mathbf{k}-\mathbf{Q}), & \ell_{1} \text{ even, } \ell_{2} \text{ odd,} \\ 0, & \text{otherwise.} \end{cases}$$

Here and in the following we have replaced  $\hat{\mathbf{k}}$  by  $\mathbf{k}$  for odd and  $\mathbf{k} + \mathbf{Q}$  for even orbitals  $\ell$  as noted in Eq. (1). For a given Fermi momentum  $\mathbf{k}$ ,  $\nu$  labels the band that crosses the Fermi energy at  $\mathbf{k}$ .

Fig. 2 shows the gap functions  $\Delta_{\ell_1\ell_2}(\mathbf{k})$  for four different combinations of orbitals  $\ell_1$  and  $\ell_2$ . From panels (a) and (b) one sees that when  $\ell_1$  and  $\ell_2$  have the same *z*-reflection symmetry, one has normal  $(\mathbf{k}, -\mathbf{k})$  pairing and the gap function  $\Delta_{\ell_1\ell_2}^N(\mathbf{k})$  is real and has even parity, i.e.,  $\Delta_{\ell_1\ell_2}^N(-\mathbf{k}) = \Delta_{\ell_1\ell_2}^N(\mathbf{k})$ . In contrast, when  $\ell_1$  and  $\ell_2$  have different *z*-reflection symmetry, one has  $(\mathbf{k}, -\mathbf{k} + \mathbf{Q})$   $\eta$ -pairing. In this case  $\Delta_{\ell_1\ell_2}^{\eta}(-\mathbf{k}) = -\Delta_{\ell_1\ell_2}^{\eta}(\mathbf{k})$ . Note that

these gaps have the same behavior under mirror reflections as the orbitally resolved gaps of Casula and Sorella [15]. Here we stress that the odd-parity and imaginary nature of these terms in orbital space arises entirely from the product of matrix-elements  $\tilde{a}_{\nu,\mathbf{k}}^{\ell_1} \tilde{a}_{\nu,-\mathbf{k}}^{\ell_2}$  and therefore is merely a reflection of the glide plane symmetry of the Fe-pnictogen/chalcogen plane. It does not reflect any exotic behavior of the pairing interaction. We also point out that time-reversal symmetry requires that  $\Delta_{\ell_1\ell_2}(\mathbf{k}) = \Delta^*_{\ell_1\ell_2}(-\mathbf{k})$  for both the normal and  $\eta$ -gaps in Eqs. (4) and (5), respectively. Because the normal gap  $\Delta_{\ell_1\ell_2}^N(\mathbf{k})$  has even parity and is purely real, it satisfies time-reversal symmetry, as does the odd parity, purely imaginary  $\eta$ -pairing gap  $\Delta_{\ell_1\ell_2}^{\eta}(\mathbf{k})$ . Both normal and  $\eta$ pairing terms, however, coexist in orbital space and contribute to the pairing condensate.

This raises the question of how these two terms combine, given their opposite parity. To study this, we transform the gap back to band representation in physical crystal momentum  $\mathbf{k}$ -space, and obtain for the normal pairing,

$$\Delta_{\nu}^{N}(\mathbf{k}) = \Delta_{\text{odd}}^{N}(\mathbf{k}) + \Delta_{\text{even}}^{N}(\mathbf{k}), \qquad (6)$$

where

2

$$\Delta_{\text{odd}}^{N}(\mathbf{k}) = \sum_{\ell_{1},\ell_{2} \text{ odd}} \tilde{a}_{\nu,\mathbf{k}}^{\ell_{1}^{*}} \tilde{a}_{\nu,-\mathbf{k}}^{\ell_{2}^{*}} \Delta_{\ell_{1}\ell_{2}}^{N}(\mathbf{k}), \qquad (7a)$$

$$\Delta_{\text{even}}^{N}(\mathbf{k}) = \sum_{\ell_{1},\ell_{2} \text{ even}} \tilde{a}_{\nu,\mathbf{k}-\mathbf{Q}}^{\ell_{1}^{*}} \tilde{a}_{\nu,-\mathbf{k}+\mathbf{Q}}^{\ell_{2}^{*}} \Delta_{\ell_{1}\ell_{2}}^{N}(\mathbf{k}) \,.$$
(7b)

Similarly, we obtain for the  $\eta$ -pairing terms,

$$\Delta^{\eta}_{\nu}(\mathbf{k}) = \Delta^{\eta}_{\text{odd-even}}(\mathbf{k}) + \Delta^{\eta}_{\text{even-odd}}(\mathbf{k}), \qquad (8)$$

where

$$\Delta_{\text{odd-even}}^{\eta}(\mathbf{k}) = \sum_{\ell_1 \text{ odd}, \ell_2 \text{ even}} \tilde{a}_{\nu, \mathbf{k}}^{\ell_1^*} \tilde{a}_{\nu, -\mathbf{k}}^{\ell_2^*} \Delta_{\ell_1 \ell_2}^{\eta}(\mathbf{k}), \qquad (9a)$$

$$\Delta^{\eta}_{\text{even-odd}}(\mathbf{k}) = \sum_{\ell_1 \text{ even}, \ell_2 \text{ odd}} \tilde{a}^{\ell_1^*}_{\nu, \mathbf{k} - \mathbf{Q}} \tilde{a}^{\ell_2^*}_{\nu, -\mathbf{k} + \mathbf{Q}} \Delta^{\eta}_{\ell_1 \ell_2}(\mathbf{k}) \,. \tag{9b}$$

Here we have used the fact that the matrix-elements  $a_{\nu,\mathbf{k}}^{\ell}$ , which provide the transformation from the orbital to the band representation in physical crystal momentum **k**-space, are given by the matrix-elements in pseudo-crystal momentum space,  $\tilde{a}_{\nu,\mathbf{k}}^{\ell}$  for  $\ell$  denoting an odd orbital, and  $\tilde{a}_{\nu,\mathbf{k-Q}}^{\ell}$  for  $\ell$  denoting an even orbital.

Then, using Eqs. (4) and (5) one can show that the gap function  $\tilde{\Delta}_{\nu}(\mathbf{k})$  calculated in the 5-orbital model in the pseudo-crystal momentum representation splits into normal and  $\eta$ -pairing terms in the physical crystal momentum space, i.e.,

$$\tilde{\Delta}_{\nu}(\mathbf{k}) = \Delta_{\text{odd}}^{N}(\mathbf{k}) + \Delta_{\text{even}}^{N}(\mathbf{k} + \mathbf{Q}) 
+ \Delta_{\text{odd-even}}^{\eta}(\mathbf{k}) + \Delta_{\text{even-odd}}^{\eta}(\mathbf{k} + \mathbf{Q}).$$
(10)



FIG. 3. (Color online) (a) The leading gap function  $\tilde{\Delta}(\tilde{\mathbf{k}})$  in the band representation calculated in the 5-orbital model in pseudo-crystal momentum space (red=positive, blue=negative). When transformed to physical crystal momentum **k**-space, the gap splits into normal even-even and odd-odd contributions  $\Delta_{\text{odd}}^N(\mathbf{k}) + \Delta_{\text{even}}^N(\mathbf{k}+\mathbf{Q})$  plotted in (b) and even-odd and odd-even  $\eta$  contributions  $\Delta_{\text{odd-even}}^{\eta}(\mathbf{k}) + \Delta_{\text{even-odd}}^{\eta}(\mathbf{k}+\mathbf{Q})$  shown in (c). In the band representation, all the contributions have even parity.

Note that the even terms have their momentum shifted by  $\mathbf{Q}$  so they appear on the same Fermi pockets as the odd terms. Fig. 3 shows a graphical representation of this relation by plotting a 3D representation of  $\tilde{\Delta}_{\nu}(\mathbf{k})$  in the top panel, its normal contribution  $\Delta_{\text{odd}}^{N}(\mathbf{k}) + \Delta_{\text{even}}^{N}(\mathbf{k}+\mathbf{Q})$ in the middle panel and its  $\eta$  contribution  $\Delta_{\text{odd-even}}^{\eta}(\mathbf{k}) +$  $\Delta_{\text{even-odd}}^{\eta}(\mathbf{k}+\mathbf{Q})$  in the bottom panel. One sees that after the transformation to band representation, the  $\eta$ -pairing term has even parity (and is real), just like the normal pairing contribution. This results from the combination of the product of matrix-elements  $\tilde{a}_{\nu,\mathbf{k}}^{\ell_1^*} \tilde{a}_{\nu,-\mathbf{k}}^{\ell_2^*}$ , which has odd parity and is purely imaginary, with the odd-parity and imaginary  $\Delta_{\ell_1\ell_2}^{\eta}(\mathbf{k})$  for odd-even combinations of  $\ell_1$ and  $\ell_2$ . Thus, as usual, an even frequency gap in the band basis has even parity for a singlet pair. From Eqs. (4– 9) it is straightforward to show that the normal and  $\eta$ contributions to the gap have the same sign and share

the same nodal structure in case of a nodal gap [18]. Thus, while the  $\eta$ -contribution is significant in the amplitude of the total gap, it does not affect its sign and nodal structure and therefore does not qualitatively alter the low temperature thermodynamic properties. This is discussed in more detail in the Supplementary Material.

Finally, we calculate the spectral function

$$A(\mathbf{k},\omega) = \sum_{\ell,\nu} |\langle \ell \mathbf{k} | \widetilde{\nu \mathbf{k}} \rangle|^2 \tilde{A}_{\nu}(\tilde{\mathbf{k}},\omega)$$

as measured in ARPES experiments in the proper 1-Fe crystal momentum **k**-space. Here,  $\tilde{A}_{\nu}(\tilde{\mathbf{k}}, \omega) = u_{\nu}^{2}(\tilde{\mathbf{k}})\delta(\omega - E_{\nu}(\tilde{\mathbf{k}})) + v_{\nu}^{2}(\tilde{\mathbf{k}})\delta(\omega + E_{\nu}(\tilde{\mathbf{k}}))$  is the BCS spectral function in the pseudo-crystal momentum space with  $E_{\nu}(\tilde{\mathbf{k}}) = \sqrt{\epsilon_{\nu}^{2}(\tilde{\mathbf{k}}) + \tilde{\Delta}_{\nu}^{2}(\tilde{\mathbf{k}})}$  and the BCS coherence factors  $u_{\nu}^{2}(\tilde{\mathbf{k}}) = [1 + \epsilon_{\nu}(\tilde{\mathbf{k}})/E_{\nu}(\tilde{\mathbf{k}})]/2$  and  $v_{\nu}^{2}(\tilde{\mathbf{k}}) = 1 - u_{\nu}^{2}(\tilde{\mathbf{k}})$ . Realizing that

$$\langle \ell \mathbf{k} | \widetilde{\nu \mathbf{k}} \rangle = \begin{cases} \tilde{a}_{\nu, \mathbf{k}}^{\ell} \delta_{\mathbf{k}, \tilde{\mathbf{k}}}, & \ell \text{ odd,} \\ \tilde{a}_{\nu, \mathbf{k} - \mathbf{Q}}^{\ell} \delta_{\mathbf{k} - \mathbf{Q}, \tilde{\mathbf{k}}}, & \ell \text{ even,} \end{cases}$$
(11)

one arrives at

$$A(\mathbf{k},\omega) = \sum_{\nu} \left[ \sum_{\ell \text{ odd}} |\tilde{a}_{\nu,\mathbf{k}}^{\ell}|^{2} \tilde{A}_{\nu}(\mathbf{k},\omega) + \sum_{\ell \text{ even}} |\tilde{a}_{\nu,\mathbf{k}-\mathbf{Q}}^{\ell}|^{2} \tilde{A}_{\nu}(\mathbf{k}-\mathbf{Q},\omega) \right]. \quad (12)$$

Thus, the superconducting gap that enters  $A(\mathbf{k}, \omega)$  as measured in ARPES experiments is given by the gap function  $\Delta_{\nu}(\mathbf{k})$  calculated in the 5-orbital 1-Fe zone in pseudo-crystal momentum space and no further transformation is necessary.  $\tilde{\Delta}_{\nu}(\mathbf{k})$  implicitly encodes the strong symmetry breaking potential associated with the pnictogen/chalcogen atom. The gap  $\tilde{\Delta}_{\nu}(\tilde{\mathbf{k}})$  entering the first  $\ell =$  "odd" term in Eq. (12) is shown in Fig. 3(a) while the gap entering the second  $\ell =$  "even" contribution which appears on the "shadow" pockets is obtained by shifting the gap by  $\mathbf{Q}$ . As in the normal state [19–23] the spectral weight in the superconducting state associated with each contribution is modulated by the orbital weights  $|\tilde{a}_{\nu,\mathbf{k}}^{\ell}|^2$  and  $|\tilde{a}_{\nu,\mathbf{k}-\mathbf{Q}}^{\ell}|^2$ , respectively, and this weight can differ substantially between the main and shadow pockets as seen in Fig. 1(c). The spectral functions for both the normal and superconducting states are discussed in more detail and shown in the Supplementary Material.

To summarize, we have carried out microscopic calculations of the superconducting gap structure in 1 Fe and 2 Fe per unit cell models and shown that  $\eta$ -pairing is an important ingredient in the superconducting condensate. We have demonstrated that it contributes with the usual even parity symmetry in band space and that time reversal symmetry is preserved, in contrast to recent proposals in the literature. Finally we have shown that the gap function, which appears in observable quantities, is identical to that found in earlier, 1 Fe per unit cell pseudo-crystal momentum calculations.

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