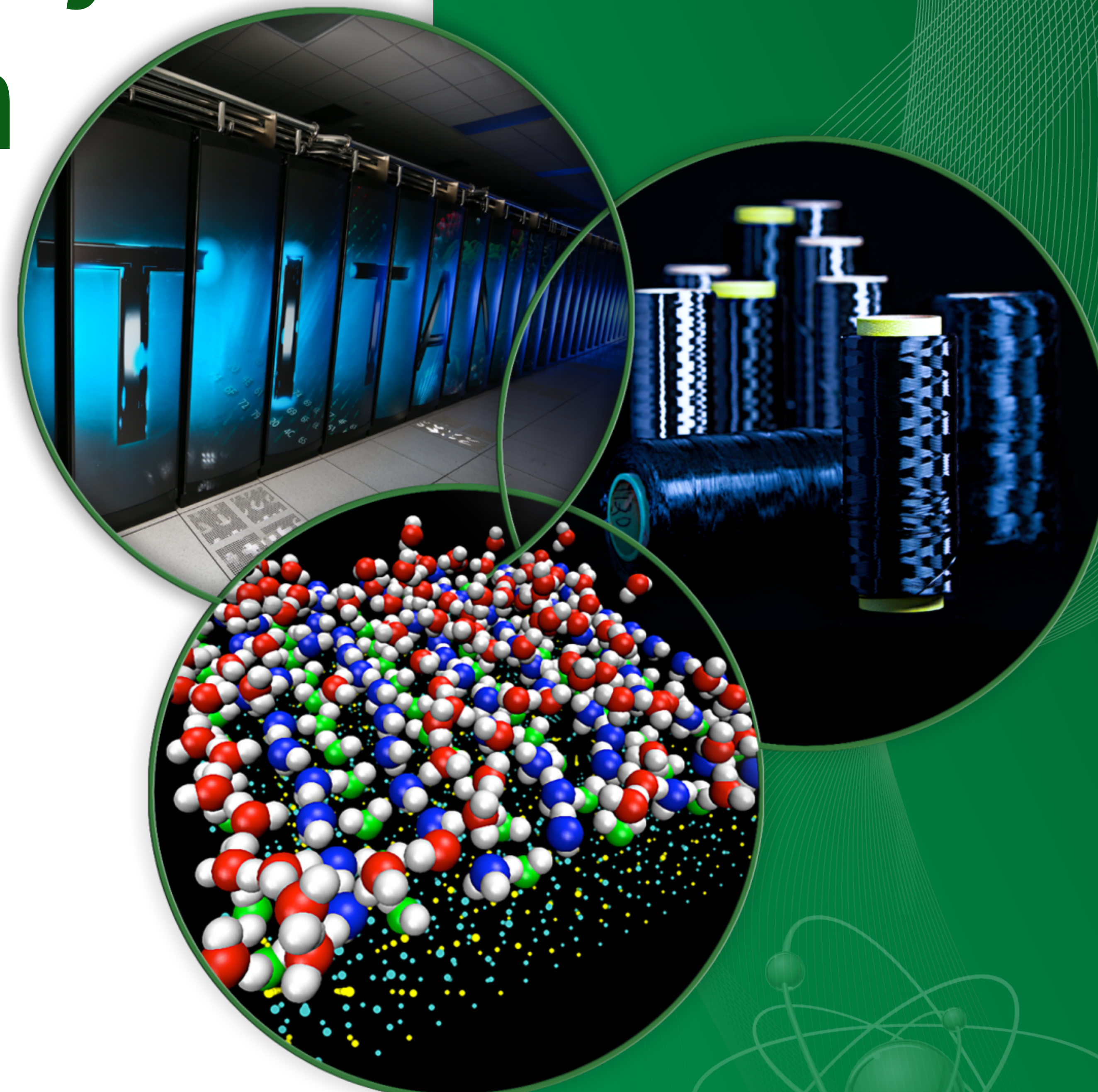
Glide plane symmetry and gap structure in iron-based superconductors



Thomas A. Maier – ORNL
Yan Wang – ORNL/UTK
Tom Berlijn – ORNL
Peter Hirschfeld – UFL
Doug Scalapino – UCSB

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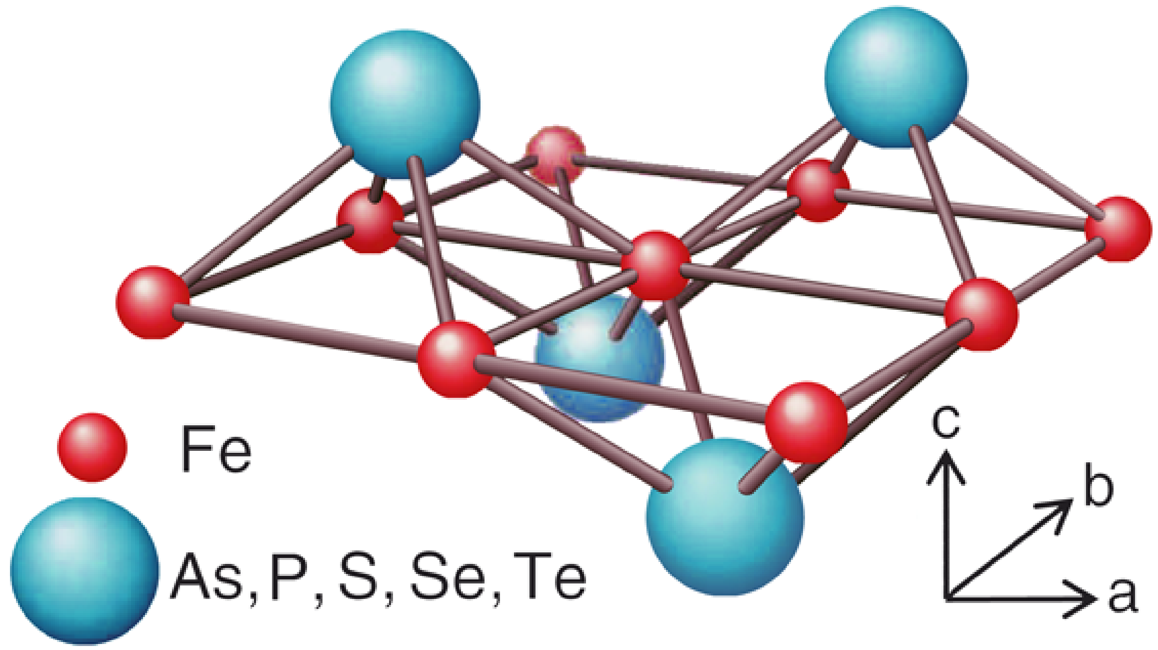
Oak Ridge National Laboratory

Glide plane symmetry in iron-based superconductors

Structure

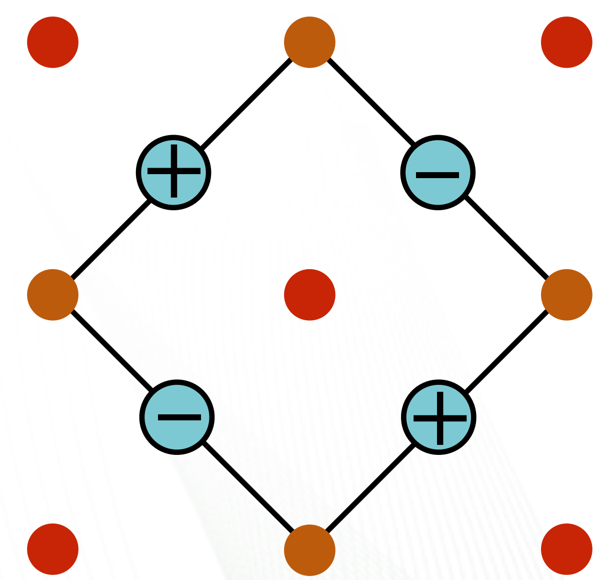
- Staggered anion positions above and below iron plane
  $[T_x,H] \neq 0; [T_y,H] \neq 0$
  (in 1 Fe unit cell)



- But **glide plane symmetry**
  $[P_z T_x,H] = 0; [P_z T_y,H] = 0$
  with P_z: z → -z requires

$$\sum_{i,j}(-1)^{i_x+i_y}\left[t_{i,j}^{xz,xy}c_{xz,i}^{\dagger}c_{xy,j} + t_{i,j}^{yz,xy}c_{yz,i}^{\dagger}c_{xy,j} + h.c.\right]$$

since $P_z|xz\rangle = -1|xz\rangle; \;\; P_z|xy\rangle = +1|xy\rangle$



Lee & Wen 2008, Lv & Philipps 2011, Lin *et al.* 2014

Why in the iron-based superconductors?

In momentum space (1-Fe BZ)

- Mixing between k and $k+Q$ with $Q=(\pi,\pi)$

$$\sum_k \left[t^{xz,xy}(k)c^\dagger_{xz}(k+Q)c_{xy}(k) + t^{yz,xy}(k)c^\dagger_{yz}(k+Q)c_{xy}(k) + h.c.\right]$$

- Mixing only for inter-orbital terms between orbitals with even parity and orbitals with odd parity in P_z
- Translational symmetry breaking in 1 Fe lattice naturally leads to η-pairing between orbitals with even and odd parity

$$\langle c_{xz,\uparrow}(k)c_{xy,\downarrow}(-k+Q)\rangle \neq 0$$

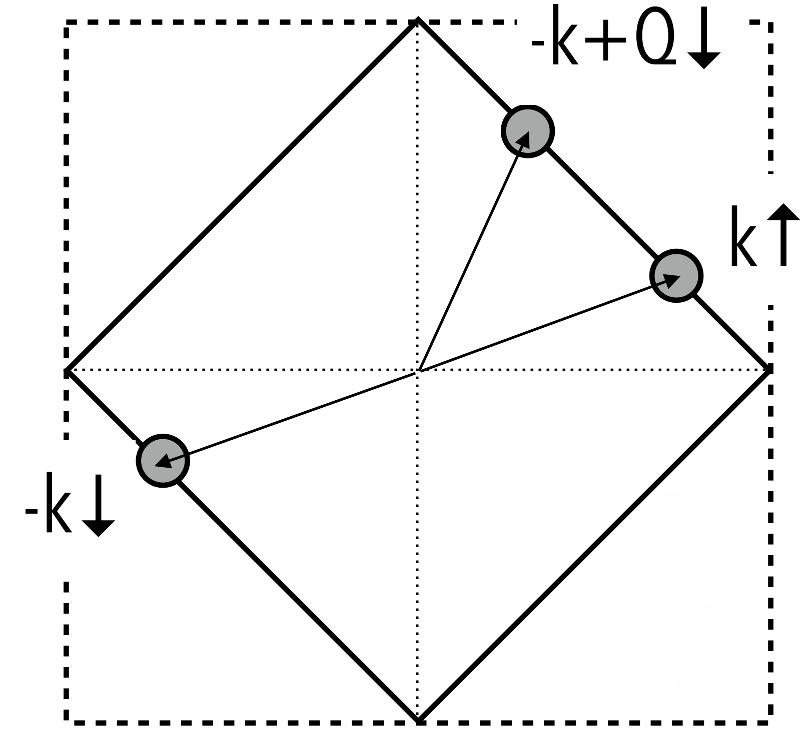
What is η-pairing?

- Pairing state with finite center of mass momentum, usually
  Q = (π,π) (C.N. Yang '89,
  R. Scalettar *et al.*, '91)
- Generally possible if **ε**(k) and **ε**(Q-k) nearly degenerate (half-filled Hubbard model, pairing in SDW phase, …)
- *Q*=0 pairing generally favored
  (Bickers '92)
- Logarithmic divergence (half-filling)

$$\chi^0_{pp}(Q=0) \propto \ln^2(\Omega_c/T)$$

$$\chi^0_{pp}(Q=(\pi,\pi)) \propto \ln(\Omega_c/T)$$

$$\langle c_{k\uparrow} c_{-k+Q\downarrow} \rangle$$



Related to

- Pair density wave
- Amperean pairing

Why odd parity singlet and time-reversal symmetry breaking?

Consider singlet state

(Scaletttar *et al.*, '91)

$$\Delta_x^\eta = \sum_r (-1)^r (c_{r\uparrow} c_{r+x\downarrow} - c_{r\downarrow} c_{r+x\uparrow})$$

$$= \sum_k (2i \sin k_x) c_{k\uparrow} c_{-k+Q\downarrow}$$

- Odd parity arises from Q=π center of mass momentum
- 2-fold degeneracy

$$\Delta(k_x, k_y) \propto \sin k_x + i \sin k_y$$

- Odd parity singlet pairing state breaks U(1) gauge symmetry, lattice translational symmetry, parity and time reversal symmetry

Why odd parity singlet and time-reversal symmetry breaking?

Consider singlet state

(Scalettar *et al.*, '91)

$$\Delta_x^\eta = \sum_r (-1)^r (c_{r\uparrow} c_{r+x\downarrow} - c_{r\downarrow} c_{r+x\uparrow})$$

$$= \sum_k (2i \sin k_x) c_{k\uparrow} c_{-k+Q\downarrow}$$

Note: Center of mass frame Q/2

$$= \sum_{k'} (2i \cos k_x) c_{k+Q/2\uparrow} c_{-k+Q/2\downarrow}$$

- Odd parity arises from Q=π center of mass momentum
- 2-fold degeneracy

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Questions raised in recent literature

$$\langle c_{xz,\uparrow}(k) c_{xy,\downarrow}(-k+Q)\rangle \neq 0$$

- Is there η-pairing in the Fe-based superconductors?
- Odd parity singlet pairing?
- Time reversal symmetry breaking?
- 1-Fe zone (5-orbital) vs. 2-Fe zone (10-orbital) calculations?

J.-P. Hu & N. Hao, PRX '12
M. Khodas & A.V. Chubukov, PRL '12
J.-P. Hu, PRX '13
M. Casula & S. Sorella, PRB '13
N. Hao & J.-P. Hu, PRB '14
C.-H. Lin, C.-P. Chou, W.-G. Yin, W. Ku, arXiv:1403.3687

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Pseudo-crystal momentum

P.A. Lee & X.-G. Wen, PRB '08

1-Fe lattice has glide plane symmetry (in 2D)

- $[P_z T_x, H] = [P_z T_y, H] = 0$
- Use eigenvalues of $P_z T_x$ and $P_z T_y$ to label eigenstates
- Use

$$\tilde{c}_e(\tilde{k}) = \sum_i e^{-i(k+Q)r} c_e(r) \quad \text{for even-parity orbitals}$$

$$\tilde{c}_o(\tilde{k}) = \sum_i e^{-ikr} c_o(r) \quad \text{for odd-parity orbitals}$$

- $k = \tilde{k}$ for odd-parity orbitals and $k + Q = \tilde{k}$ for even-parity orbitals
- Hamiltonian is diagonal in $\tilde{k}$

5-Orbital model in pseudo crystal momentum space

Microscopic Hamiltonian – Multi-orbital Hubbard-Hund model

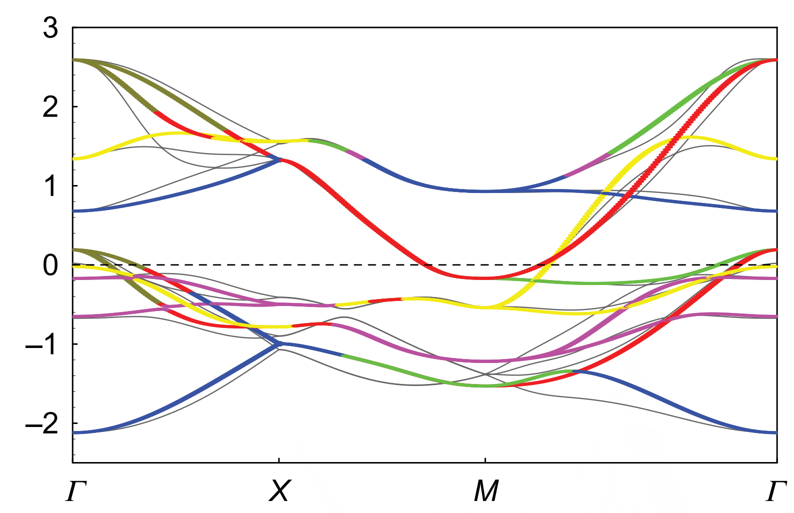
$$H = H_0$$

$$+ U \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + U' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'}$$

$$+ J \sum_{i,\ell'<\ell,\sigma\sigma'} c^{\dagger}_{i\ell\sigma} c^{\dagger}_{i\ell'\sigma'} c_{i\ell\sigma'} c_{i\ell'\sigma}$$

$$+ J' \sum_{i,\ell'\neq\ell} c^{\dagger}_{il\uparrow} c^{\dagger}_{i\ell\downarrow} c_{i\ell'\downarrow} c_{i\ell'\uparrow}$$

5-orbital tight-binding model from fitting LDA bandstructure with 10-band model and gauge transformation on B-sublattice

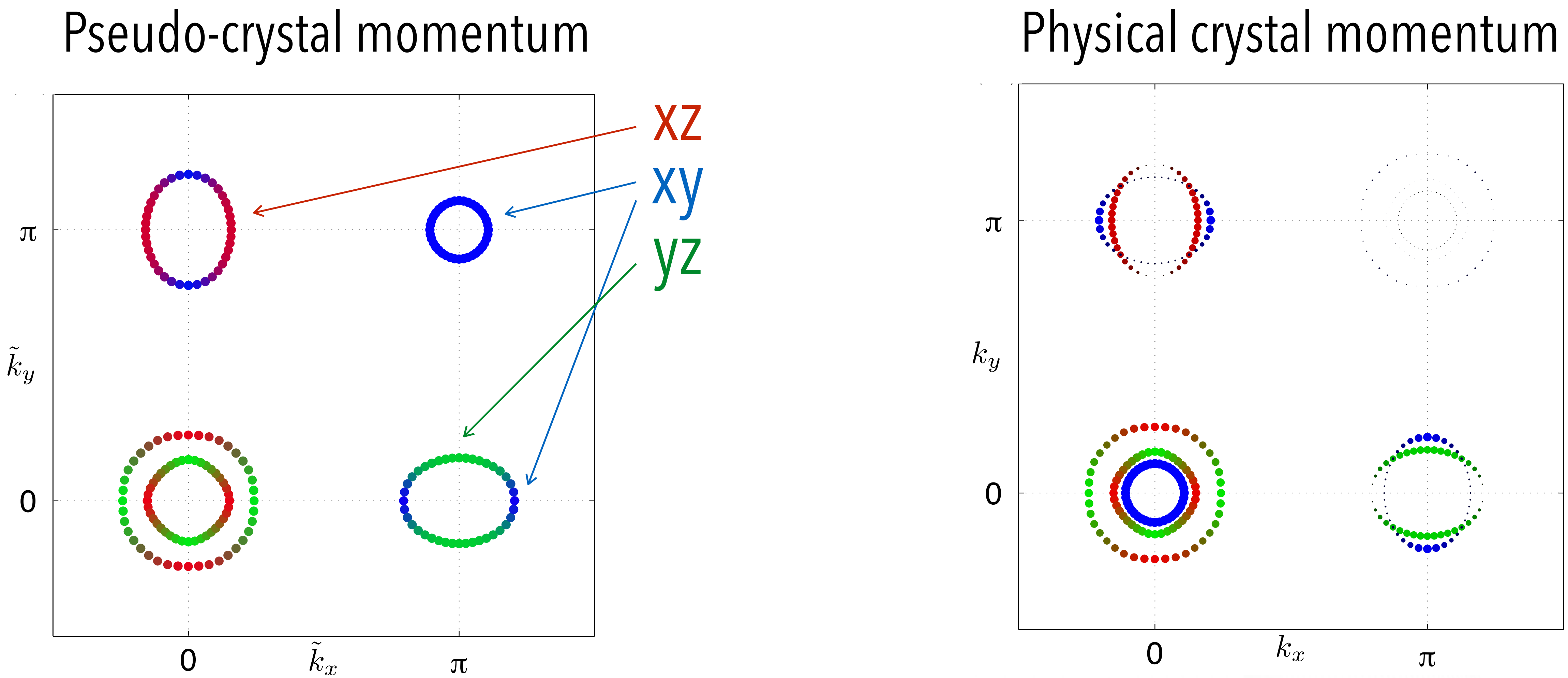


Intra- and inter-orbital Coulomb interactions

Hund's rule coupling

Pair-hopping term

Transformation from pseudo-crystal to physical crystal momentum space



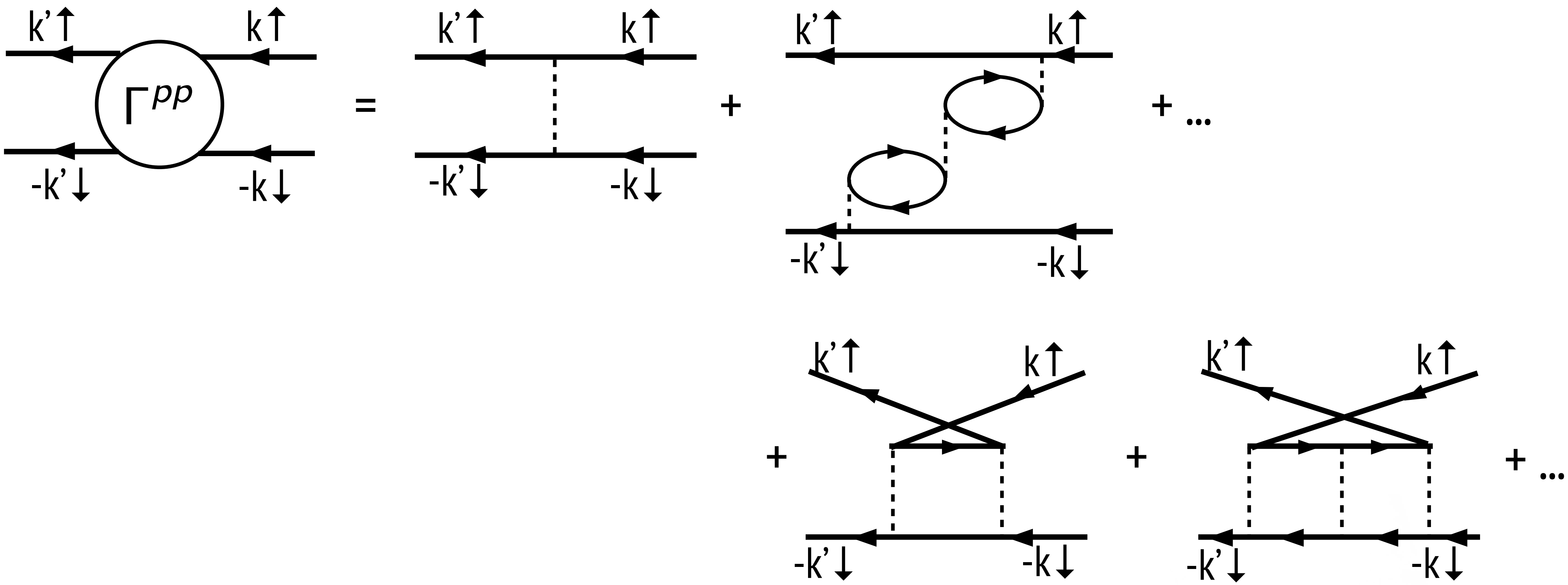
$$-\frac{1}{\pi}\Im\sum_n \tilde{G}_{nn}(\tilde{k},\omega)$$

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\Im\left[\sum_{n\in\,\mathrm{odd}} \tilde{G}_{nn}(\tilde{\mathbf{k}},\omega) + \sum_{n\in\,\mathrm{even}} \tilde{G}_{nn}(\tilde{\mathbf{k}}+\mathbf{Q},\omega)\right]$$

see also: Lv & Philipps 2011, Lin *et al.* 2014

RPA pairing interaction

Berk, Schrieffer 1966



$$\Gamma^{pp}_{\ell_1\ell_2\ell_3\ell_4}(\tilde{k},\tilde{k}') = \left[\frac{3}{2}U^s\chi^s_{RPA}(\tilde{k}-\tilde{k}')U^s - \frac{1}{2}U^c\chi^c_{RPA}(\tilde{k}-\tilde{k}')U^c + \frac{1}{2}(U^s+U^c)\right]_{\ell_1\ell_2\ell_3\ell_4}$$

Spin fluctuations Charge/orbital fluctuations

RPA pairing

Pairing strength from eigenvalue equation

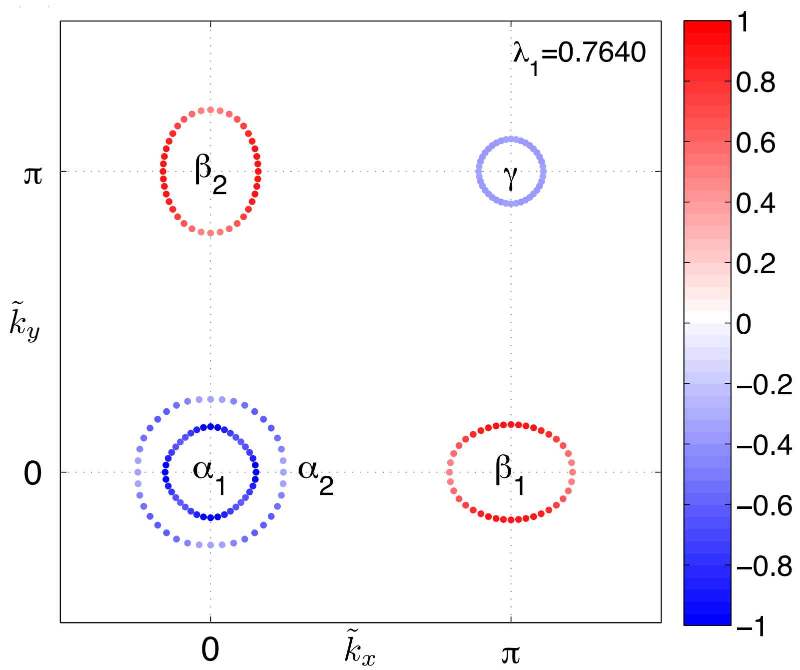
$$-\sum_j \oint_{C_j} \frac{d\tilde{\mathbf{k}}'_{\|}}{2\pi v_F(\tilde{\mathbf{k}}'_{\|})} \Gamma_{ij}(\tilde{\mathbf{k}},\tilde{\mathbf{k}}') g_\alpha(\tilde{\mathbf{k}}') = \lambda_\alpha(\tilde{\mathbf{k}}) g_\alpha(\tilde{\mathbf{k}})$$

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

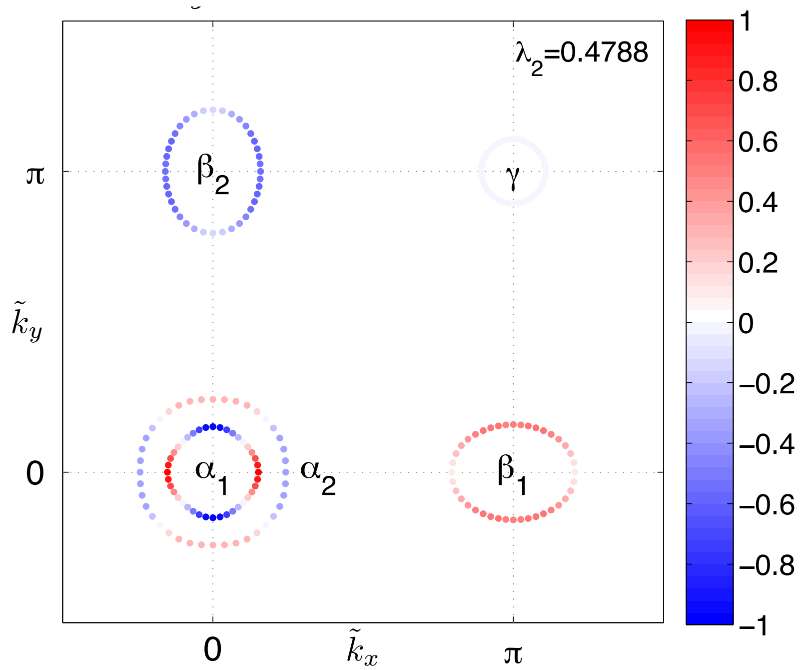
$$\tilde{a}_\nu^\ell(\tilde{\mathbf{k}}) = \langle \ell\tilde{\mathbf{k}} | \nu\tilde{\mathbf{k}} \rangle$$

RPA gap structures in pseudo-crystal momentum space

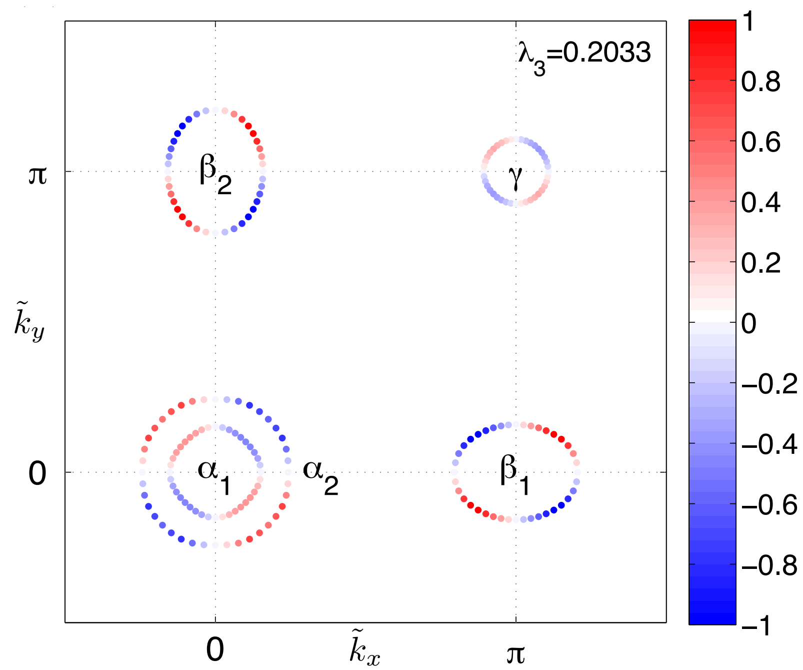
s±, λ=0.76



$d_{x^2-y^2}$, λ=0.48



d_{xy}, λ=0.20



Graser *et al.* , NJP 2009

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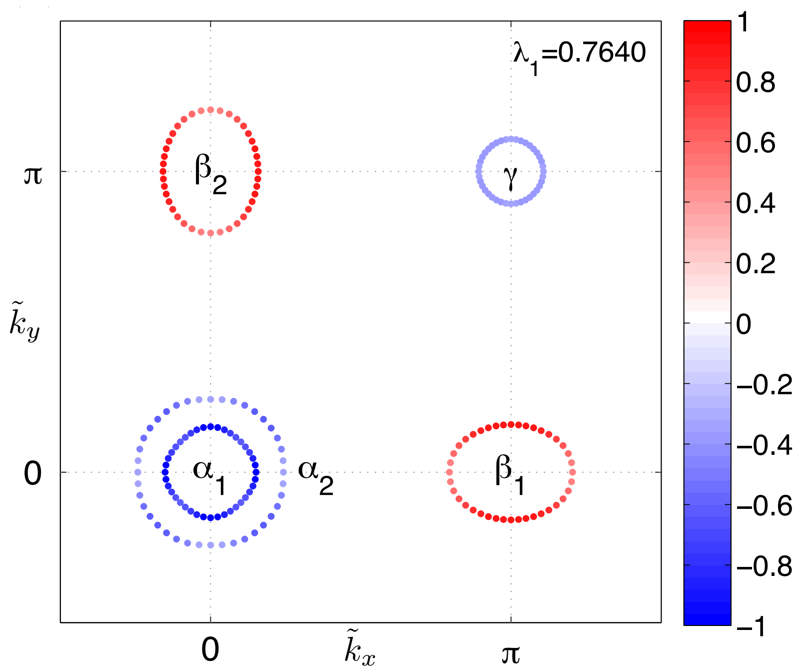
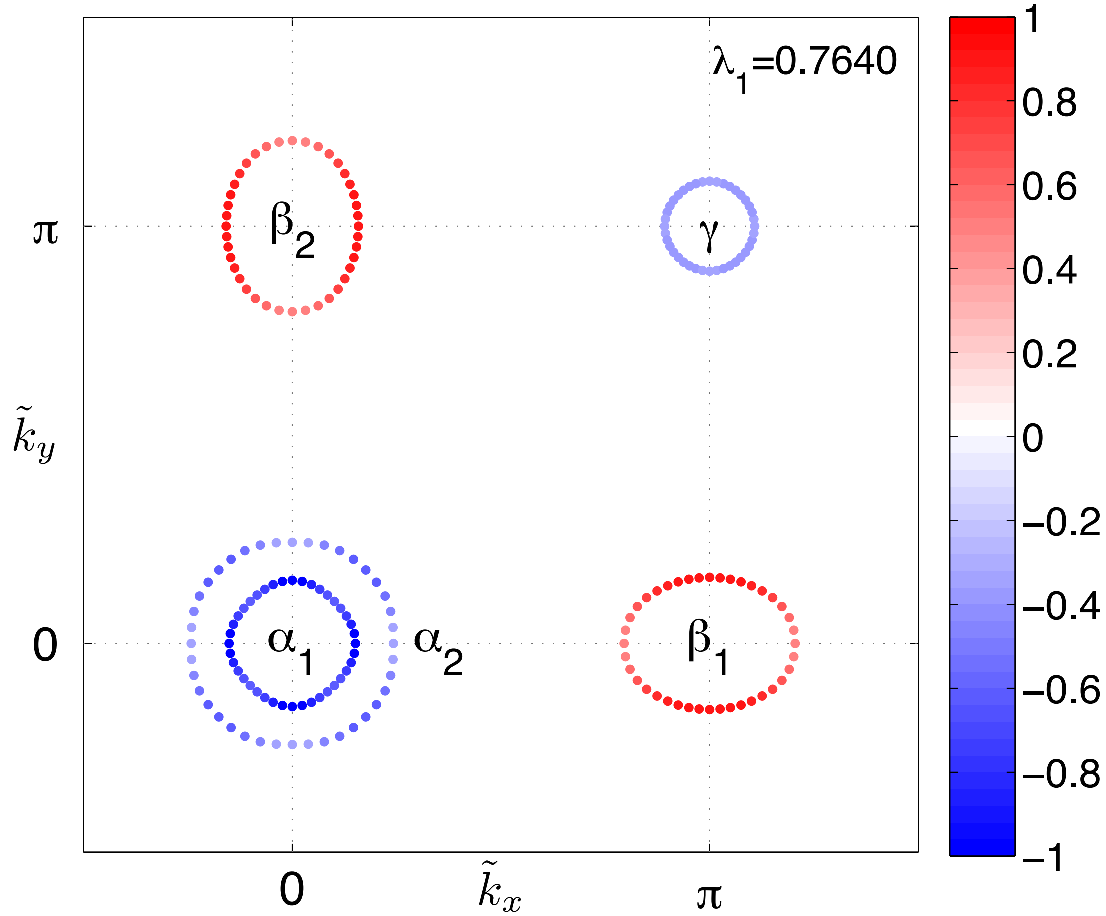
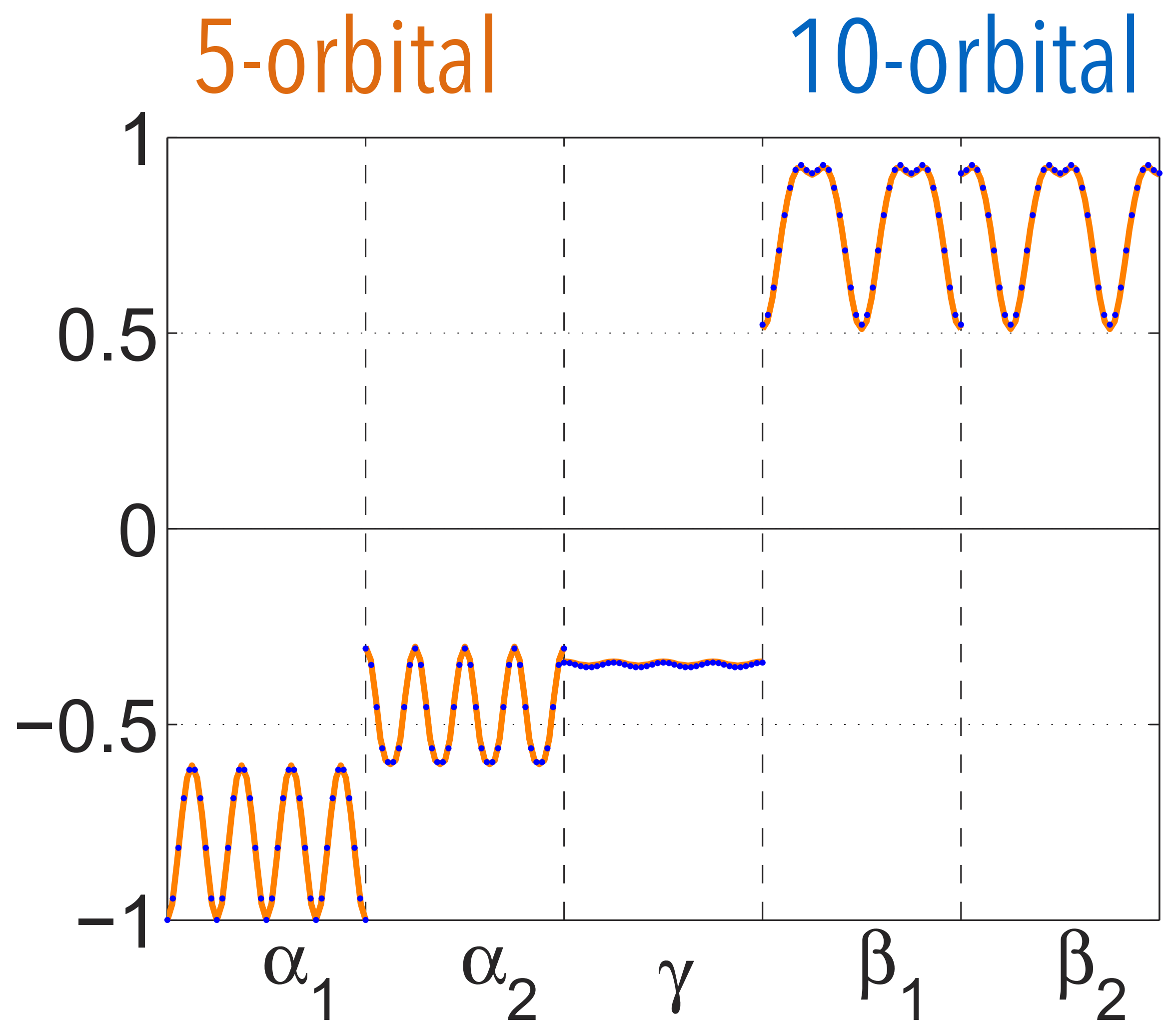


Graser *et al.* , NJP 2009

Results from 10-orbital model





- **1 Fe/5-orbital calculation agrees with full 2 Fe/10-orbital calculation**

Transformation to orbital space

Normal pairing terms

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

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

η - pairing terms

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

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

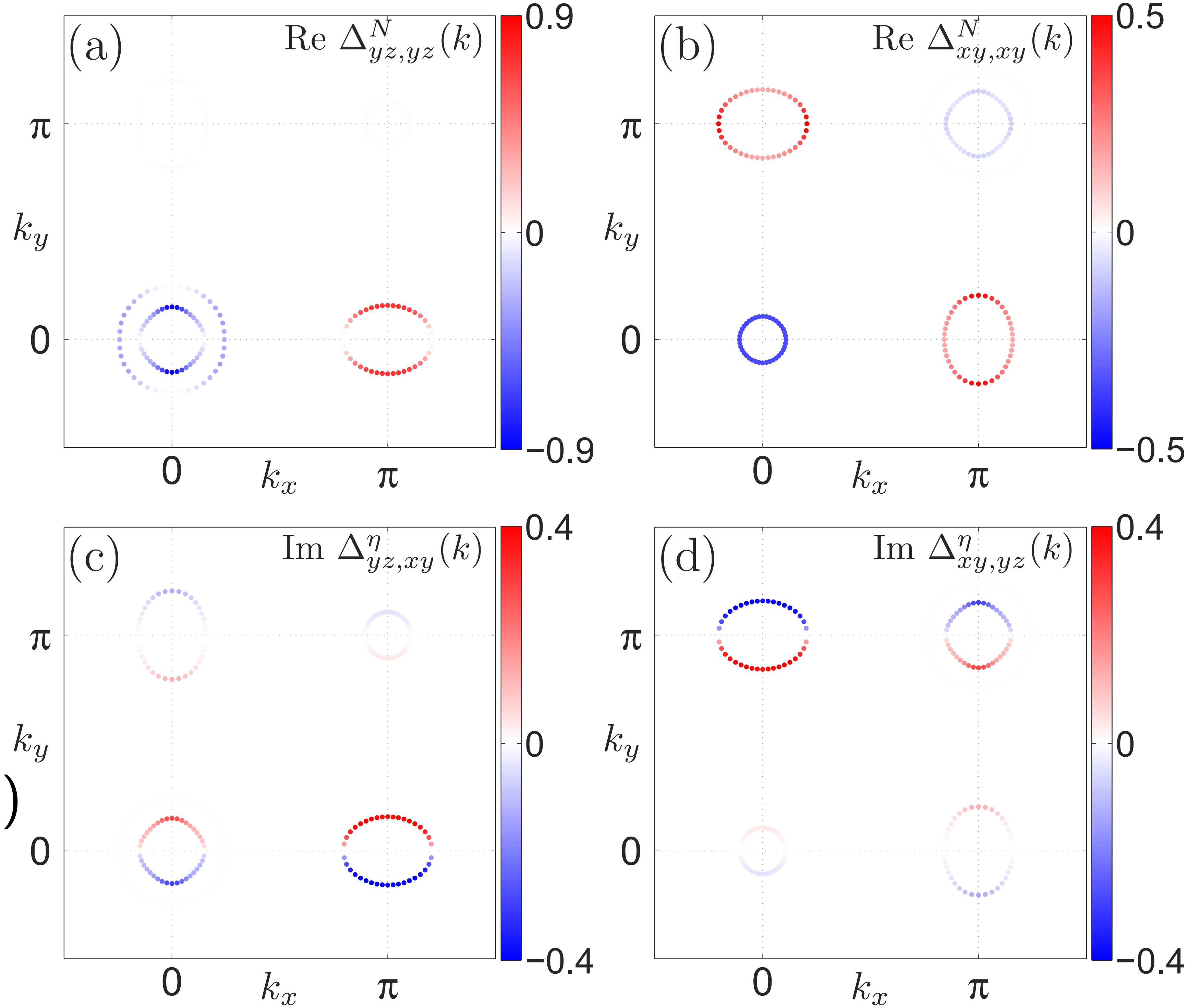
Gap functions in orbital basis/physical momentum

Normal pairing (*k*,-*k*)

- $\Delta_{\ell_1 \ell_2}(k)$ real
- $\Delta_{\ell_1 \ell_2}(k) = \Delta_{\ell_1 \ell_2}(-k)$

η-pairing (*k*,-*k*+*Q*)

- $\Delta_{\ell_1 \ell_2}(k)$ imaginary
- $\Delta_{\ell_1 \ell_2}(k) = -\Delta_{\ell_1 \ell_2}(-k)$



No time reversal symmetry breaking!

Consider singlet pair

$$\langle c^\dagger_{\ell_1\uparrow}(\mathbf{k})c^\dagger_{\ell_2\downarrow}(-\mathbf{k}) - c^\dagger_{\ell_1\downarrow}(\mathbf{k})c^\dagger_{\ell_2\uparrow}(-\mathbf{k})\rangle \propto \Delta_{\ell_1\ell_2}(\mathbf{k})$$

Time reversal symmetry requires that

$$\Delta_{\ell_1\ell_2}(\mathbf{k}) = \Delta^*_{\ell_1\ell_2}(-\mathbf{k})$$

- normal pairs

$$\Delta_{\ell_1\ell_2}(\mathbf{k}) = \Delta_{\ell_1\ell_2}(-\mathbf{k})$$

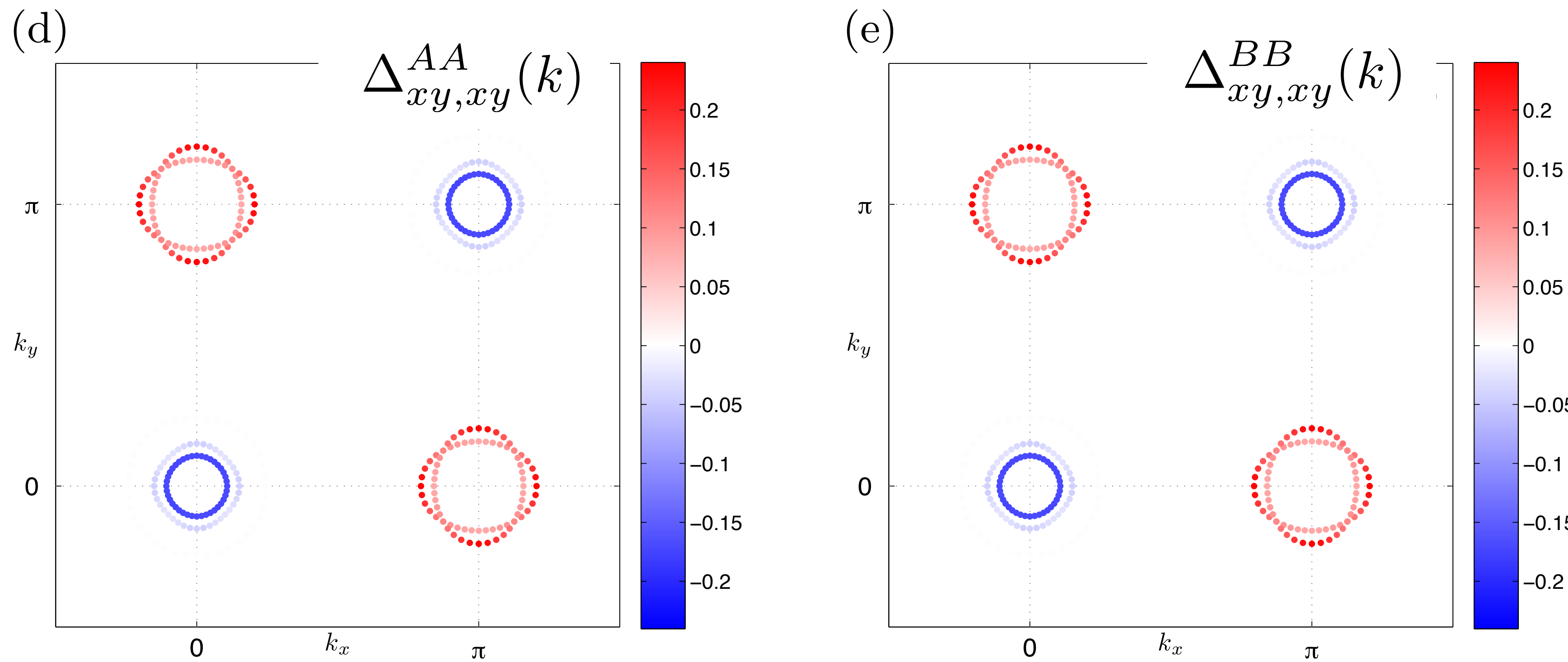
- η pairs

$$\Delta_{\ell_1\ell_2}(\mathbf{k}) = -\Delta_{\ell_1\ell_2}(-\mathbf{k})$$

Pair amplitudes in 2 Fe zone on A- and B-sublattices

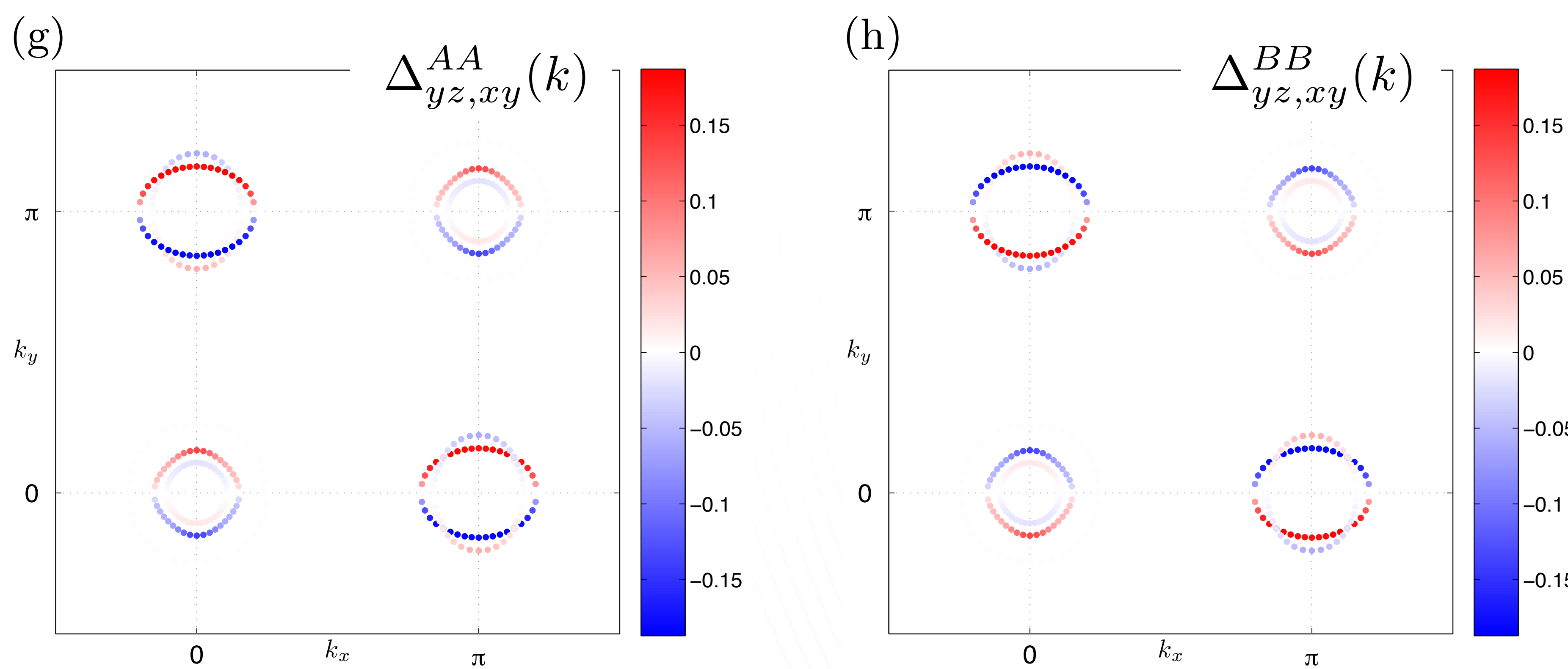
even-even

- $\Delta^{AA}_{xy,xy}(k) = \Delta^{BB}_{xy,xy}(k)$
- even parity



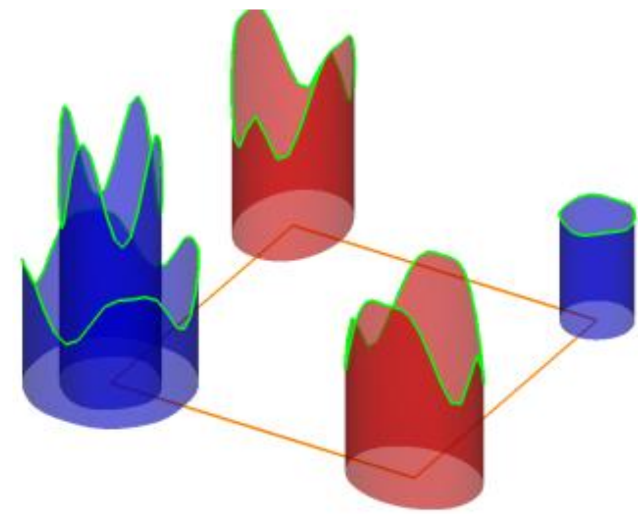
odd-even

- $\Delta^{AA}_{yz,xy}(k) = -\Delta^{BB}_{yz,xy}(k)$
- odd parity



Normal and η-gaps in band space

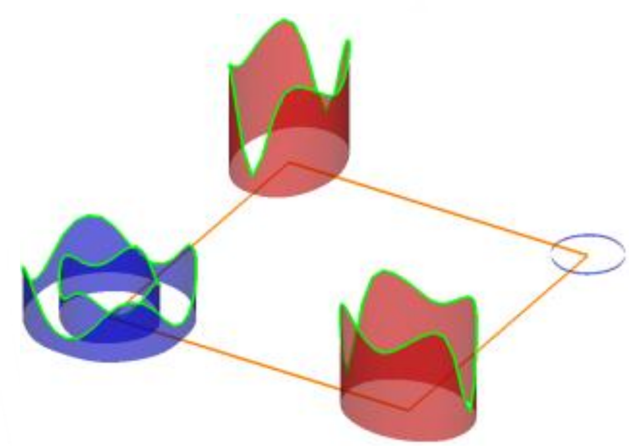
Transform back to band space



- normal pairing $\Delta_\nu^N(\mathbf{k}) = \Delta_{odd}^N(\mathbf{k}) + \Delta_{even}^N(\mathbf{k})$

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

$$\Delta_{\text{even}}^N(\mathbf{k}) = \sum_{\ell_1,\ell_2 \text{ even}} \tilde{a}_{\nu,\mathbf{k}-\mathbf{Q}}^{\ell_1^*} \tilde{a}_{\nu,-\mathbf{k}+\mathbf{Q}}^{\ell_2^*} \Delta_{\ell_1\ell_2}^N(\mathbf{k})$$



- η-pairing $\Delta_\nu^\eta(\mathbf{k}) = \Delta_{odd-even}^\eta(\mathbf{k}) + \Delta_{even-odd}^\eta(\mathbf{k})$

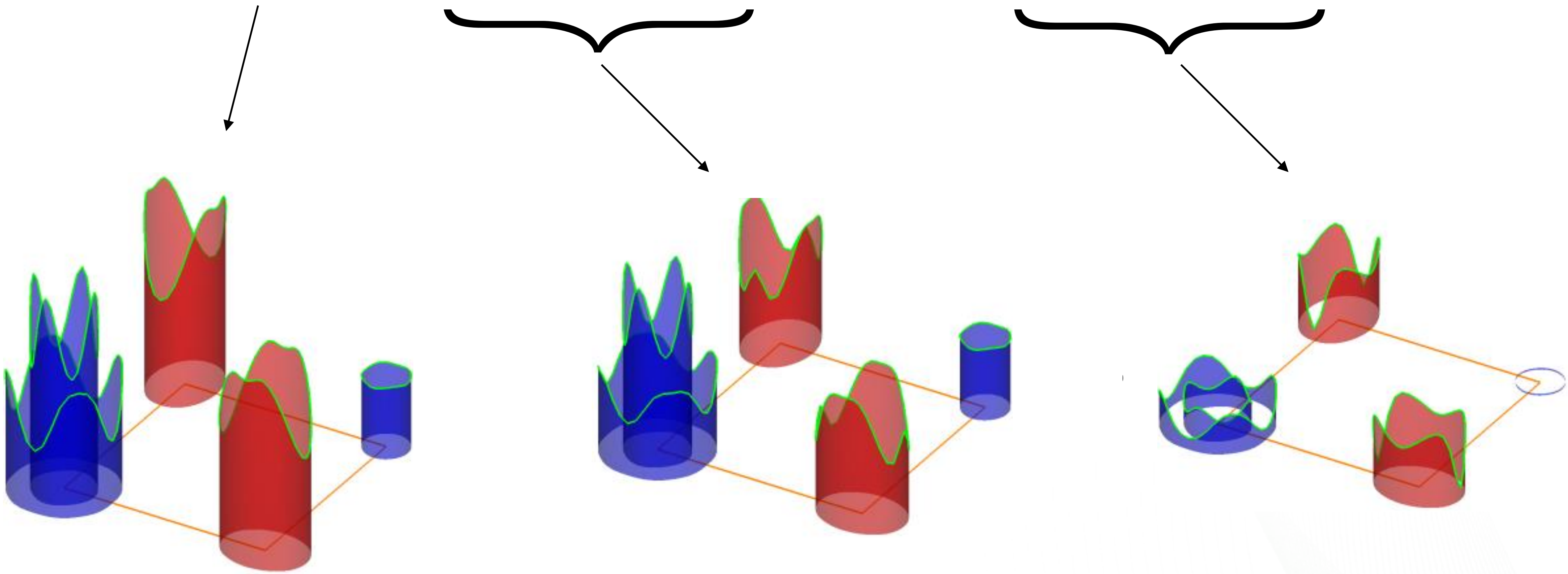
$$\Delta_{odd-even}^\eta(\mathbf{k}) = \sum_{\ell_1 \text{ odd}, \ell_2 \text{ even}} \tilde{a}_{\nu,\mathbf{k}}^{\ell_1^*} \tilde{a}_{\nu,-\mathbf{k}}^{\ell_2^*} \Delta_{\ell_1\ell_2}^\eta(\mathbf{k})$$

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

▸ **η-gap has even parity in band space**

Normal and η-gaps in band space

$$\tilde{\Delta}_\nu(\mathbf{k}) = \Delta^N_{odd}(\mathbf{k}) + \Delta^N_{even}(\mathbf{k}+\mathbf{Q}) + \Delta^\eta_{odd-even}(\mathbf{k}) + \Delta^\eta_{even-odd}(\mathbf{k}+\mathbf{Q})$$



- Gap calculated in 1 Fe pseudo-crystal momentum basis splits into normal and η-pairing gaps in physical momentum basis

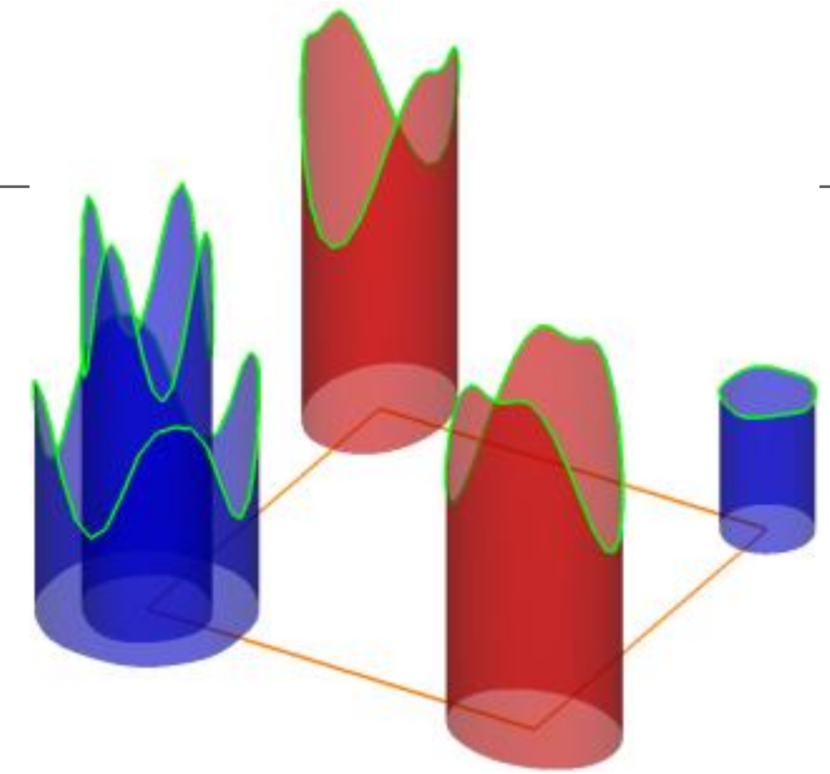
What does ARPES see?

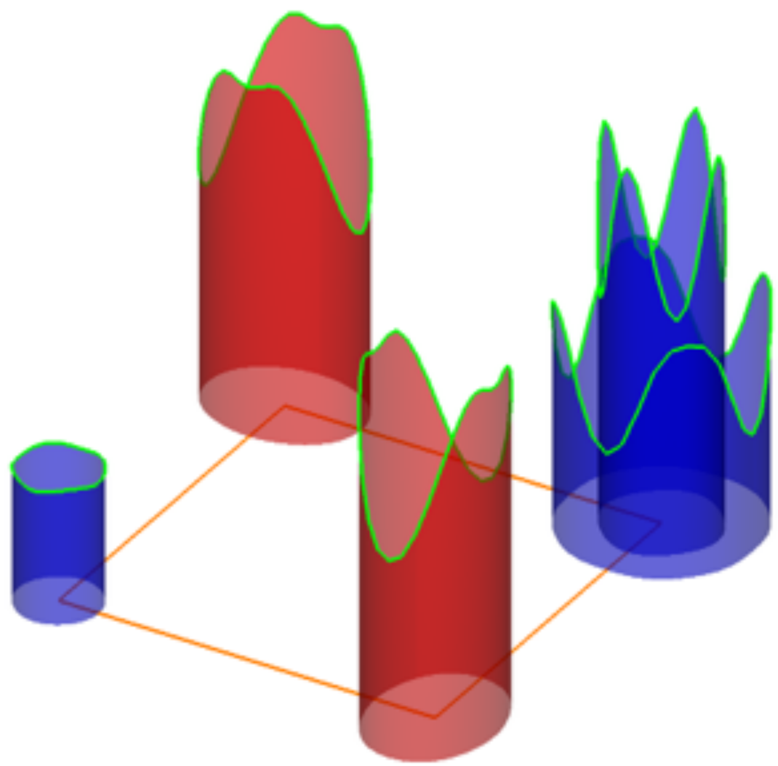
$$A(\mathbf{k},\omega) = \sum_{\ell,\nu} |\langle \ell\mathbf{k}|\nu\tilde{\mathbf{k}}\rangle|^2 \tilde{A}_\nu(\tilde{\mathbf{k}},\omega)$$

$$\tilde{A}_\nu(\tilde{\mathbf{k}},\omega) = \delta(\omega - \sqrt{\epsilon_\nu^2(\tilde{\mathbf{k}}) + \tilde{\Delta}_\nu^2(\tilde{\mathbf{k}})})$$

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

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





- **ARPES sees the gap calculated in the 1 Fe zone pseudo-crystal momentum space**

Summary & Conclusions

- η-pairing in the Fe-based superconductors appears in the 1 Fe zone because of broken translational symmetry
- It is implicitly included in 1 Fe zone calculations in pseudo-crystal momentum basis
- The gap calculated in the 1 Fe zone pseudo-crystal momentum representation is the gap that enters observables
- 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 η-pairing

3D effects?

C.-H. Lin, C.-P. Chou, W.-G. Yin, W. Ku, arXiv:1403.3687

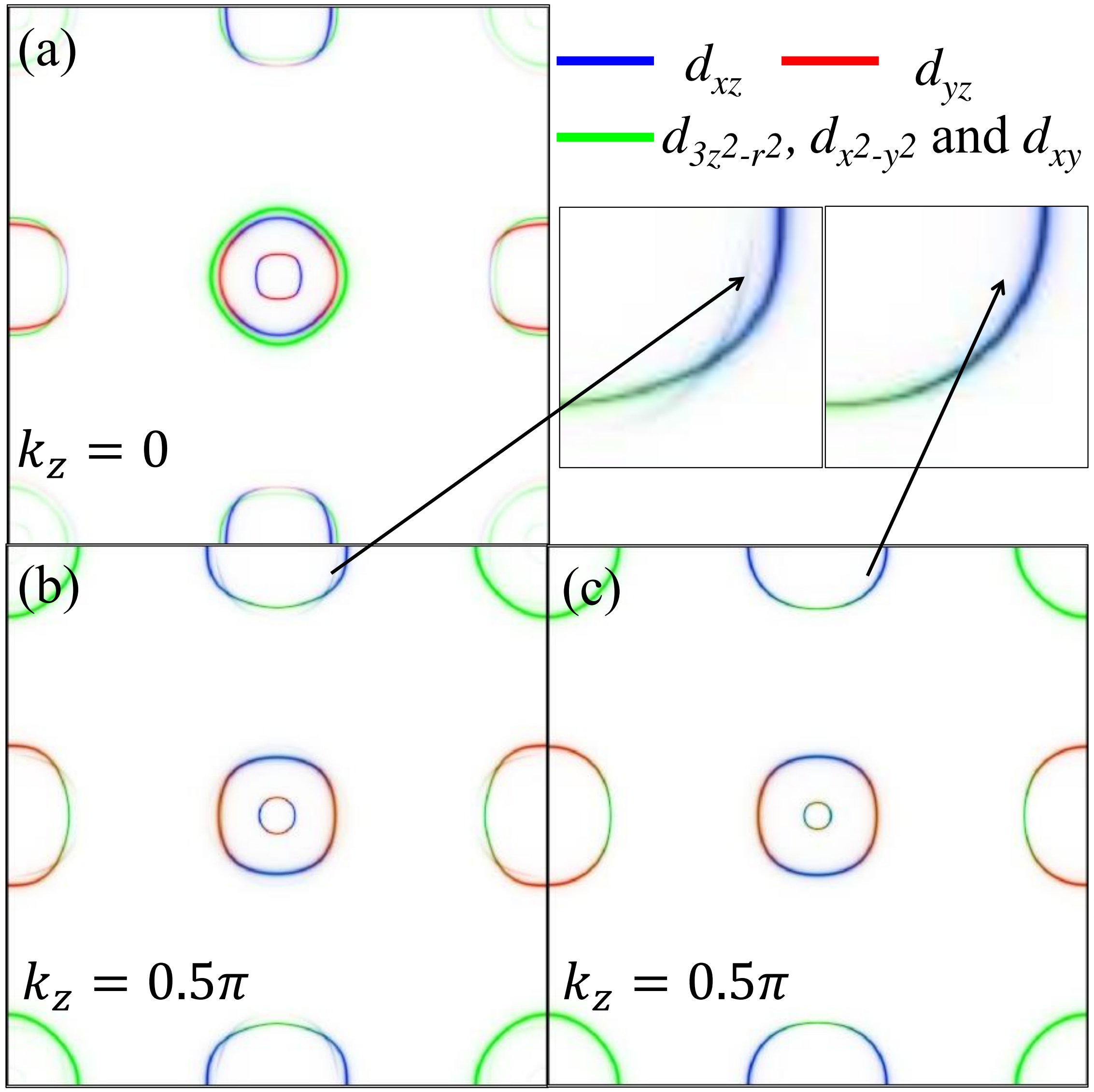


FIG. 1: (a) The unfolded one-particle spectral function $A_n(k, \omega = 0)$ at the Fermi energy calculated from the first-principles FeTe Wannier orbitals (see Ref. 22 for details). The spectral function in the local gauge space $\tilde{A}_n(\tilde{k}, \omega = 0)$ (b) with and (c) without the symmetry breaking part of $H_0^{\perp}$. The enlargements show that the folded spectral weights due to $H_0^{\perp}$ are hardly visible in (b) and vanish in (c).