Spin/Orbital correlation, disordered impurities, and glide translational symmetry of Fe-based superconductors

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Outlines

- Spin/orbital correlation
  - Ferro-orbital & AFM
  - Effect of itinerant electrons on spin dynamics & fluctuation
- Glide translational symmetry:
  - 1-Fe vs 2-Fe description
  - novel pairing structure
- Effects of disordered impurities:
  - Substitution of Fe: doping or not?
  - Fe vacancy: “violation” of Luttinger theorem
  - Ru substitution: realization of superdiffusion

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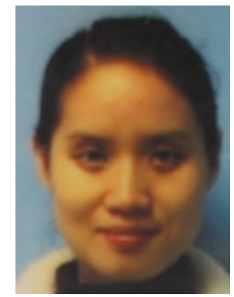

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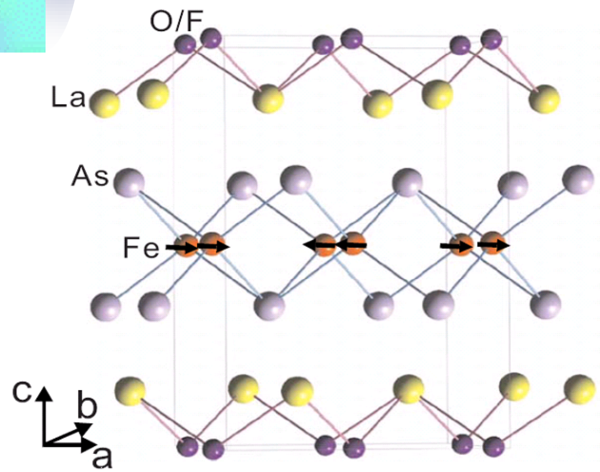
Spin & orbital: Ferro-orbital order & anisotropic magnetic structure in 1111 (&122)

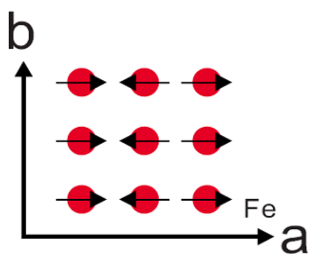
Chi-Cheng Lee, Wei-Guo Yin & Wei Ku

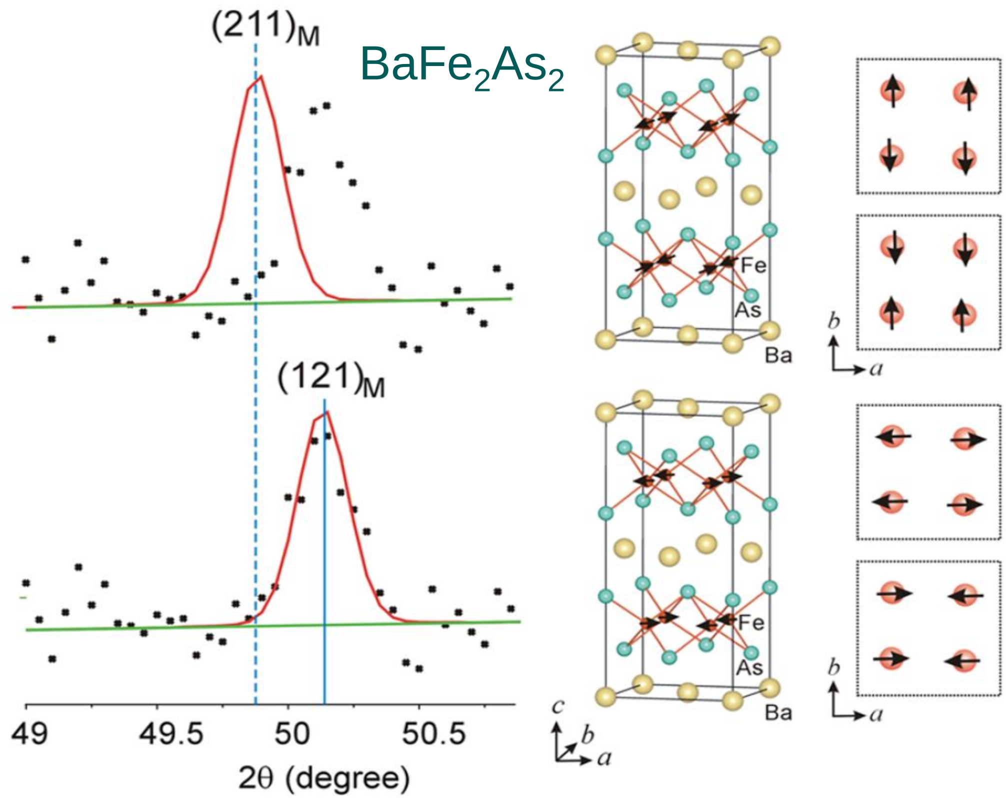
Phys. Rev. Lett. **103**, 267001 (2009)

Stripy magnetic and lattice structure



Phys. Rev. B **78**, 054529 (2008)

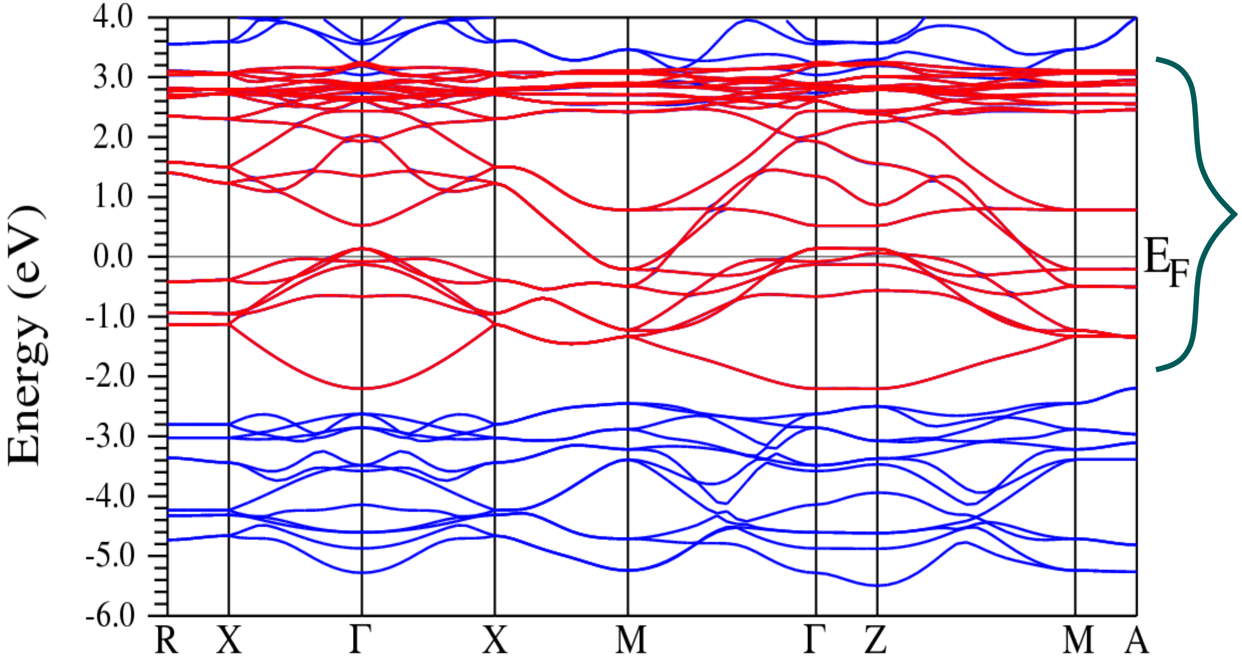




Q. Huang et al., PRL **101**, 257003 (2008)

- Structure transition at 155k; Stripy AFM order at 137K (AF bond longer?)
- What drives the magnetic transition?
  Fermi surface instability? (SDW due to nesting?)
- What drives the structural transition?
  Transition temperature so close to magnetic T_N : related?
- Implications to electronic structure and superconductivity?

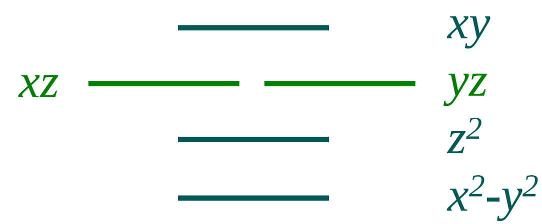
Energy resolved, symmetry respecting Wannier function



$$|\vec{R}n\rangle = \sum_{\vec{k}m}^{\text{(energy window)}} |\vec{k}m\rangle\langle\vec{k}m|\vec{R}n\rangle$$

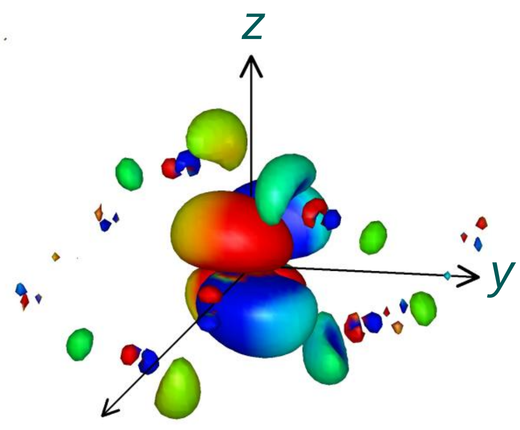
$$= \frac{1}{\sqrt{N_{cell}}} \sum_{\vec{k}m} |\vec{k}m\rangle e^{-i\vec{k}\cdot\vec{R}} U_{mn}^{(\vec{k})}$$

$$= \frac{1}{\sqrt{N_{cell}}} \sum_{\vec{k}} \left(\sum_{m} U_{mn}^{(\vec{k})} |\vec{k}m\rangle \right) e^{-i\vec{k}\cdot\vec{R}}$$

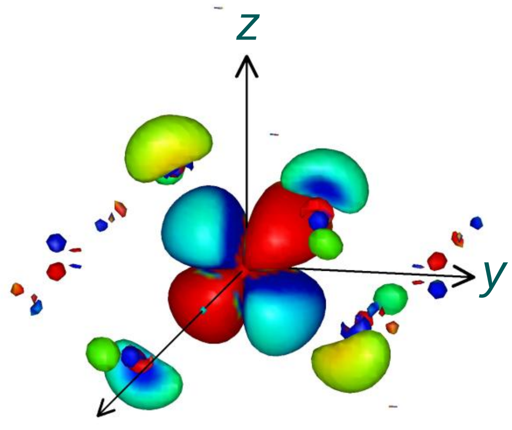


NM onsite energy (eV)

z^2	-0.03
x^2-y^2	-0.20
yz	0.10
xz	0.10
xy	0.34



d_{xz}



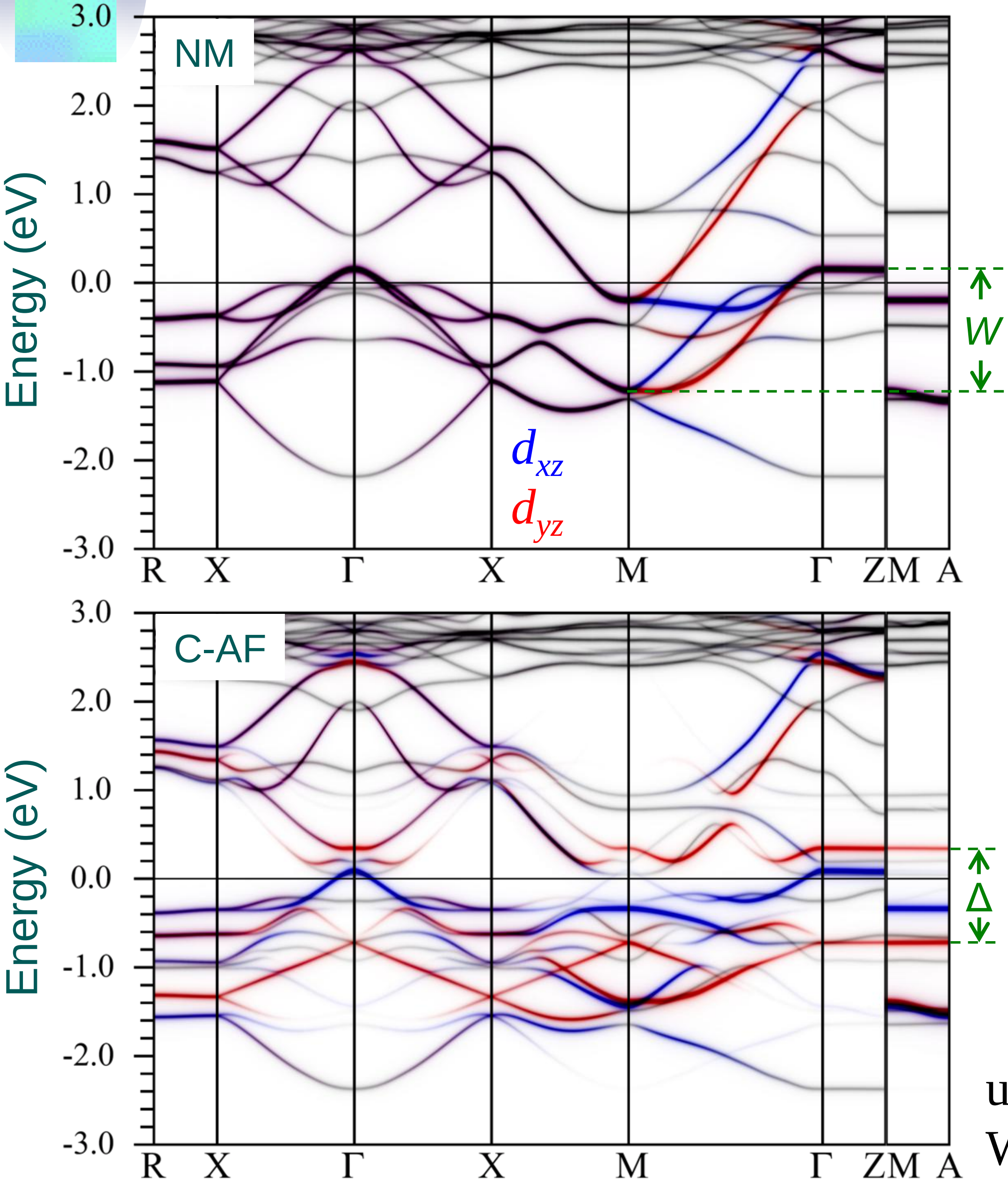
d_{yz}

- small crystal field splitting
- degenerate *xz* and *yz*

→ orbital freedom !

methods see: W. Ku et al., PRL **89**, 167204 (2002); W. Yin et al., PRL **96**, 116405 (2006)

Comparing LDA band structures



- in NM 1st-BZ
- d_{xz} & d_{yz} most relevant to the low-E
- Only d_{yz} splits strongly near E_F
- d_{yz} more spin polarized ~0.34μ_B than d_{xz} (~0.15μ_B)
- more different with U=2eV 0.58 vs. 0.23μ_B

→ orbital symmetry broken

- Δ ~ W

→ large (ω,**k**)-space involved

→ local picture more suitable

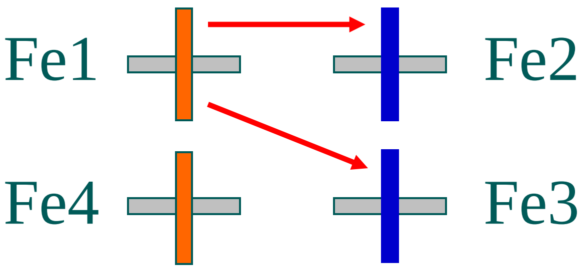
→ Fermi surface nesting not essential

→ SDW less convenient

unfolding methods see:
Wei Ku *et al.*, PRL **104**, 216401 (2010)

Anti-intuitive hopping parameters

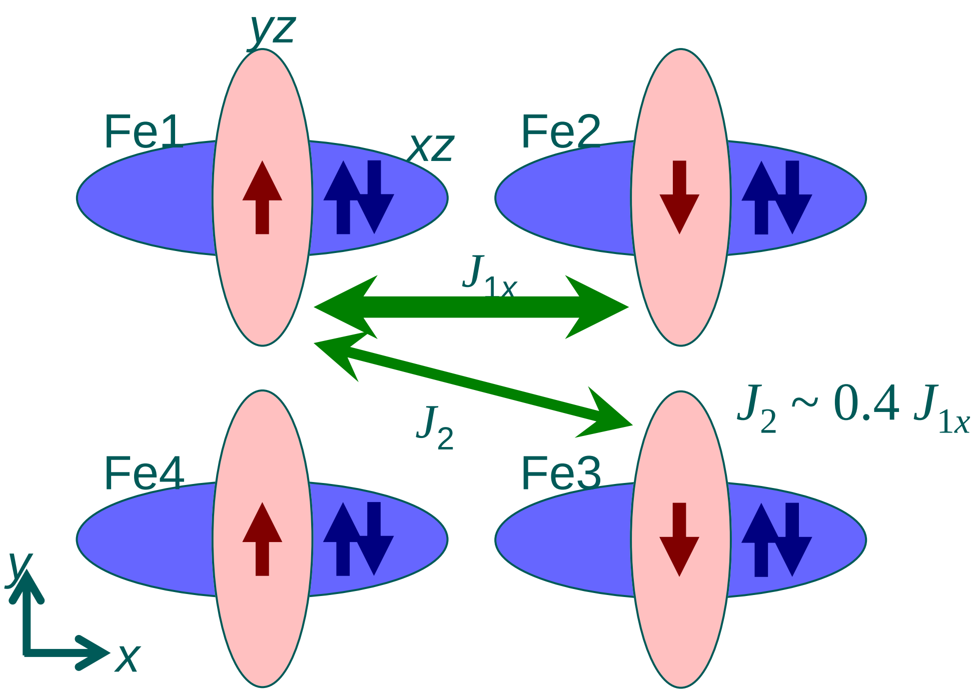
<WFs|H|WFs>	Fe1 z^2	x^2-y^2	yz	xz	xy
Fe2 (Fe4) z^2	0.13	0.31 (-0.31)	-0.10 (0.00)	0.00 (0.10)	0.00
x^2-y^2	0.31 (-0.31)	-0.32	0.42 (0.00)	0.00 (0.42)	0.00
yz	-0.10 (0.00)	0.42 (0.00)	-0.40 (-0.13)	0.00	0.00 (0.23)
xz	0.00 (0.10)	0.00 (0.42)	0.00	-0.13 (-0.40)	-0.23 (0.00)
xy	0.00	0.00	0.00 (0.23)	-0.23 (0.00)	-0.30
Fe3 z^2	0.06	0.00	-0.08	0.08	0.26
x^2-y^2	0.00	-0.10	0.12	0.12	0.00
yz	0.08	-0.12	0.25	-0.07	-0.05
xz	-0.08	-0.12	-0.07	0.25	0.05
xy	0.26	0.00	0.05	-0.05	0.16

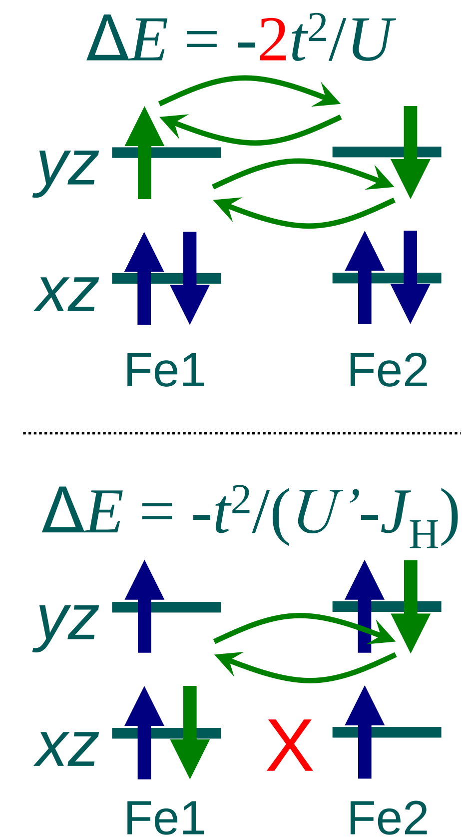


- Unusual coupling direction
- Cubic symmetry broken seriously by As
  → Fe-As phonon modes important
- Perpendicular hopping direction!

Chi-Cheng Lee *et al.*, PRL **103**, 267001 (2009)

C-AF magnetic structure and ferro-orbital order





- Strongly anisotropic super-exchange: $J_{1x} > J_2 >> J_{1y}$
  → no competition with G-AF at all ! $J_1 \sim 2J_2$ irrelevant !
  → Heisenberg model inadequate
- Orbital polarization and ferro-orbital correlation important
  Unusual coupling direction and strong anisotropic hoppings !
  → $a > b$: AF across long bond (rare)
  → strong in-plane nematic-like anisotropic response
  transport, optical, and lattice properties

Chi-Cheng Lee *et al.*, PRL **103**, 267001 (2009)

Effects of itinerant carriers:
Rich magnetic orders & strong moment fluctuation

Weiguo Yin, Chi-Cheng Lee & Wei Ku
Phys. Rev. Lett. **105**, 107004 (2010)

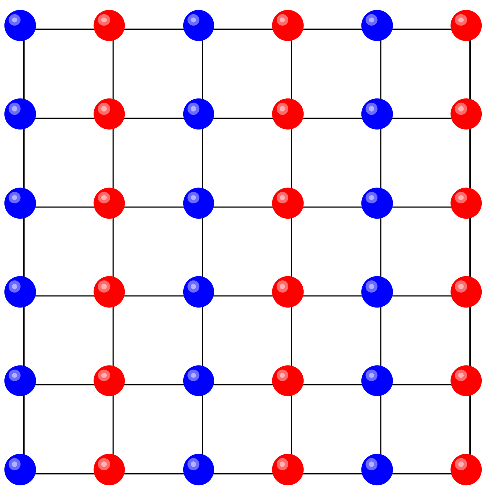
Weiguo Yin, Chia-Hui Lin & Wei Ku
Phys. Rev. B **86**, 081106(R) (2012)

Yuting Tam, Daoxin Yao, & Wei Ku
preprint

Magnetic structures of parent compounds

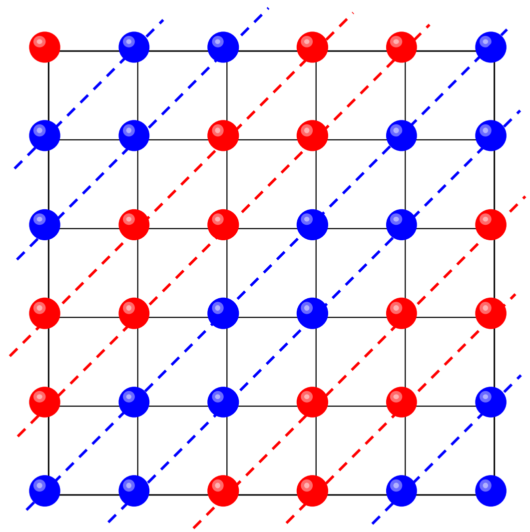
W. Bao *et al.*, arXiv:1102.3674

Collinear
C-type
$(\pi, 0)$



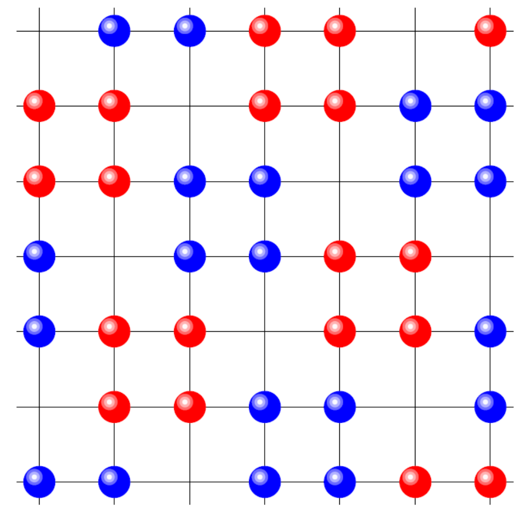
1111 (e.g. $LaO_{1-x}F_xFeAs$)
122 (e.g. $Ba_{1-x}K_xFe_2As_2$)

Bi-collinear
E-type
$(\pi, -\pi)$



11 (e.g. $FeTe_{1-x}Se_x$)

Block checkerboard
X-type
$(3\pi/5, \pi/5)$



245 ($K_{0.8}Fe_{1.6}Se_2$)

magnetic insulator
finally a Mott insulator?

- Fermi surface are similar
  → not simple nesting

Questions about magnetism in Fe-SC

- Large local moment with small ordered moment, for example

TABLE I: local moment and ordered moment in several systems

System	local moment(μ_B)	ordered moment(μ_B)
LaFeAsO	$1.1 \sim 2.4$ [2]	0.36 [6]
CeFeAsO	1.3 [7]	0.8 [8]
PrFeAsO	1.3 [9]	0.35 [10]
FeTe	$2 \sim 3$ [1]	$0.4 \sim 2$ [11]
$BaFe_2As_2$	1.3 [9]	0.87[12]
$SrFe_2AS_2$	2.1 [7]	0.94 [13]

  - fluctuation at different length scales
  - spatial fluctuation, not a mean-field behavior
- Local moment and itinerant carriers: roles of itinerant carriers
  - stability of states
  - roles in moment fluctuation
  - effects of nesting

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Simplest coupling: spin-fermion model

$$H = -\sum_{ij\gamma\gamma'\sigma} \left(t_{ij}^{\gamma\gamma'} d^{\dagger}_{i\gamma\sigma} d_{j\gamma'\sigma} + h.c.\right) - K\sum_{i} \vec{s}_i \cdot \vec{S}_i + \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

- "Itinerant" electrons: d & s
- "Localized" spins: S

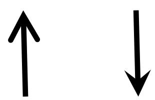
Background

- *Solvation of U but not J.* Sawatzky et al., *EPL* 86, 17006 (2009).
  - *U*=2 eV, *J*=0.8 eV, Yang et al., PRB 80, 014508 (2009).
- *Reversed strong anisotropy in the n.n. hoppings of xz and yz*
  - Lee et al., PRL 103, 267001 (2009).
- *Strongly spin-dependent electron transport in $BaFe_2As_2$.*
  - Chuang et al., *Science* 327, 181 (2010).

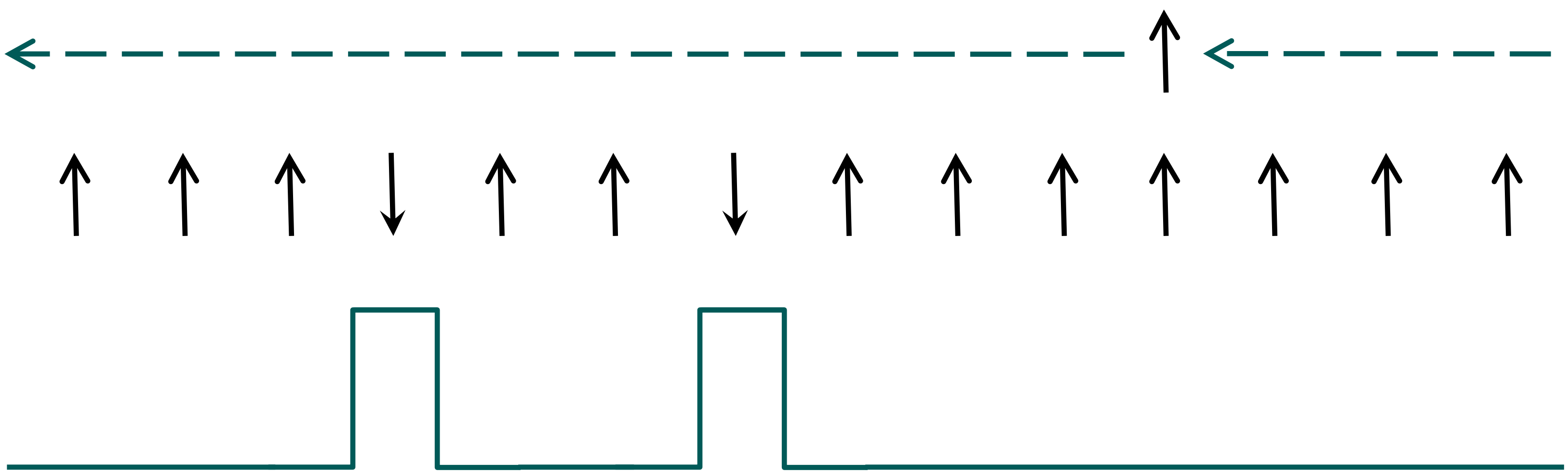
W.-G. Yin *et al*, PRL **105**, 107004 (2010)
See also P. Phillips, ZY Weng, E. Dagotto

Super exchange vs. double exchange

- Super exchange between local moments → local AF coupling

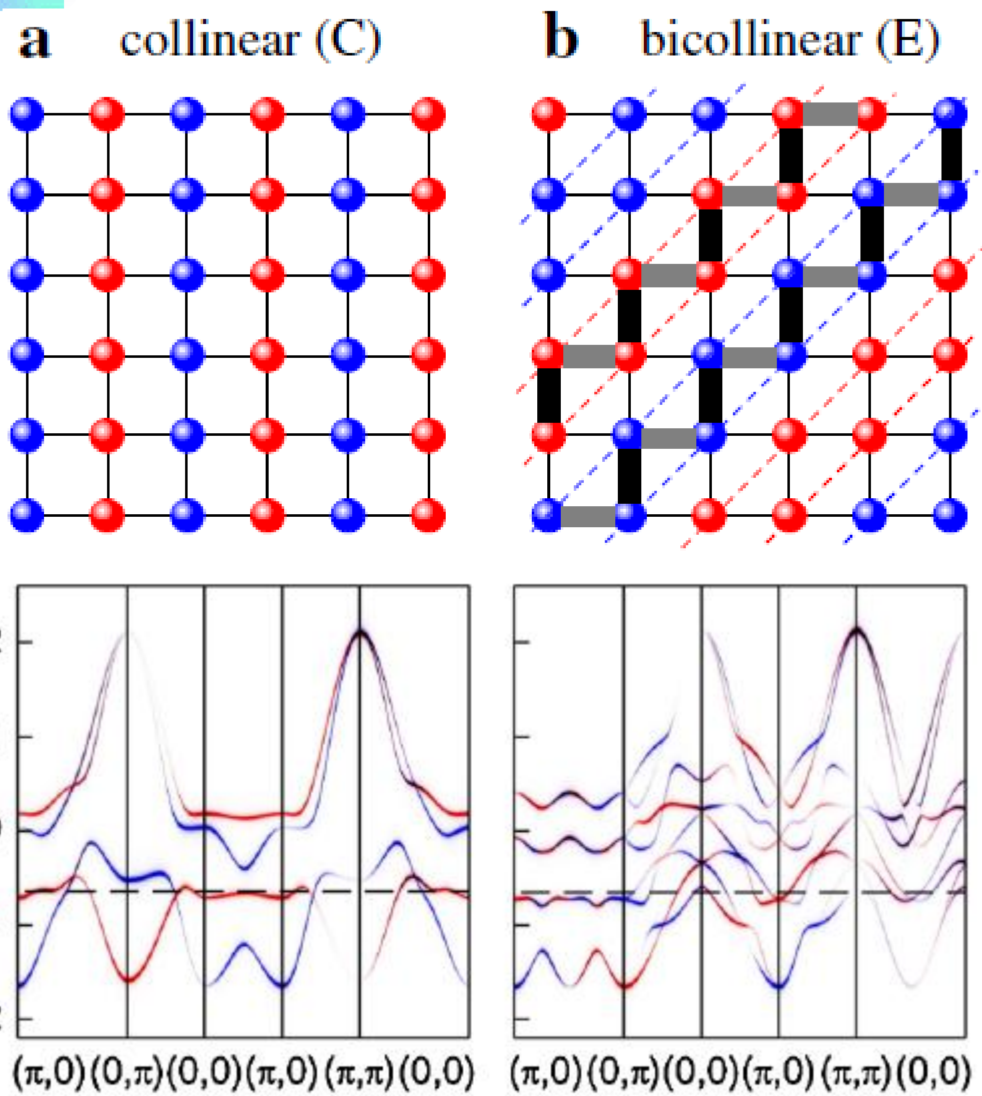


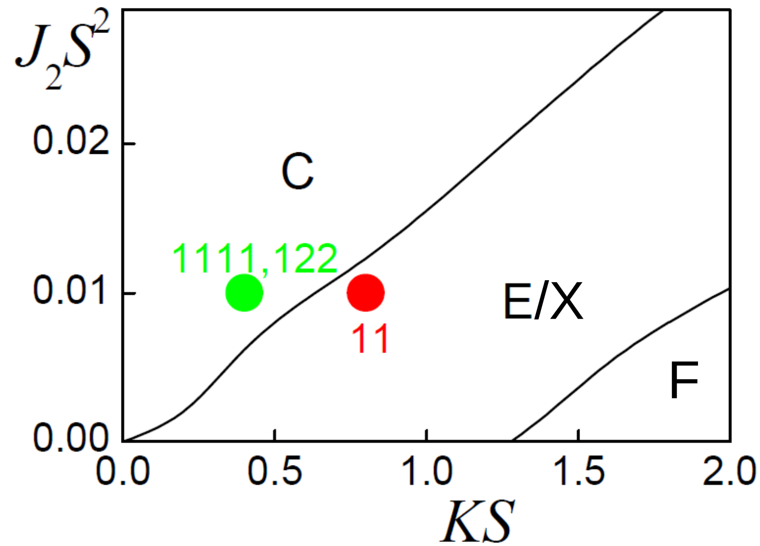
- Double exchange effects → range-dependent FM coupling



→ intrinsic instability with AF-coupled 1D FM chains
or, "dimerization" to strengthen local bonds
→ strong *T*-dependent scattering of carriers against spin

Rich magnetic structures

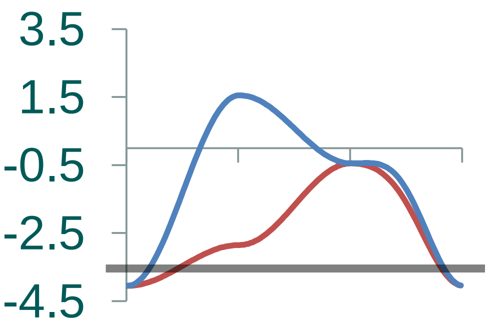


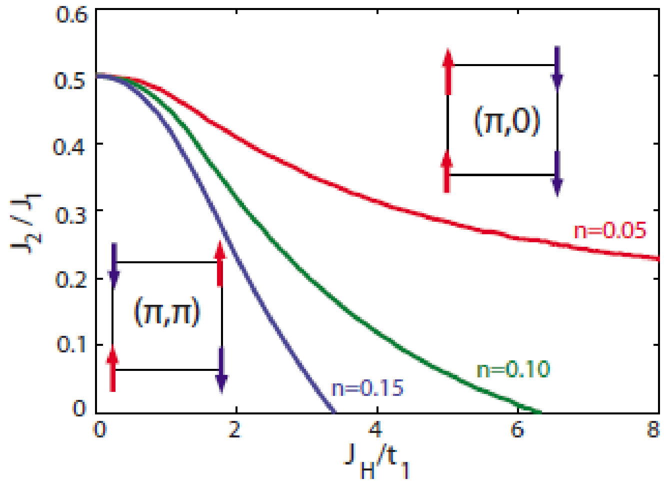


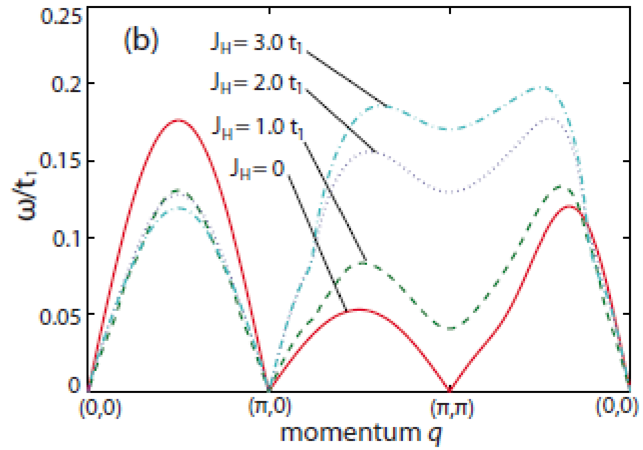
- C-type ← J_2S^2
- E-type ← KS & KE
- Weak OO in E-type

W.-G. Yin *et al*, PRL **105**, 107004 (2010)
W.-G. Yin *et al.*, PRB **86**, 081106(R) (2012)

Phase stability and renormalization of spin waves

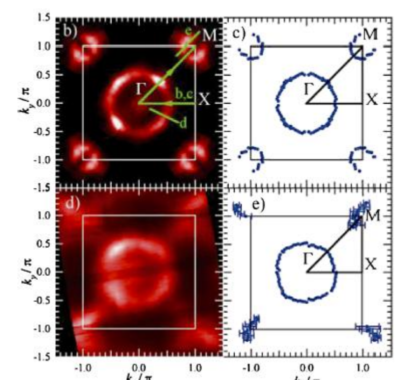






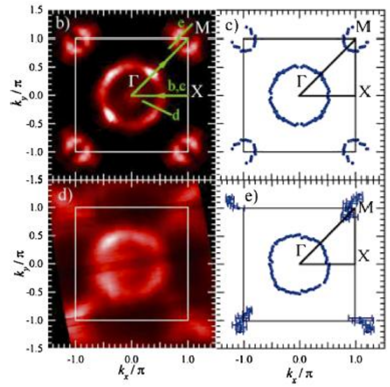
Lv, W., F. Krüger, et al. PRB.82.045125(2010).

- Introduction of small number of "free" carriers
  → generates stronger coupling along FM neighbors (double exchange)
  → enhance stripe state
  → higher spin wave energy near (π,π)
- Nesting physics absent ☹

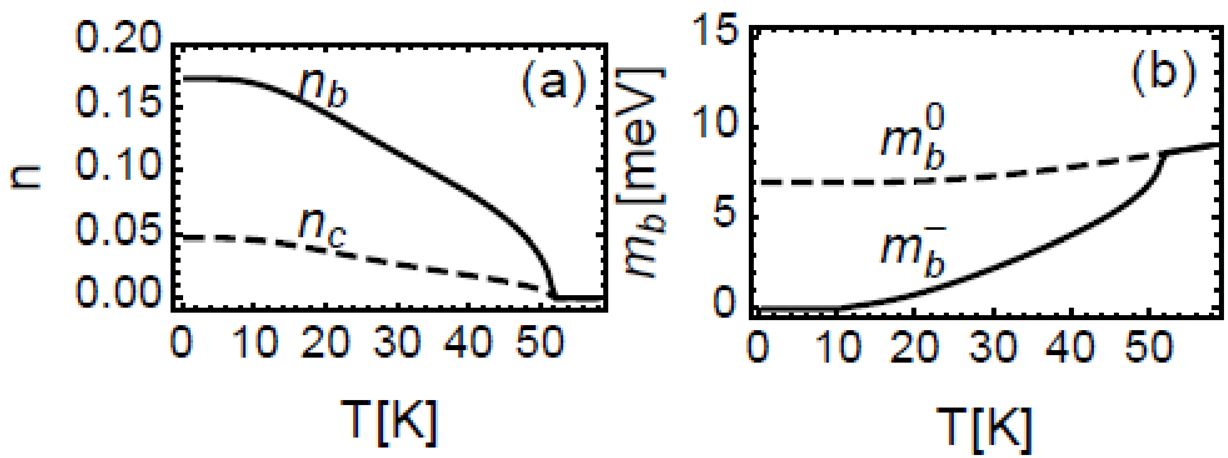


H. Ding et al. arXiv:0812.0534.

Role of nesting?



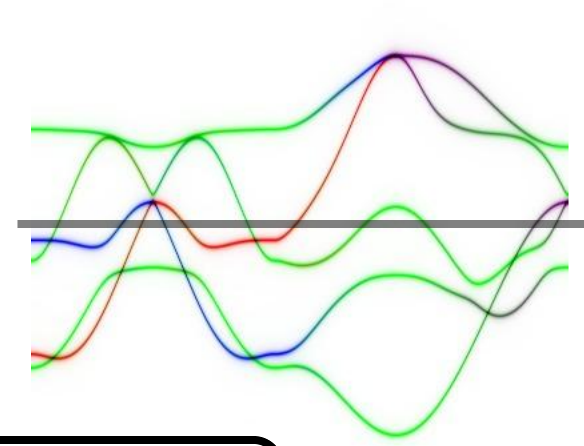
H. Ding et al. arXiv:0812.0534.



Yi-Zhuang You and Zheng-Yu Weng, NJP **16**, 023001 (2014)

- Intuitively, nesting of itinerant carriers should help stabilize the stripe phase.
- You & Weng: Itinerant and local join force to give strong stripe order.

Method



DFT

→ Wannier function

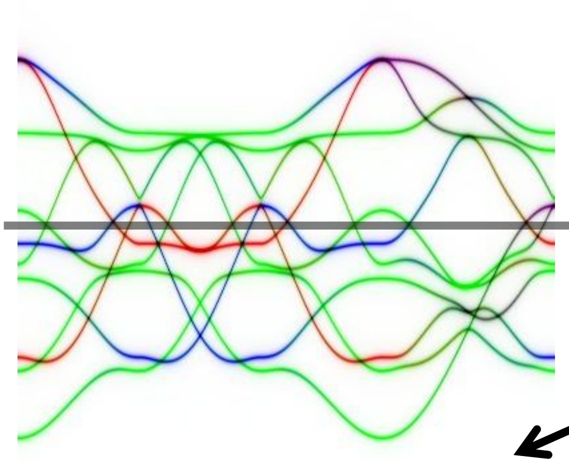
$H^{10\text{-band}}$

→ Local gauge transform

$2D\ H^{5\text{-band}}$

→ Spin-rotation

$2D\ H^{10\text{-band}}$



→ Integrate out itinerant carriers (Lv et al, PRB 2010)

Renormalized linear spin wave H^{SW}

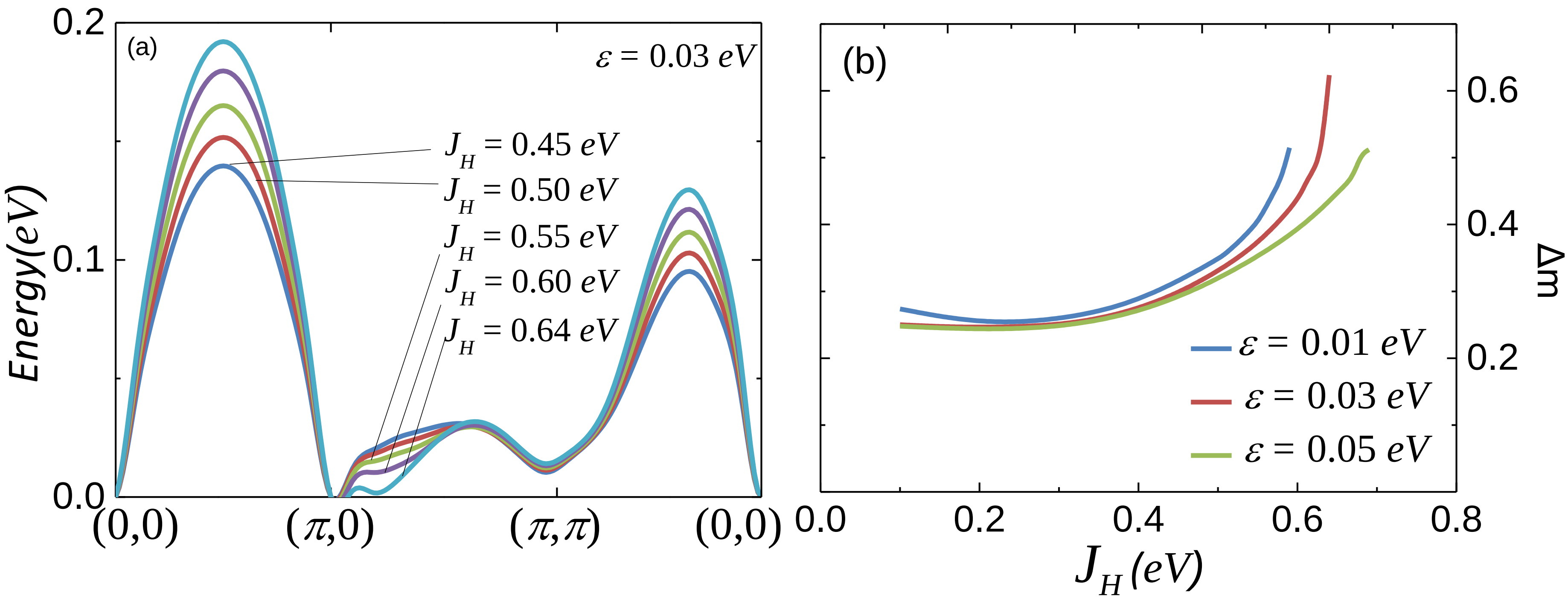
→ Spin wave theory

Dispersion & fluctuation

- Include the ferro-orbital order parameter ε in $H^{5\text{-band}}$

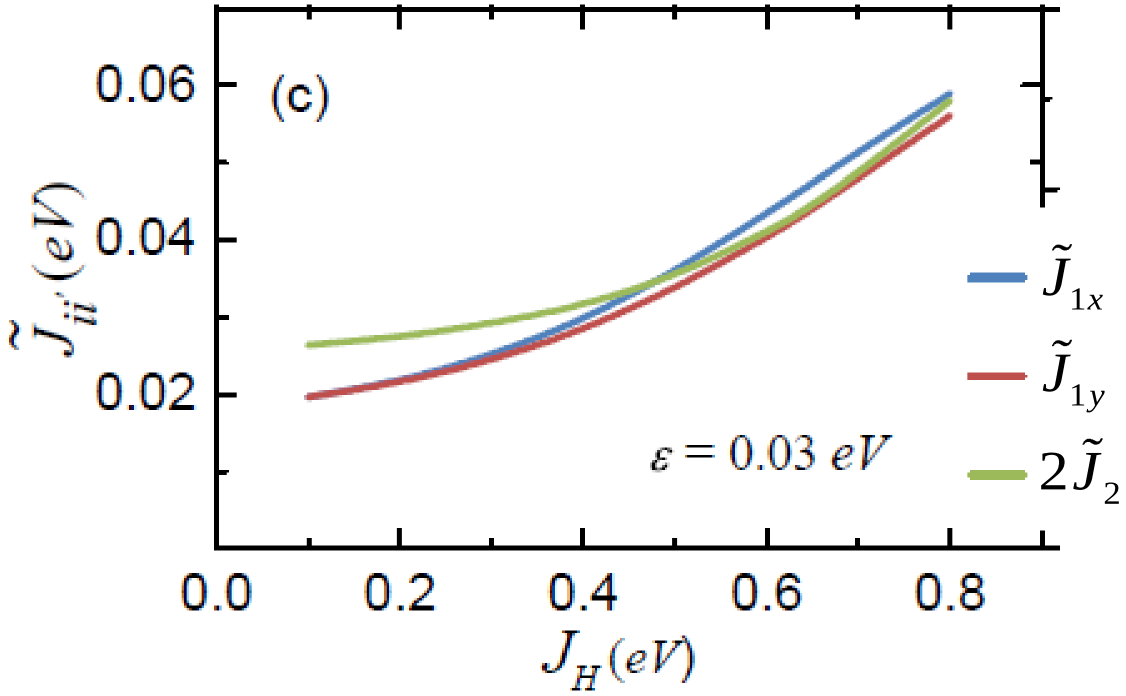
Effects of itinerant carriers

$S = 1,\ J_1 = 0.019\ eV,\ J_2 = 0.013\ eV$



- Larger J_H: stronger moment fluctuation easily 60% suppression
- Fluctuate along (π,q) direction
- Not a FM double exchange effect, but an AFM effect !
- Temporal and spatial fluctuation
- Significant reduction of ordered moment

Renormalization of real-space couplings



- Enhancement of short-range AFM couplings
- Not a FM double exchange effect, but an AFM effect !
- Fluctuation along (π, q) enhanced as $2J_2$ approaches J_{1y}.

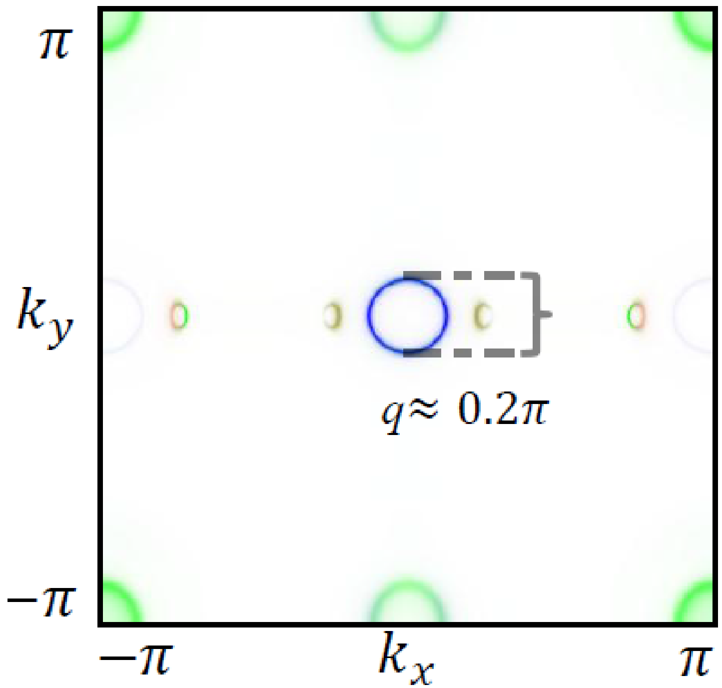
Long-rang couplings

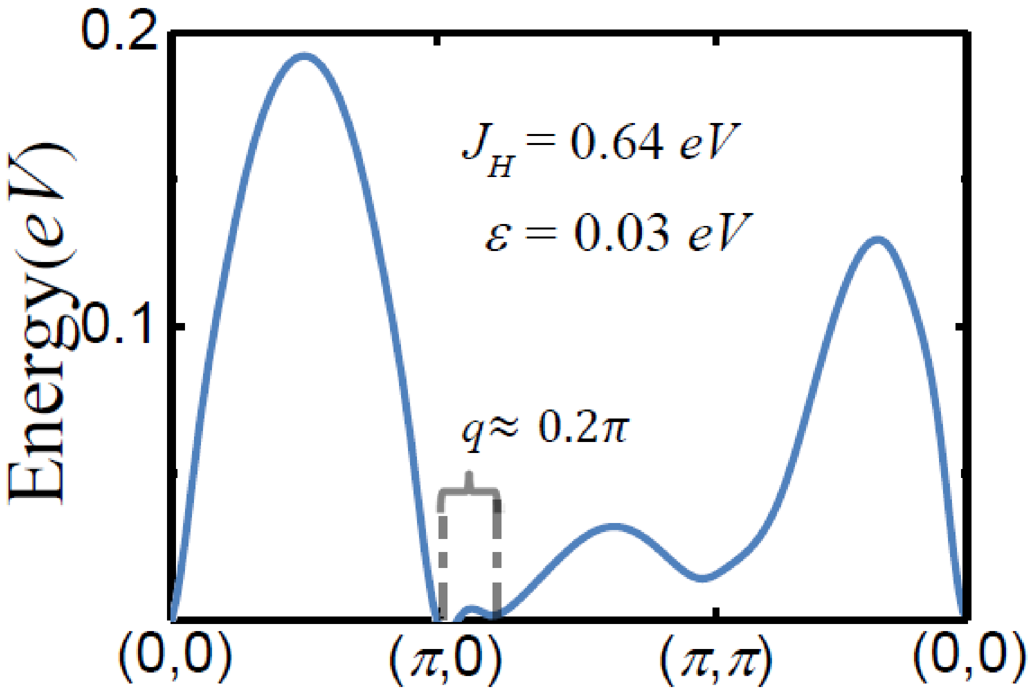
TABLE II: Importance of induced long-range coupling

$J_H = 0.6\,ev$, $\epsilon = 0.03\,ev$	$q = (\pi, \frac{\pi}{5})$ full/up-to-$\tilde{J}_2$	$q = (\pi, \pi)$ full/up-to-$\tilde{J}_2$
A_q	0.1534/0.1558	0.0134/0.0316
B_q	-0.1527/-0.1532	0.0022/-0.0049
w_q	0.0103/0.0281	0.0132/0.0312

- Itinerancy → long-range (RKKY-like) couplings with power-law decay
- Long-range effects comparable to short-range ones
- Spatial fluctuation in addition to temporal fluctuation

Nesting ⟷ Long rang interaction

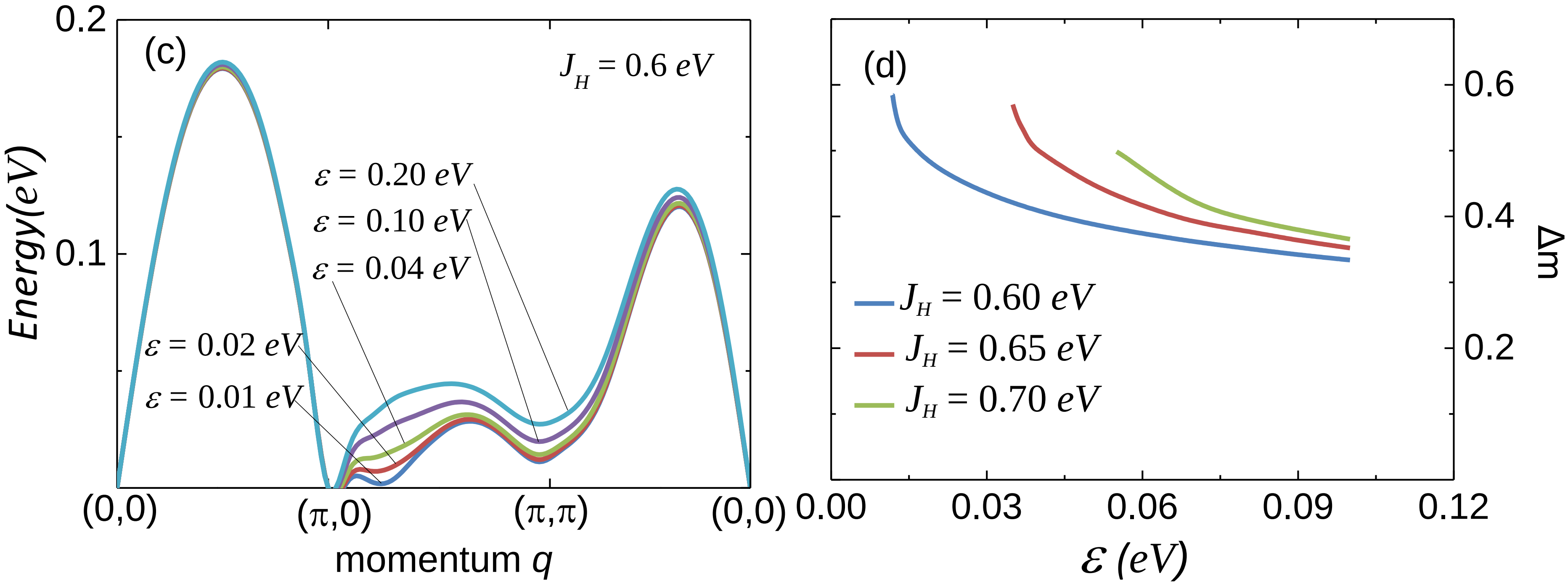




- Fermi surface nesting of the ordered state
  → pinpoint most fluctuating momentum region
  → strong long-range spatial fluctuation

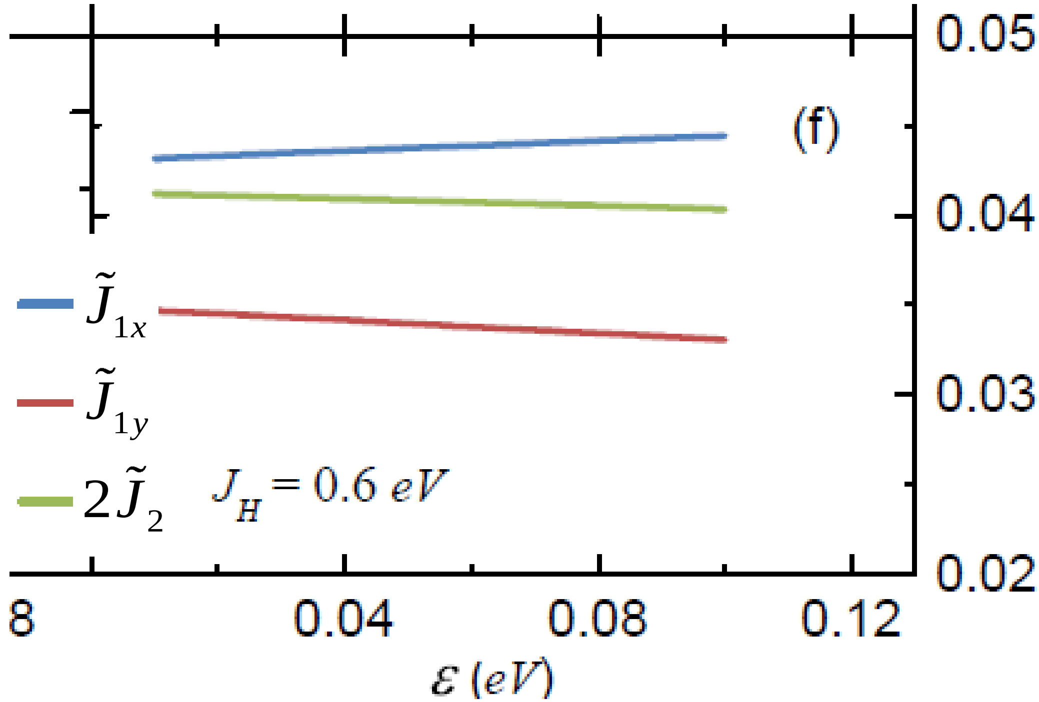
Effects of ferro-orbital order

$S = 1, J_1 = 0.019\ eV, J_2 = 0.013\ eV$



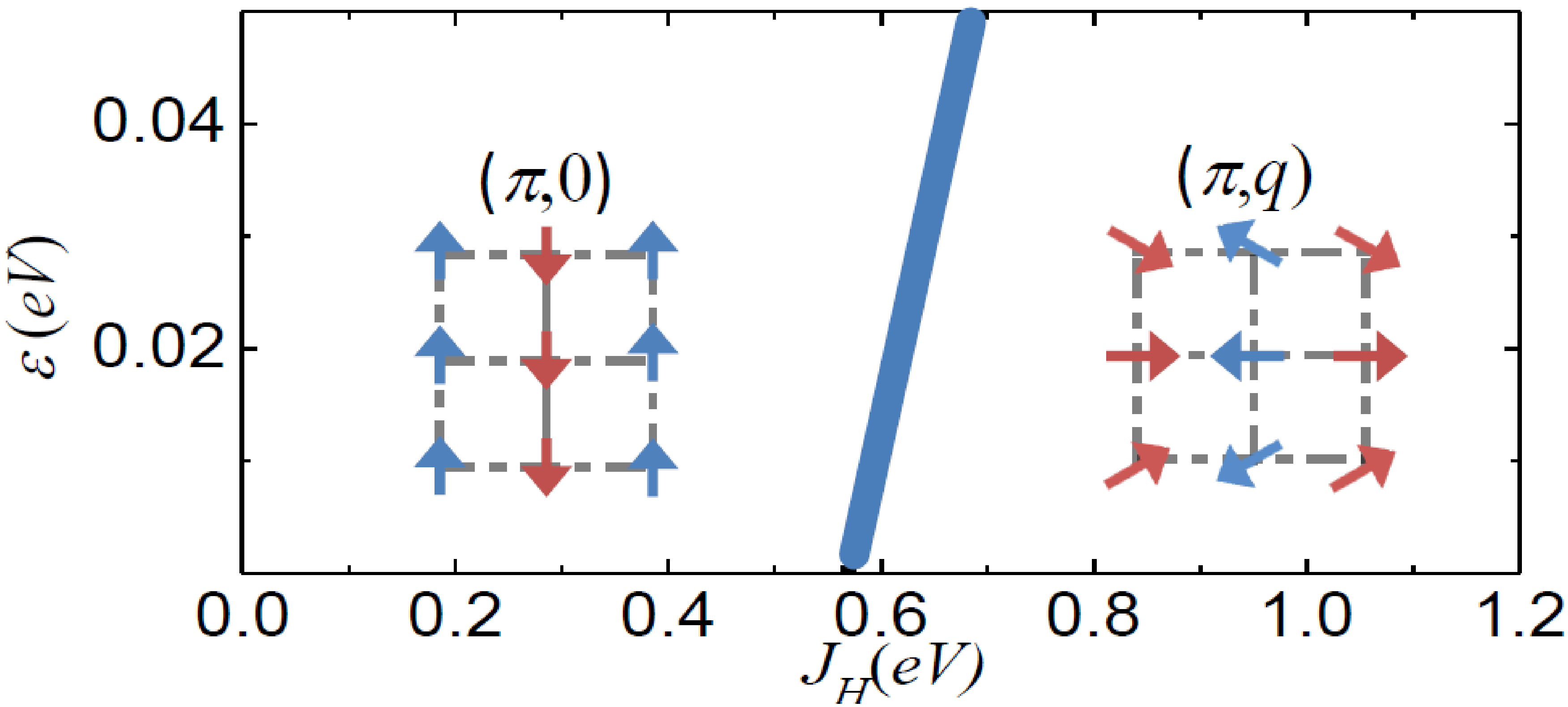
- Ferro-orbital order helps stabilize the stripe phase
- strengthen dispersion along FM direction, look like DE effect !?
  → fitting to short-range spin model highly unreliable and misleading
- FO order suppresses fluctuation, to ~40% suppression
- Spin fluctuation strongly sensitive to FO

Ferro-orbital correlation & anisotropy



- FO order enhances anisotropy $J_{1x} > J_{1y}$:
  → help stabilize stripe phase
  → suppress slightly fluctuation

Stability of the $(\pi,0)$ C-AFM phase



- For realistic value of J_H, FO order is necessary to stabilize the stripe order.

Summaries

- Why is the ordered moment so much smaller than local moment?
  → Itinerant carriers introduce long-range spin fluctuation
  → temporal and spatial fluctuation
- Does nesting of the itinerant carriers stabilize stripe phase?
  → No, it generates large $J_{1x} > J_{1y} \sim 2J_2$,
  → Not the FM double exchange physics, but AFM nesting effect
- Small long-range couplings integrate to ~50% effects for stripe phase.
- FO order enhances anisotropy, further suppresses fluctuation to ~40% moment suppression.

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- Useful discussion: Fan Yang
- Warm hospitality: Beijing Computational Research Science Center

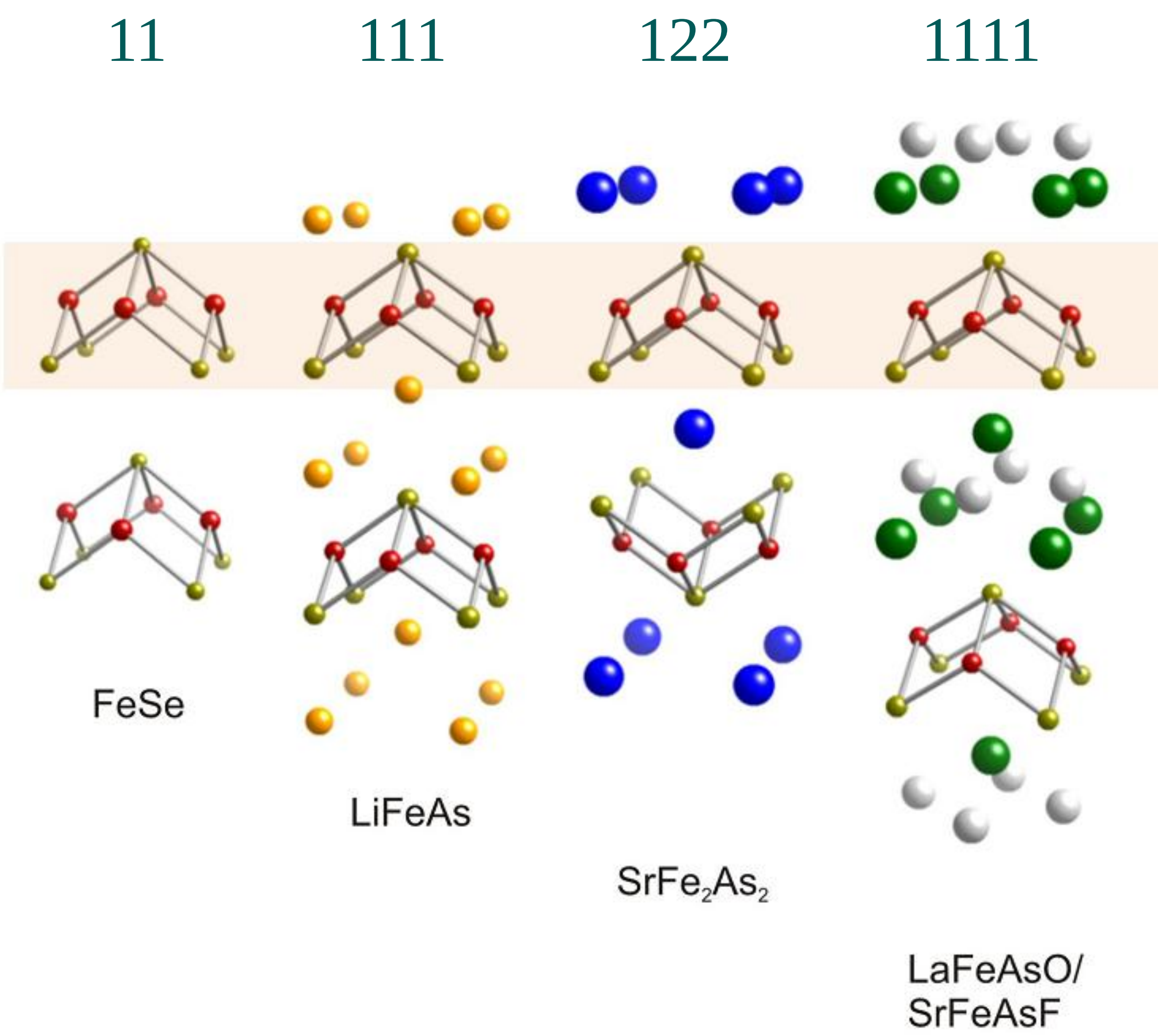
Glide translational symmetry:
One-Fe vs two-Fe picture

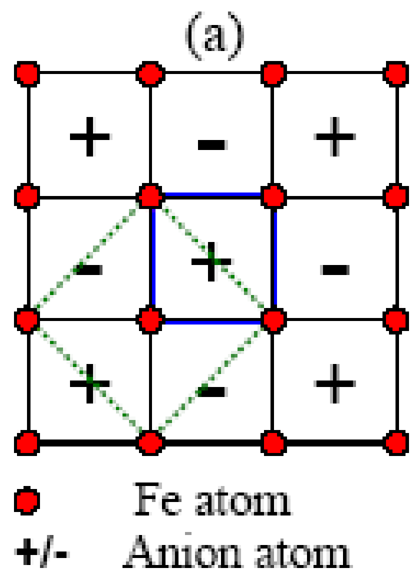
Chia-Hui Lin, Tom Berlijn, Limin Wang, Chi-Cheng Lee,

Wei-Guo Yin, & Wei Ku

Phys. Rev. Lett. **107**, 257001 (2011)

Crystal structure & lack of 1Fe-translational symmetry



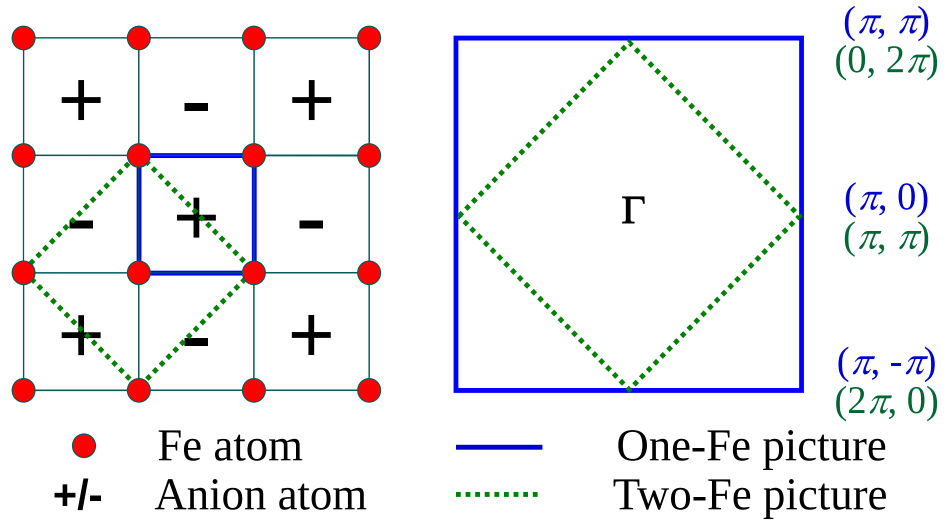


J. Paglione and R. L. Greene, Nature Phys. 2010

One-Fe vs. two-Fe description

Periodicity of the system

- Structure → 2-Fe

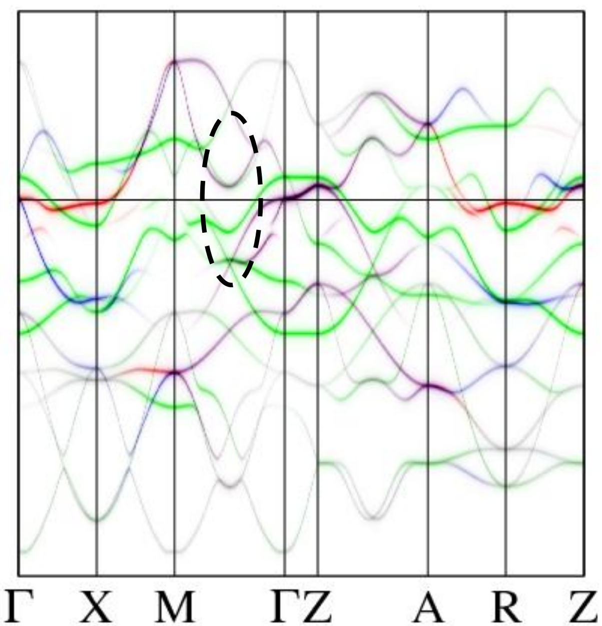


- Neutron → 1-Fe
  - J. T. Park *et al.*, Phys. Rev. B **82**, 134503 (2010).
  - Z. Xu *et al.*, Phys. Rev. B **82**, 104525 (2010).
  - H.-F. Li *et al.*, Phys. Rev. B **82**, 140503(R) (2010).
  - M. D. Lumsden *et al.*, Nature Phys. **6**, 182 (2010).
- Theories of superconductivity (1-band – 5-band) → 1-Fe
  - S. Graser et al., New J. Phys. **11**, 025016 (2009).
  - A. V. Chubukov et al., Phys. Rev. B **78**, 134512 (2008).
  - R. Arita and H. Ikeda, J. Phys. Soc. Jpn. **78**, 113707 (2009).

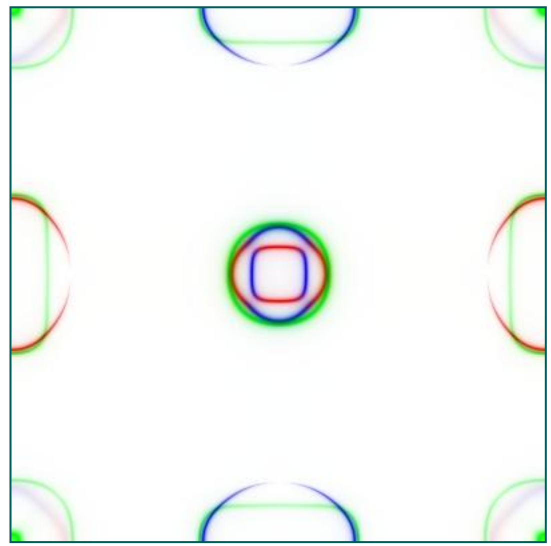
What is the effects of translational symmetry breaking?

S_4 symmetry is not a small perturbation from C_4

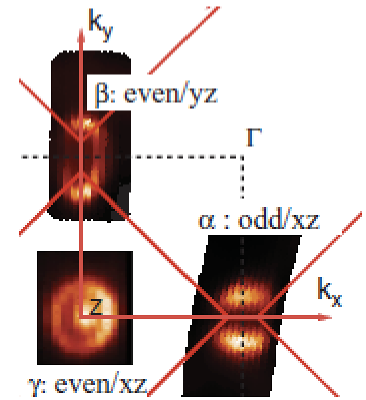
Large gap in *eV*

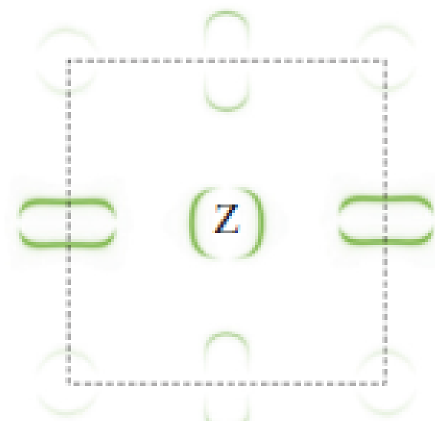


Incomplete pockets



Experimental confirmation





$Ba(Fe_{0.92}Co_{0.08})_2As_2$

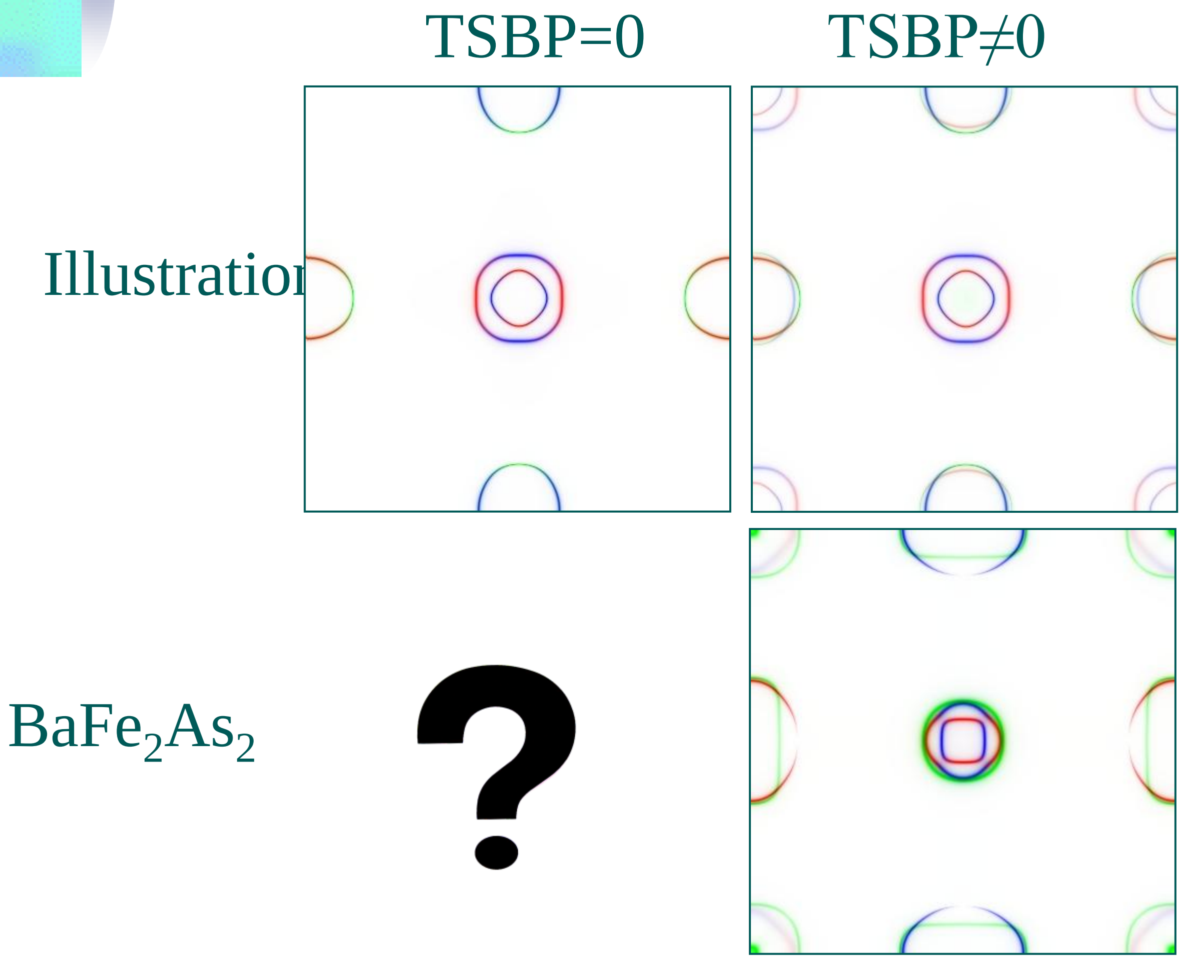
Wei Ku *et al*, *Phys. Rev. Lett.* **104**, 216401 (2010)

Chia-Hui Lin *et al*, *Phys. Rev. Lett.* **107**, 257001 (2011)

V. Brouet *et al*, *Phys Rev B* **6**, 075123 (2012)

L. Moreschini *et al*, *Phys. Rev. Lett.* **112**, 087602 (2014)

Incomplete electron pockets



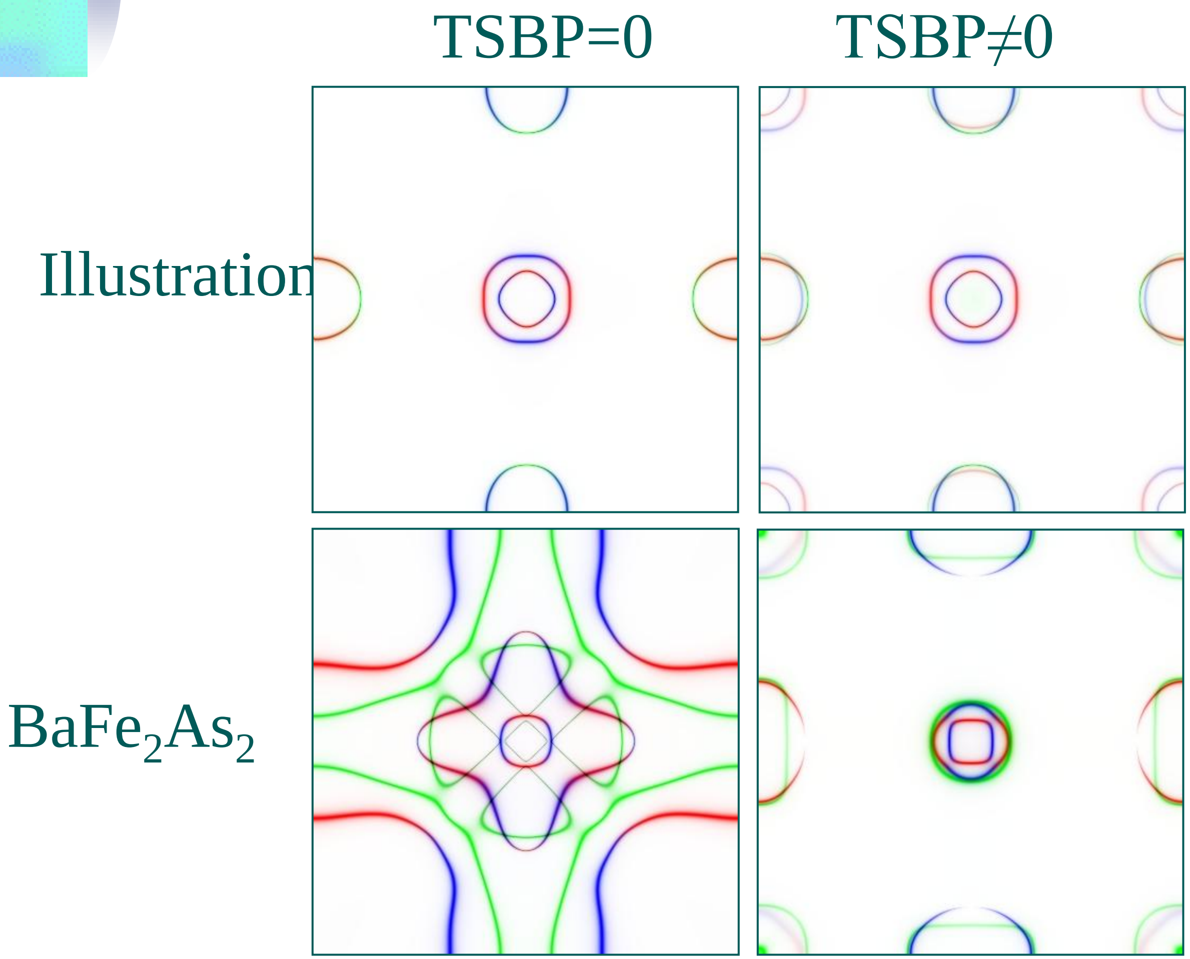
- One can understand this through a complicated matrix elements

  V. Brouet et al, *Phys Rev B* **6**, 075123 (2012)

- Or one can think directly in terms of the unfolded basis

  Chia-Hui Lin *et al*, *Phys. Rev. Lett.* **107**, 257001 (2011)

Creation of electron pockets in Fe-superconductors



- Electron pockets are formed by coupling bands from k and $k+q^{TSBP}$
  - → Electron pockets form via translational symmetry breaking
  - → Intrinsic 2-Fe physics, cannot be properly produced from 1-Fe models

Chia-Hui Lin *et al*, *Phys. Rev. Lett.* **107**, 257001 (2011)

Glide translational symmetry: Novel pairing structure

Chia-Hui Lin, Chung-Pin Chou, Wei-Guo Yin, & Wei Ku

arXiv:1403.3687

Crystal structure & glide translational symmetry

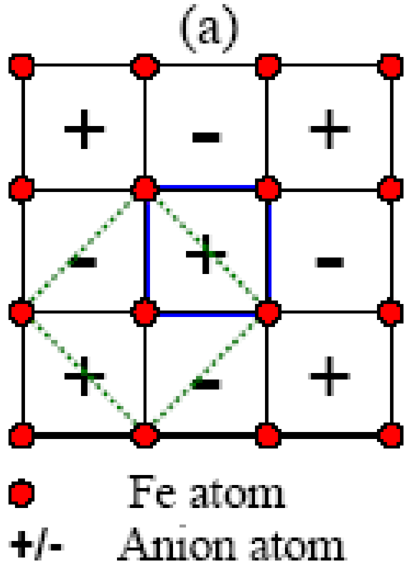
- Lack of 1Fe in-plane translational symmetry $T_{\|}$

$$\left[T_{\perp}, H\right] = 0 \quad \text{but} \quad \left[T_{\|}, H\right] \neq 0$$

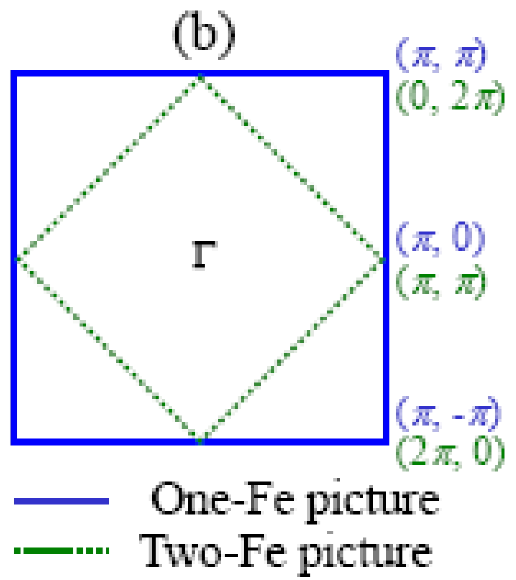
- Glide translational symmetry $P_z T_{\|}$

$$\left[T_{\perp}, H\right] = 0, \quad \left[P_z T_{\|}, H\right] = 0 \quad \text{but} \quad \left[P_z T_{\|}, T_{\perp}\right] \neq 0$$

P. A. Lee & X.-G. Wen, *Phys. Rev. B* **78**, 144517 (2008)



- 3D momentum is not a good quantum number
- QP does not live in physical 3D momentum space
- What ARPES observed is only components of QP
- Two rigorous approaches:
  - Choose $T_{\perp}$ → double the unit cell in the plane
  - Choose $T_{\|} = U^{\dagger} P_z T_{\|} U$ → mix k_z with $-k_z$
  - Always have to deal with 10 *d*-bands ☹



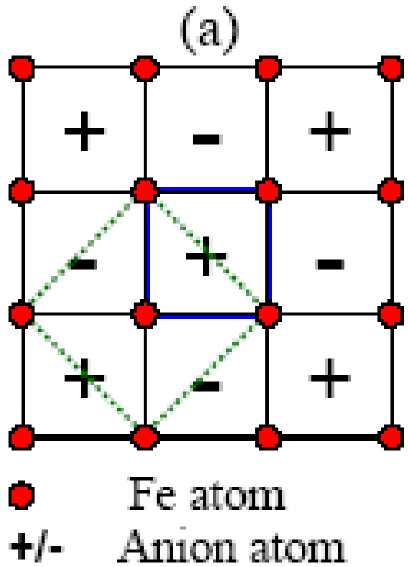
A good approximate representation

- Local gauge transform for the even orbitals in odd lattice sites

$$\hat{c}_{i,e} = -\hat{a}_{i,e}$$

$$\hat{c}_e\left(\tilde{k}\right) = \hat{a}_{i,e}\left(k+Q\right)$$

$$Q = \left(\pi,\pi,0\right) \text{ (orth)} \quad \text{or} \quad \left(\pi,\pi,\pi\right) \text{ (bct)}$$



- Transformed $H = H_{\parallel} + H_{\perp}$

  $H_{\parallel}$ respects translational symmetry

  $H_{\perp}$ still breaks translational symmetry, but perhaps only weakly

  ~ 5-band picture ☺

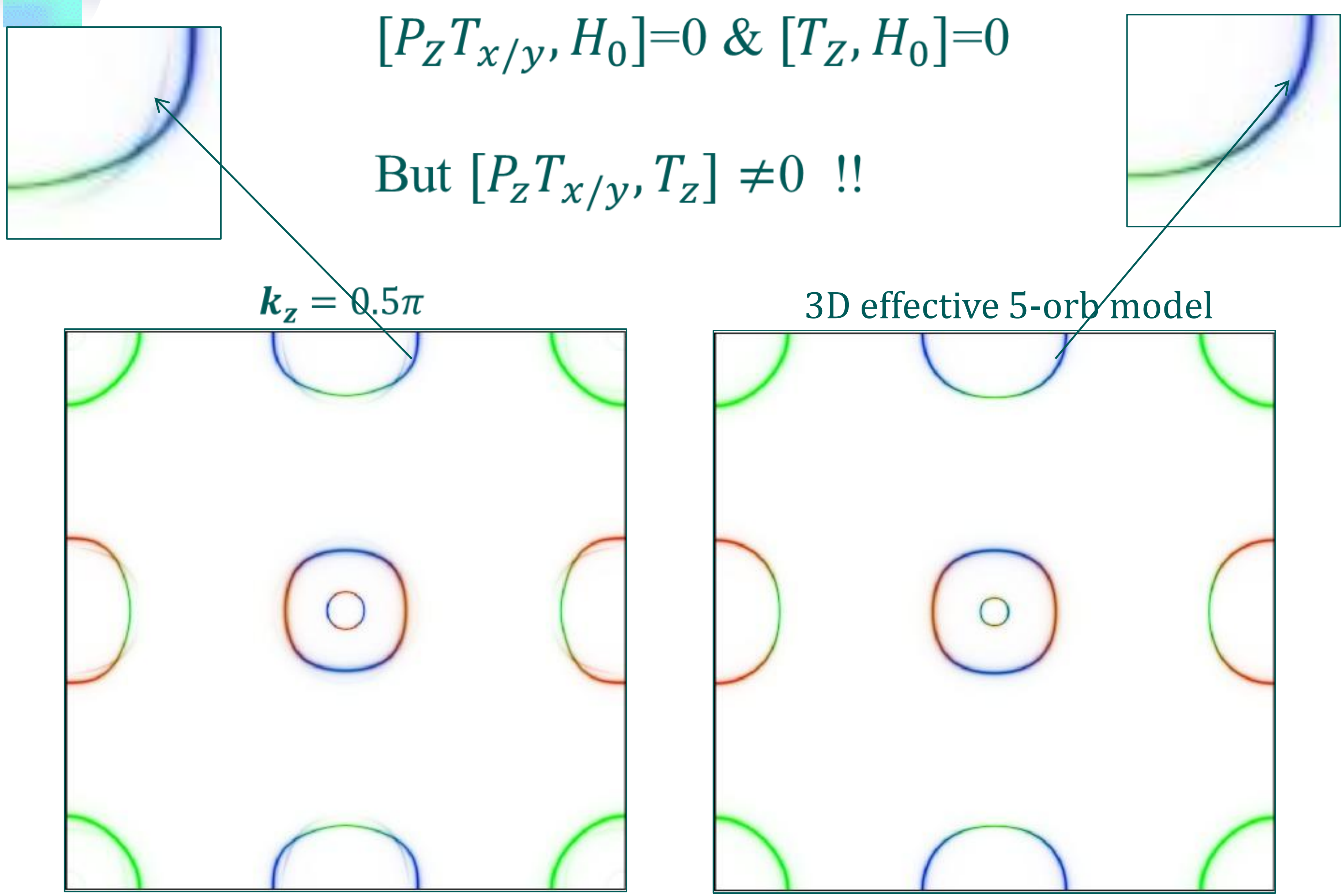
- $\tilde{k}$ is the pseudo-crystal momentum
  - almost a good quantum
  - defines QP in gauged space

Wen & Lee ,*Phys. Rev. B* (2008)

Remaining symmetry breaker can be weak

$$[P_Z T_{x/y}, H_0]=0 \ \& \ [T_Z, H_0]=0$$

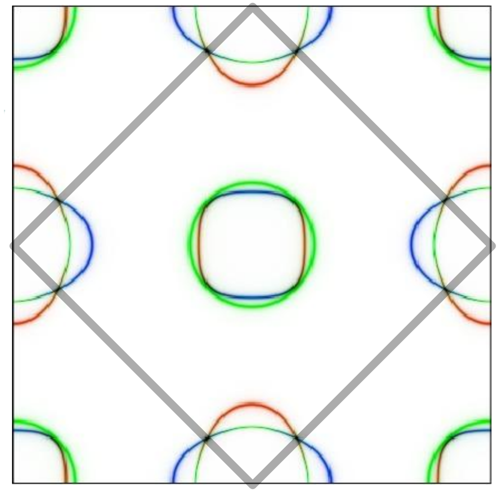
But $[P_z T_{x/y}, T_z] \neq 0$!!



Splitting QP cleanly in physical momentum space

$$A_o(k,w) = A_o(k,w)$$

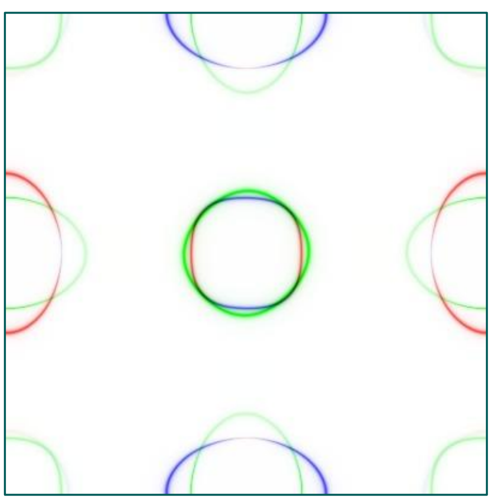
$$A_e(k+Q,w) = A_e(k,w)$$



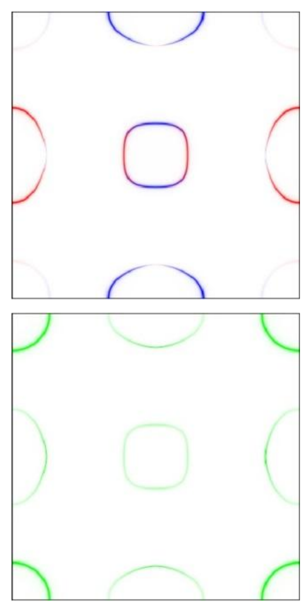
$\hat{a}_{xz}(k)$
$\hat{a}_{xy}(k)$

$\hat{c}_{xz}(k)$
$\hat{c}_{xy}(k+Q)$

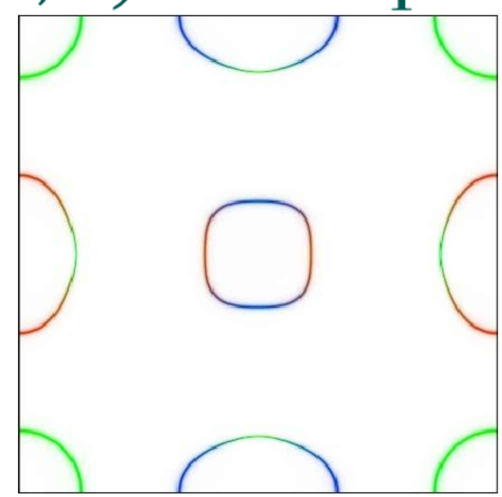
A($\boldsymbol{k}$, $\boldsymbol{\omega}$)



k=physical momentum



A($\tilde{\boldsymbol{k}}$, $\boldsymbol{\omega}$) in math space



$\tilde{\boldsymbol{k}}$ =pseudo-crystal momentum

Rich gap structure in physical momentum

- A regular Cooper pair $\left\langle c_{-k,n,\uparrow} c_{k,m,\downarrow} \right\rangle$ transformed into three coexisting contributions of similar strength:

$$\left\langle a_{-k,o,\uparrow} a_{k,o,\downarrow} \right\rangle$$

$$\left\langle a_{-k+Q,e,\uparrow} a_{k+Q,e,\downarrow} \right\rangle$$

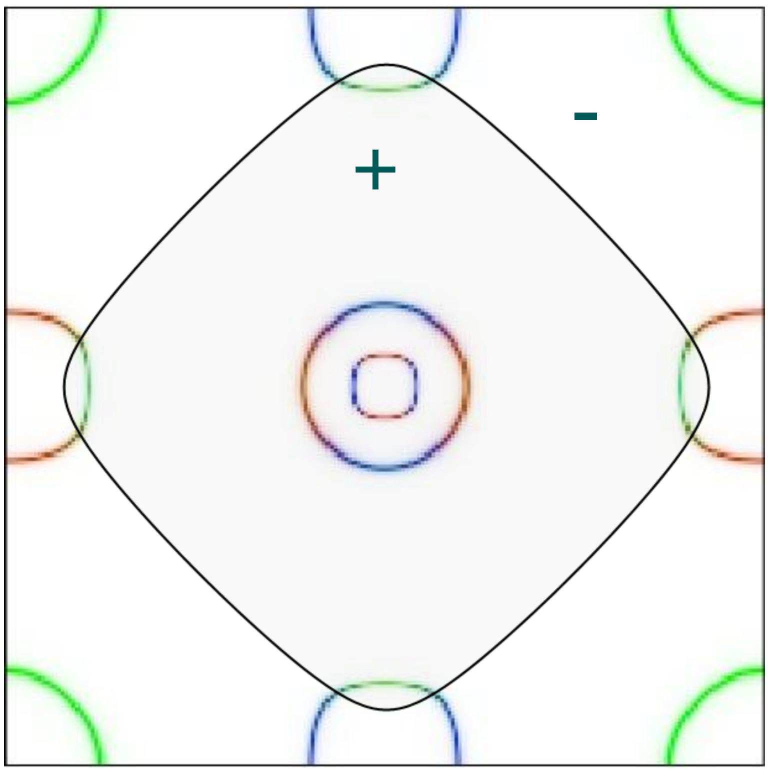
} pair with orbitals of same parity
→ relative shift by Q !

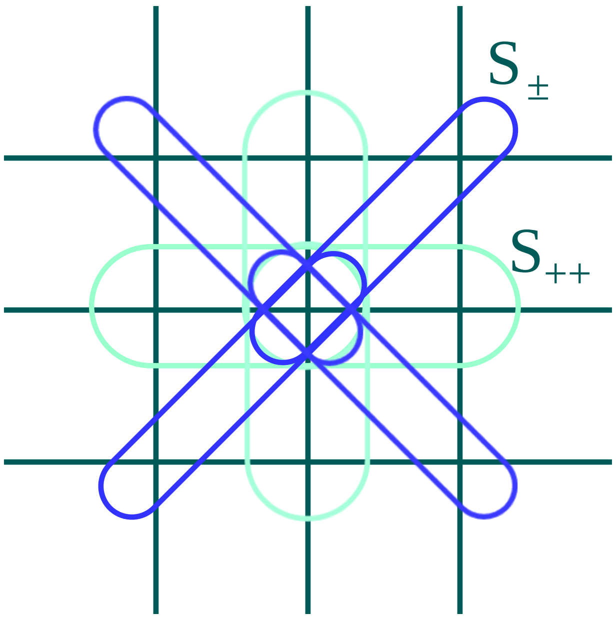
$$\left\langle a_{-k,o,\uparrow} a_{k+Q,e,\downarrow} \right\rangle$$

→ pair with orbitals of opposite parity
→ η-pairing of momentum Q
→ spin singlet with odd form factor
→ break time reversal symmetry

Single Gap Structure in Math Space

$$\tilde{\Delta}(\tilde{k}) = 4\tilde{\Delta}_{s_+}(\cos\tilde{k}_x \cos\tilde{k}_y) + 2\,\tilde{\Delta}_{s_{++}}(\cos\tilde{k}_x + \cos\tilde{k}_y) + \tilde{\Delta}_s$$



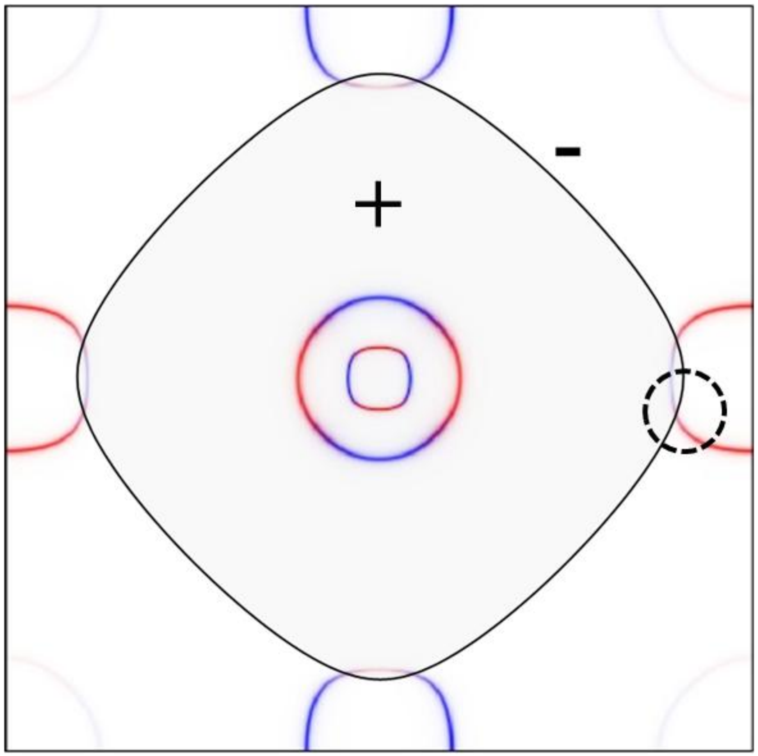


d_{xz} d_{yz} d_{z^2}, $d_{x^2-y^2}$ and d_{xy}

Observing gap nodes in different k points

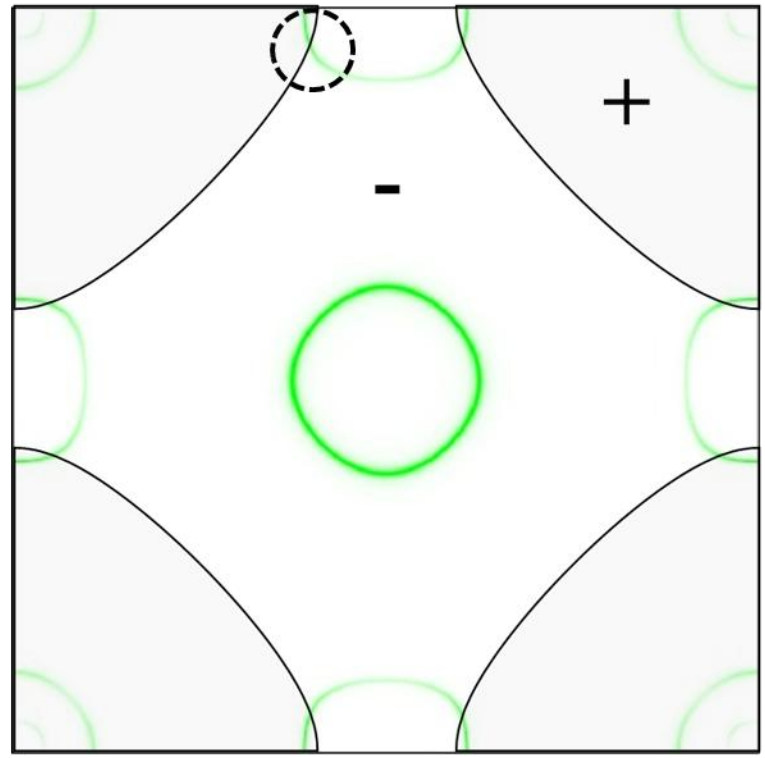
$$\tilde{\Delta}_{s_{++}} = 10\tilde{\Delta}_{s_{\pm}} \qquad \tilde{\Delta}_{s} = 0$$

Odd pairt



$$\Delta(odd, k) \sim 4\tilde{\Delta}_{s_{\pm}}(\cos k_x \cos k_y) + 2\tilde{\Delta}_{s_{++}}(\cos k_x + \cos k_y)$$

Even pairty



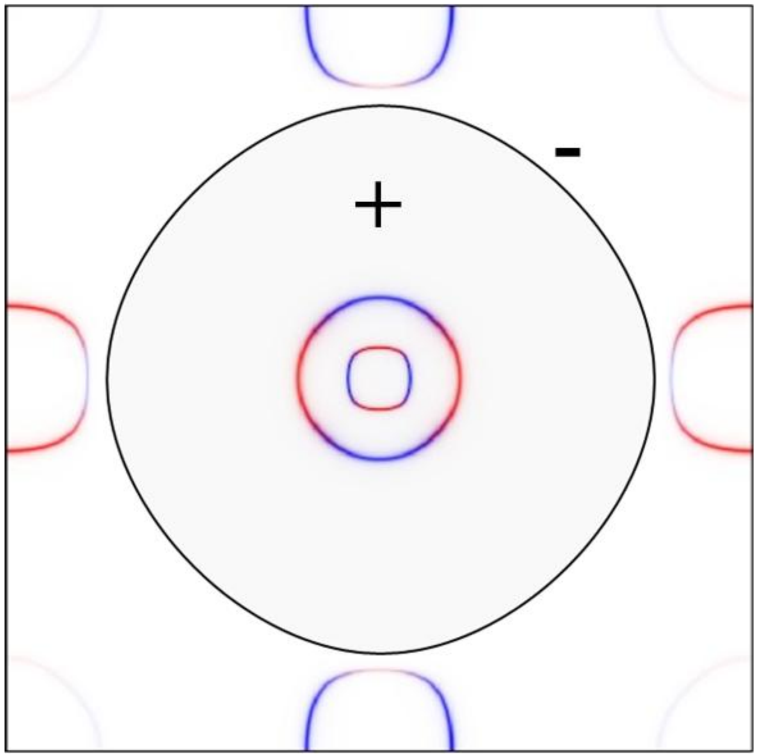
$$\Delta(even, k) \sim 4\tilde{\Delta}_{s_{\pm}}(\cos k_x \cos k_y) - 2\tilde{\Delta}_{s_{++}}(\cos k_x + \cos k_y)$$

d_{xz} d_{yz} d_{z2}, $d_{x2\text{-}y2}$ and d_{xy}

Orbital-parity distinct nodal structure

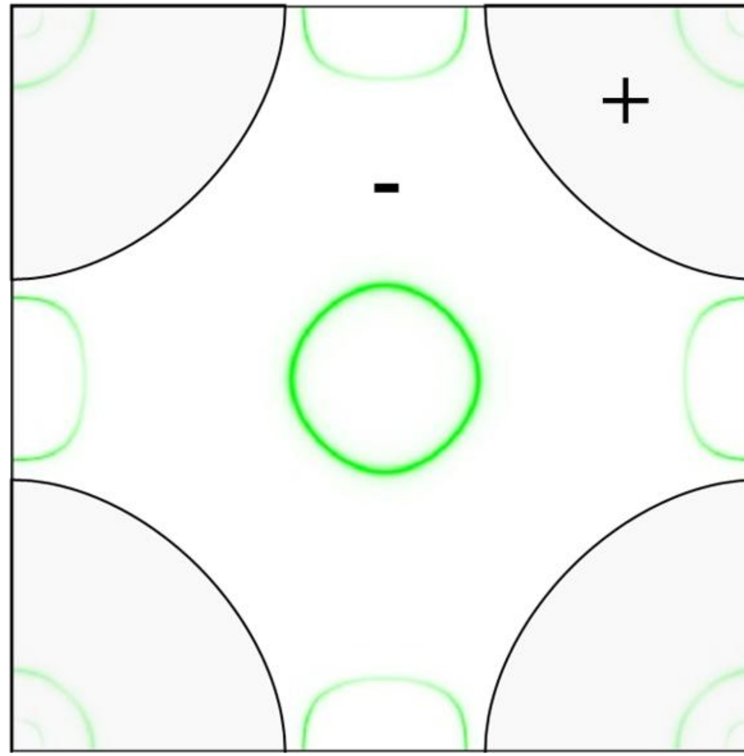
$\widetilde{\Delta}_{s_{++}} = 4\widetilde{\Delta}_{s_{\pm}} \qquad \widetilde{\Delta}_{s} = 0$

Odd pairt



$$\Delta(odd, k) \sim 4\widetilde{\Delta}_{s_{\pm}}(\cos k_x \cos k_y) + 2\widetilde{\Delta}_{s_{++}}(\cos k_x + \cos k_y)$$

Even pairty

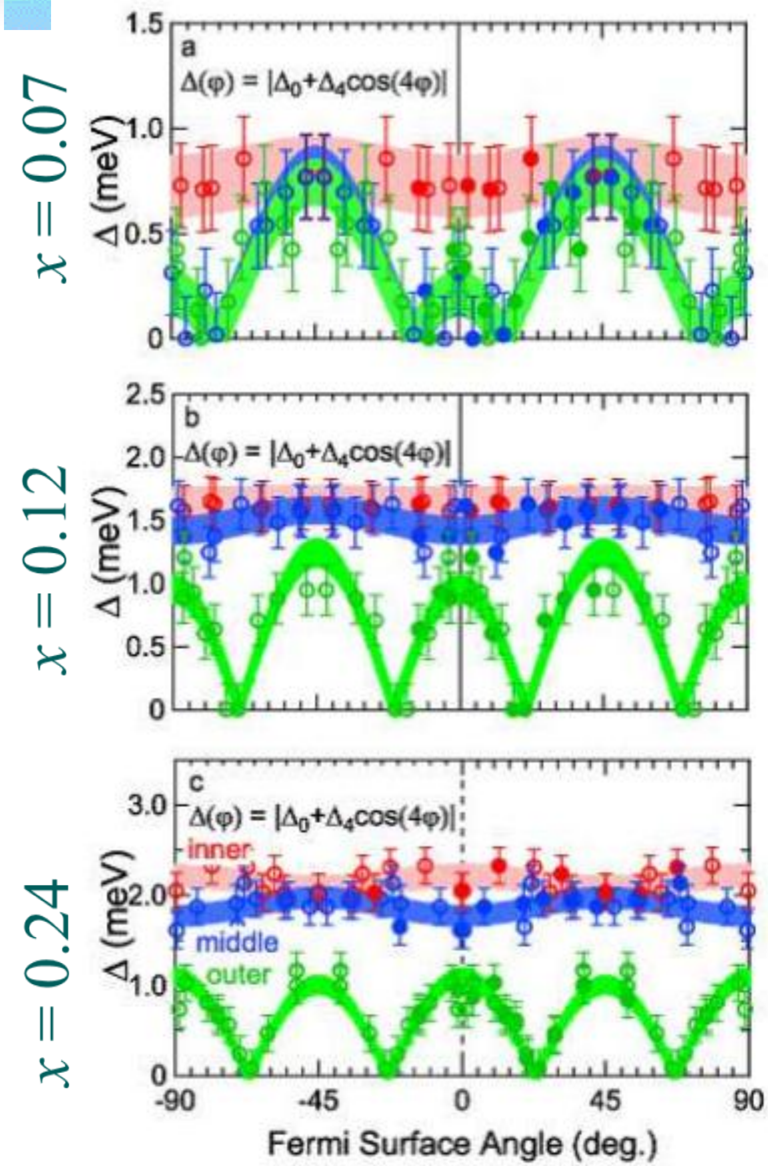


$$\Delta(even, k) \sim 4\widetilde{\Delta}_{s_{\pm}}(\cos k_x \cos k_y) - 2\,\widetilde{\Delta}_{s_{++}}(\cos k_x + \cos k_y)$$

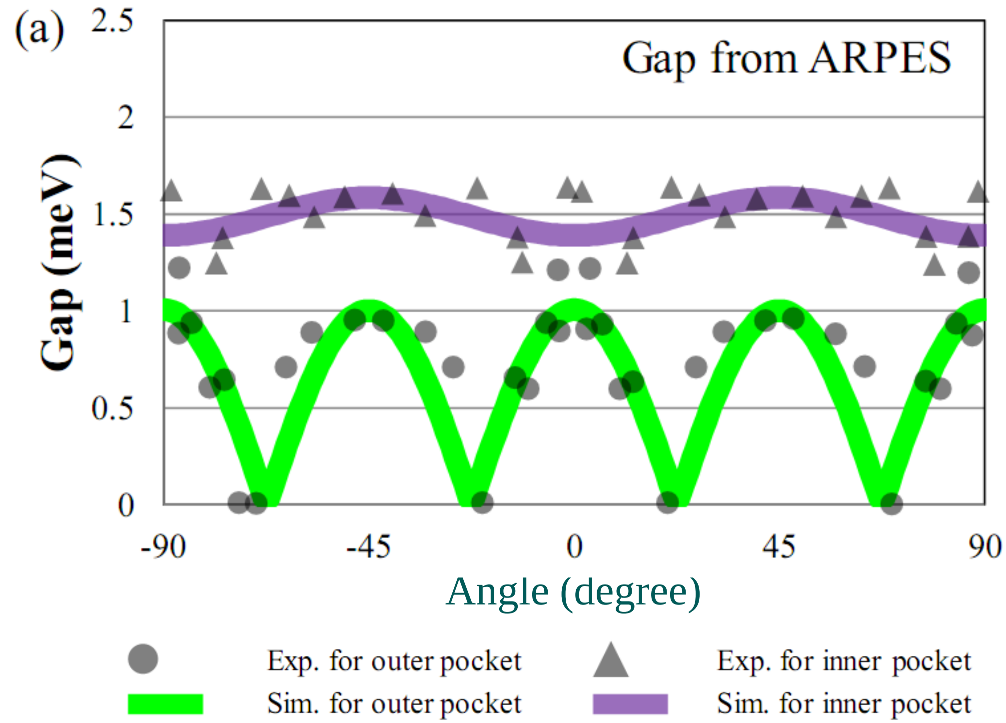
d_{xz} (blue) d_{yz} (red) d_{z^2}, $d_{x^2-y^2}$ and d_{xy} (green)

Distinct gap structure hole pockets from ARPES

$(Ba_xK_{1-x})Fe_2As_2$



Ota *et. al.*, arXiv 1307.7922

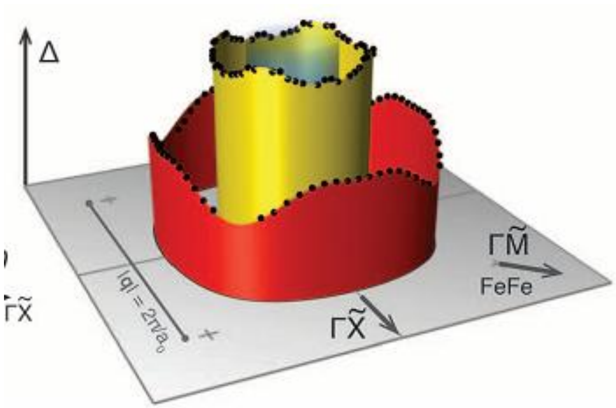


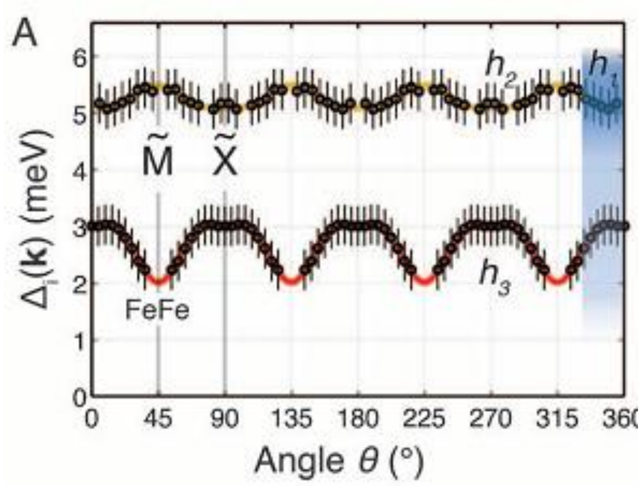
$(\widetilde{\Delta}_{s_\pm}, \widetilde{\Delta}_{s_{++}}, \widetilde{\Delta}_{s})_{inner} = (.25, 2.3, -3.0)$ meV

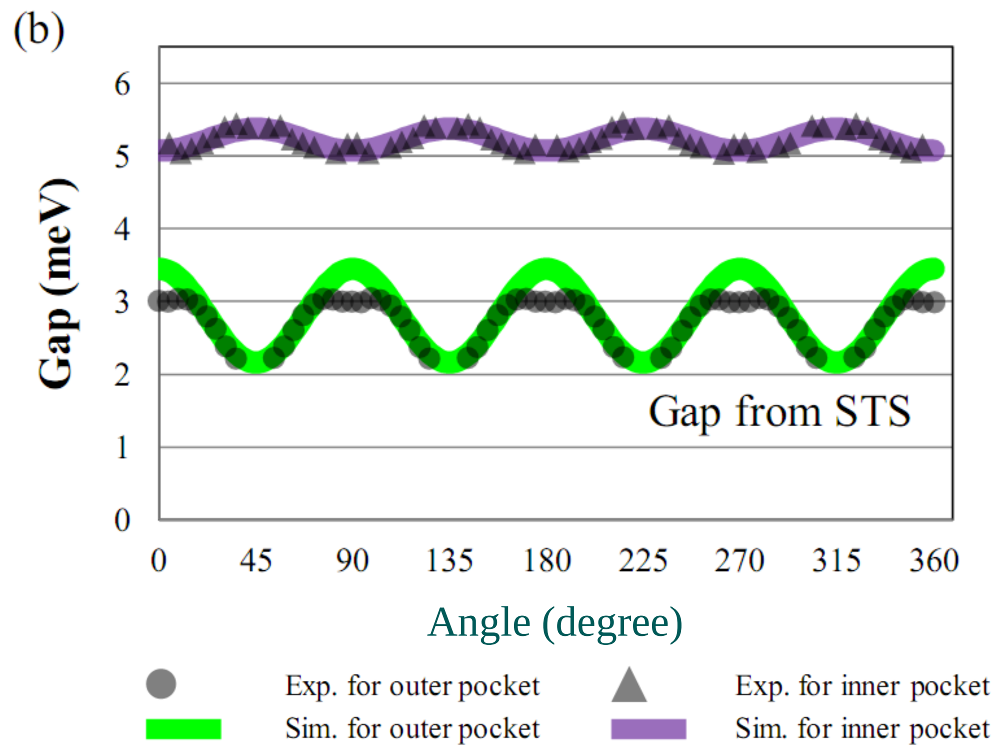
$(\widetilde{\Delta}_{s_\pm}, \widetilde{\Delta}_{s_{++}}, \widetilde{\Delta}_{s})_{outer} = (1.3, -4.2, 7.0)$ meV

Anti-phase gap structure on hole pockets from STS

LiFeAs





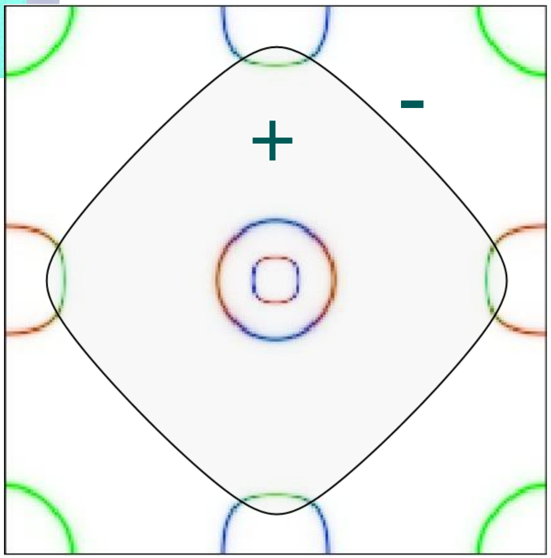


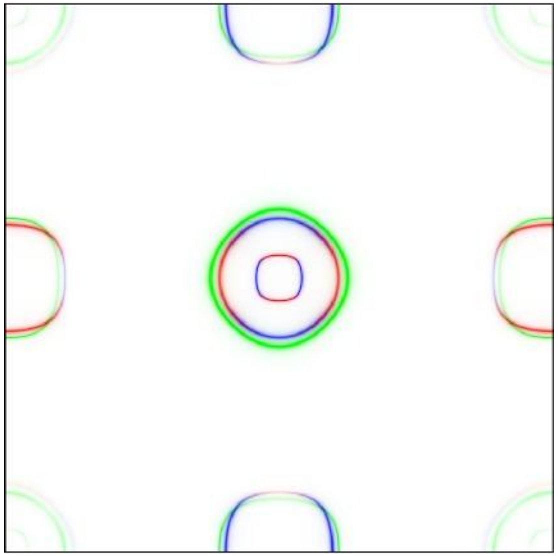
$(\widetilde{\Delta}_{s_{\pm}}, \widetilde{\Delta}_{s_{++}}, \widetilde{\Delta}_{s})_{inner} = (0.0, 3.0, -3.3)$ meV

$(\widetilde{\Delta}_{s_{\pm}}, \widetilde{\Delta}_{s_{++}}, \widetilde{\Delta}_{s})_{outer} = (0.0, -2.0, 3.8)$ meV

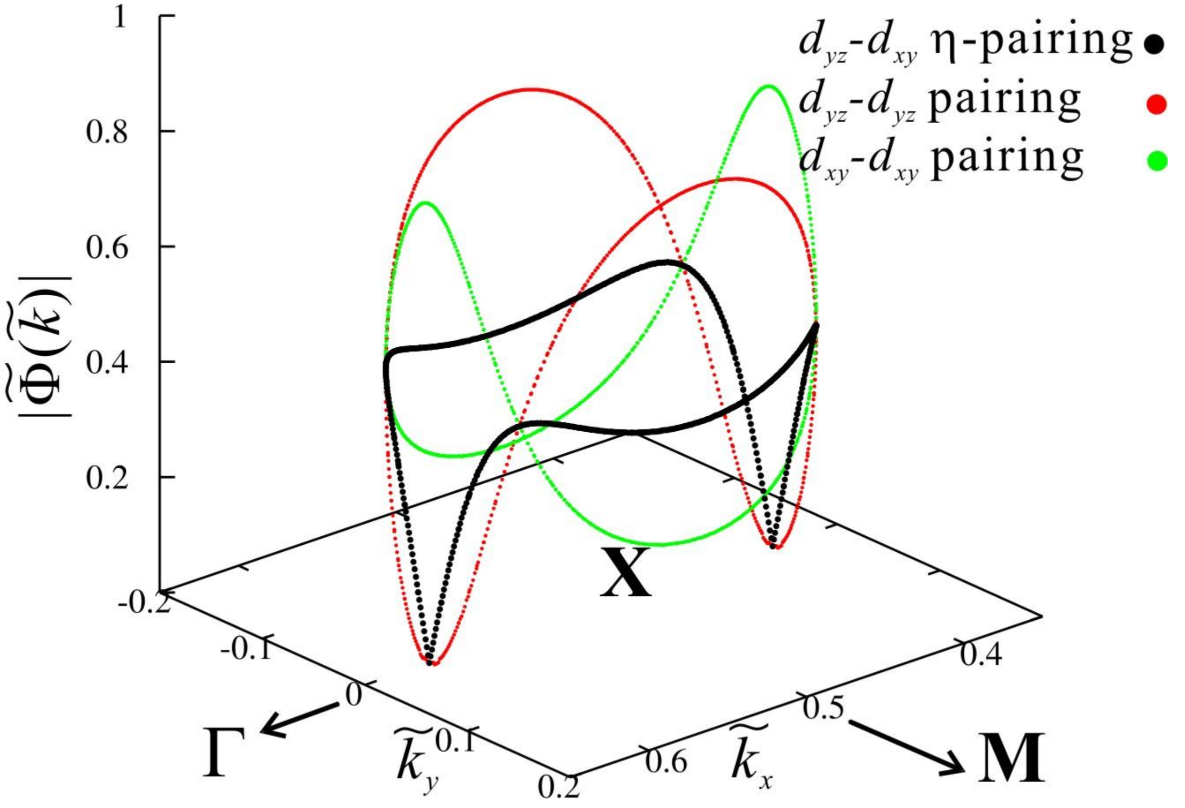
Allen *et. al.*, Science 336, 563 (2012)

Coexisting finite-momentum pairing





$$\langle a_{-k,xy} a_{k+Q,yz} \rangle = \langle c_{-\tilde{k},xy} c_{\tilde{k},yz} \rangle$$
$$= \tilde{\Delta}(\tilde{k}) \phi_{xy}(-\tilde{k}) \phi_{yz}(\tilde{k})$$



C. N. Yang, PRL 63, 2144 (1989).
Scalettar, Singh, and Zhang, PRL 67, 370 (1991)
Hu and Hao, Phys. Rev. X 2, 021009 (2012).

Summary

- Lack of 1Fe translational symmetry (not a small perturbation!)
- Glide translational symmetry
- Approximate treatment via local gauge transform & pseudo-momentum
- Clean splitting of QP in momentum by a (π,π) shift
- Cooper pairs transform into three components in physical momentum
- Orbital parity distinct pairing structure with Q-shift
  - Distinct gap anisotropy seen in ARPES
  - Anti-phase gap anisotropy seen in STS
- Coexisting η-pairing of finite momentum Q

  → spin singlet with odd form factor

  → break time reversal symmetry

Treating materials with disordered impurities

T. Berlijn, D. Volja, and Wei Ku, PRL **106**, 077005 (2011)

For various applications, see

T.S. Herng, *et al*., *Phys. Rev. Lett.* **105**, 207201 (2010)

Tom Berlijn, *et al*., *Phys. Rev. Lett.* **108**, 207003 (2012)

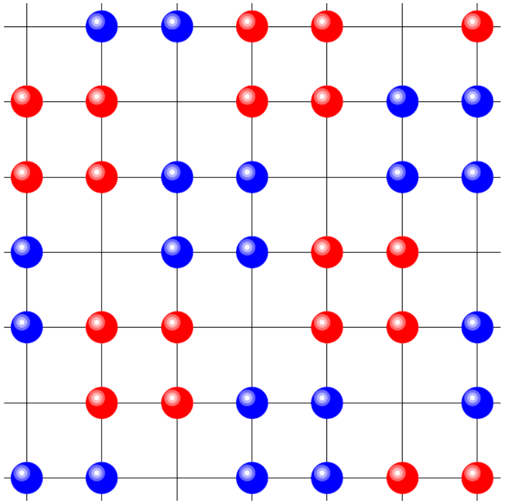
Tom Berlijn, *et al*., *Phys. Rev. Lett.* **109**, 147003 (2012)

L.-M. Wang, *et al*., *Phys. Rev. Lett.* **110**, 037001 (2013)

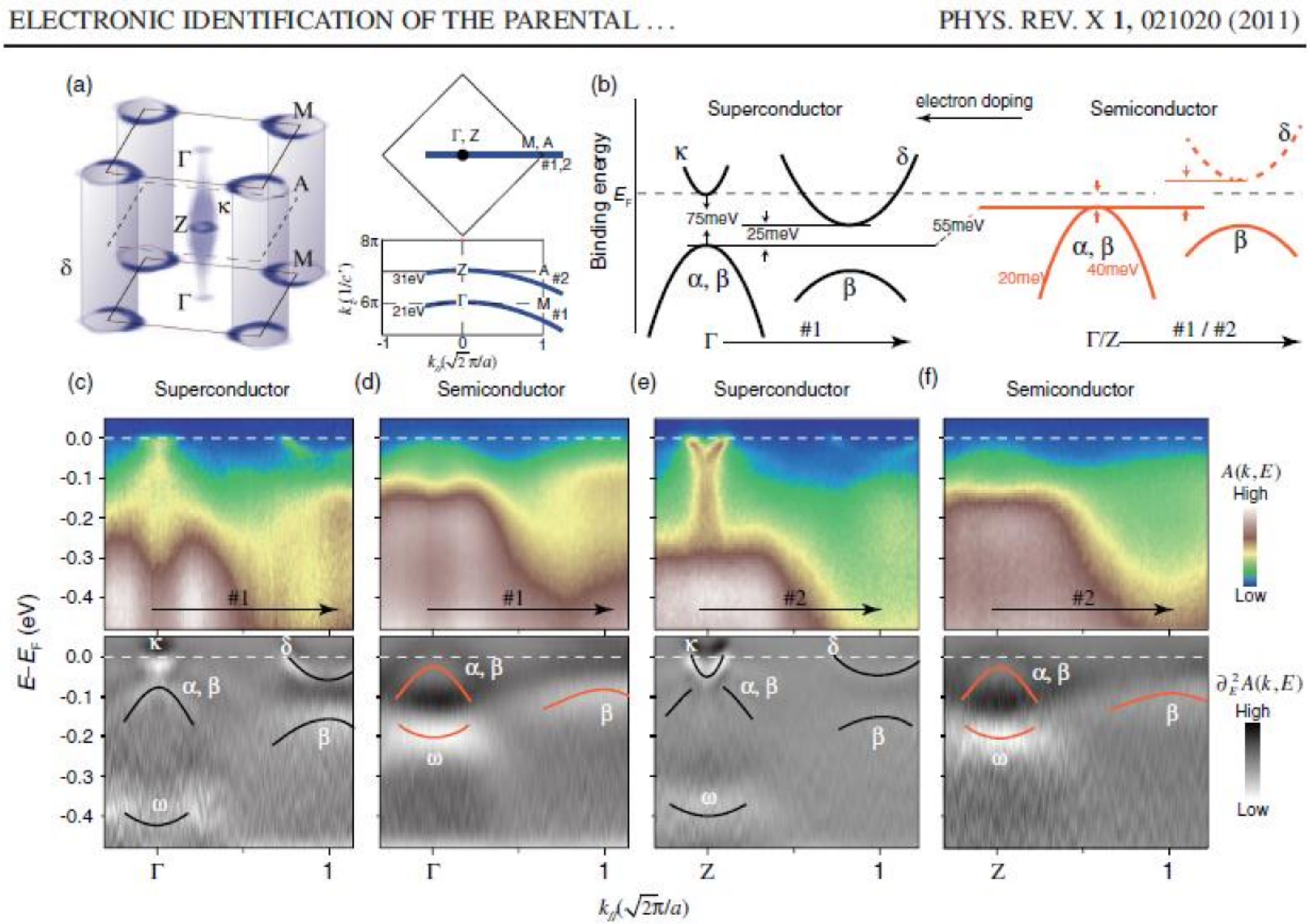
Fe vacancy in $K_2Fe_4Se_5$

T. Berlijn, P. Hirschfeld, & Wei Ku

PRL **109**, 147003 (2012)

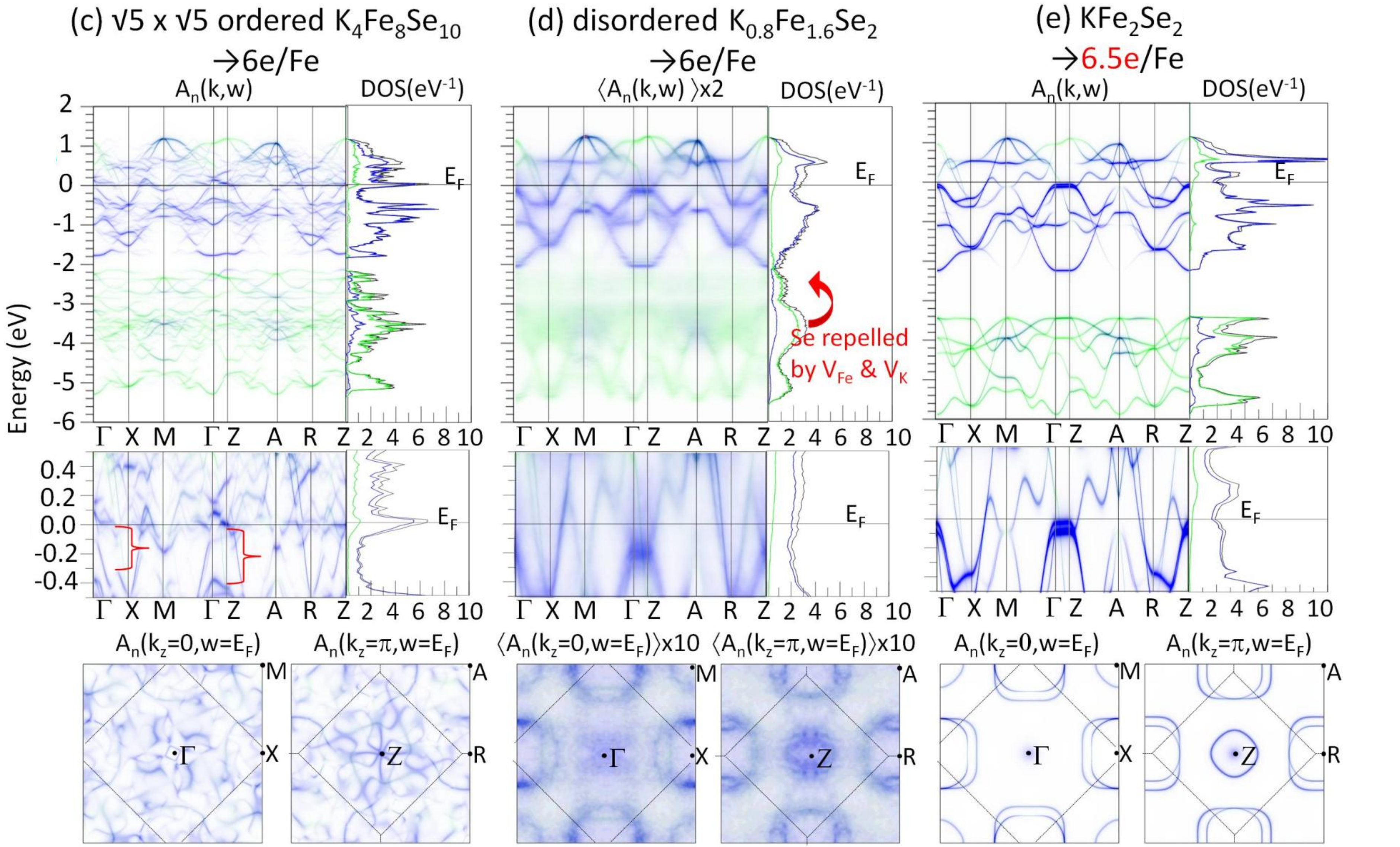


A heavily electron doped system?



F. Chen et al. Phys. Rev. X **1**, 021020 (2011)

Effective "doping" with Fe vacancy: Luttinger theorem?



Appears to be heavily doped ~ 0.5 e / Fe with disordered Fe vacancy

Tom Berlijn, Peter Hirschfeld, and Wei Ku, **109**, 147003 (2012)

Summary of the talk

- Spin/orbital correlation
  - Ferro-orbital & AFM
  - Effect of itinerant electrons on spin dynamics & fluctuation
- Glide translational symmetry:
  - 1-Fe vs 2-Fe description
  - novel pairing structure
- Effects of disordered impurities:
  - Substitution of Fe: doping or not?
  - Fe vacancy: “violation” of Luttinger theorem
  - Ru substitution: realization of superdiffusion