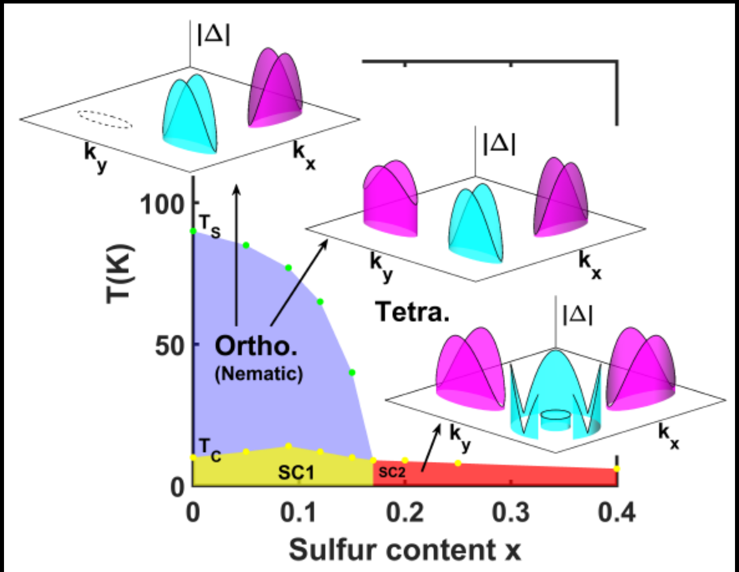
Ultranodal pair states in iron-based superconductors

P. Hirschfeld, U. Florida

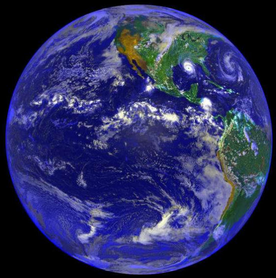


PJH, Comptes Rendus Physique 17, 197 (2016)
C. Setty, S. Bhattacharyya, A. Kreisel and PJH, arXiv 1903.00481

UNF 2019

Collaborators

from U. Florida Dept. of Physics:



from rest of world:

Chandan Setty

Shinibali
Bhattacharyya

Yifu Cao

Andreas Kreisel
U. Leipzig

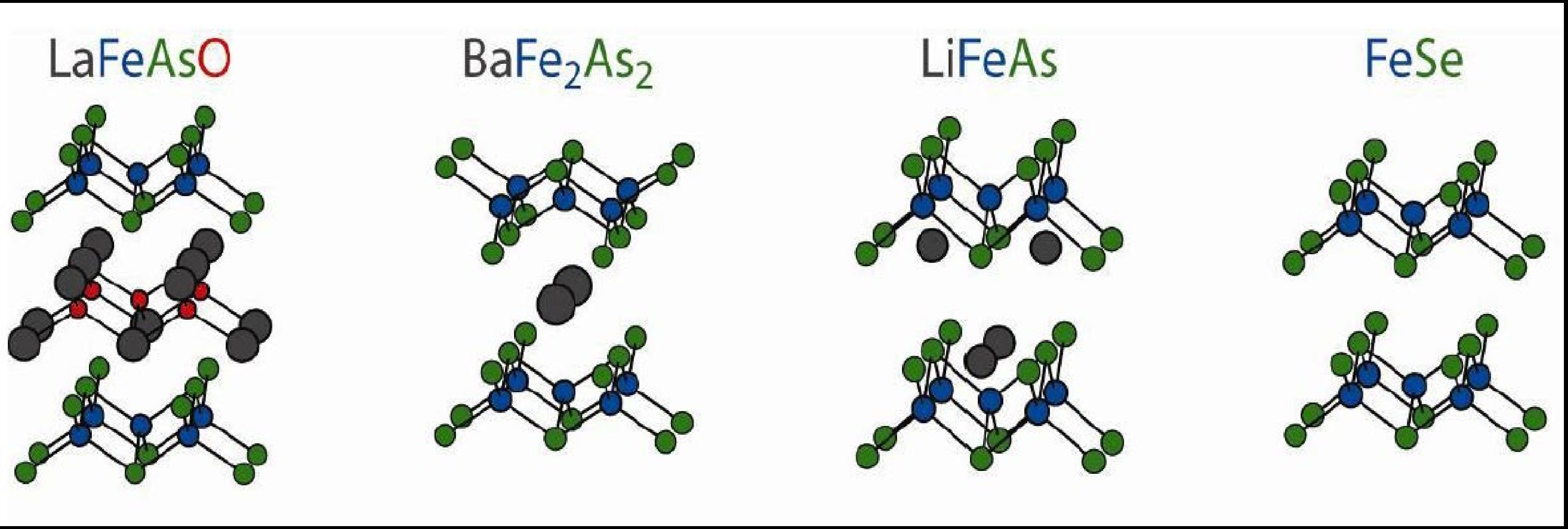
"The theoretical oriented scientist cannot be envied, because nature, i.e. the experiment, is a relentless and not very friendly judge of his work. In the best case scenario it only says "maybe" to a theory, but never "yes" and in most cases "no". If an experiment agrees with theory it means "perhaps" for the latter. If it does not agree it means "no". Almost any theory will experience a "no" at one point in time - most theories very soon after they have been developed."

Albert Einstein,

Theoretical Remark on the Superconductivity of Metals

Iron-based superconductors

Recent reviews: Paglione & Greene Nat Phys 2010; Johnston Adv. Phys. 2010



T_c=28K
(55K for Sm)

- Kamihara et al JACS (2008)
- Ren et al Chin. Phys. Lett. (2008)

T_c=38K

- Rotter et al. arXiv: PRL (2008)
- Ni et al Phys. Rev. B 2008 (single xtals)

T_c=18K

Wang et al
Sol. St. Comm. 2008

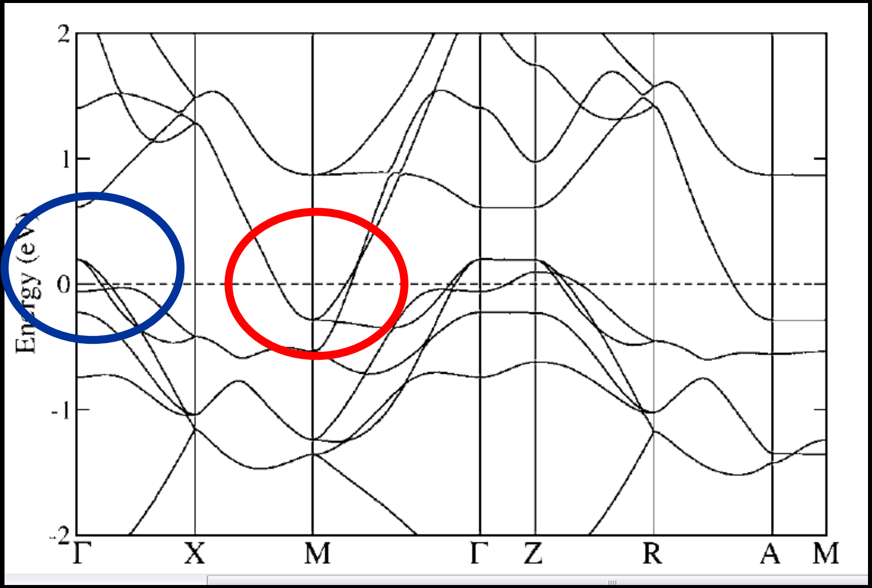
T_c=8K

Hsu et al
PNAS 2008

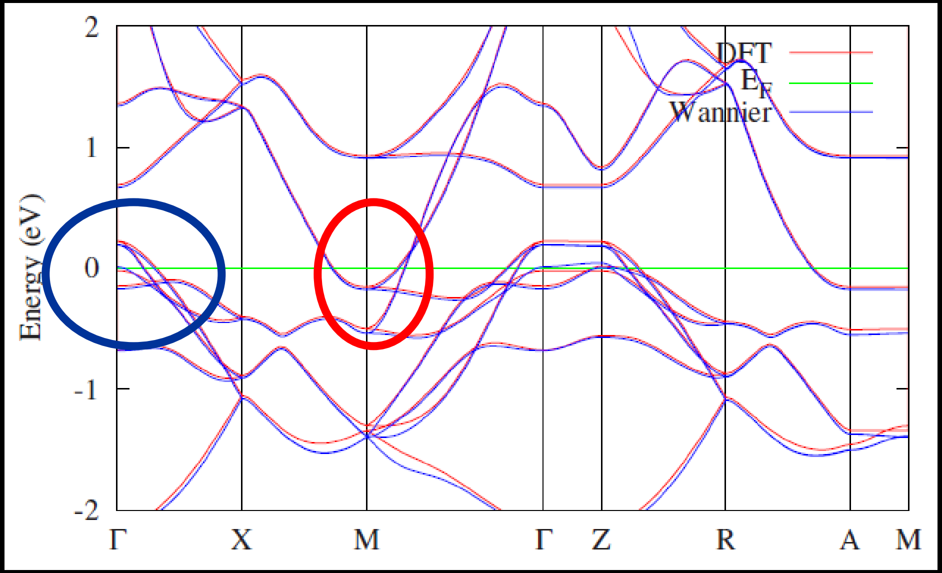
No arsenic ☺!

Electronic structure calculations

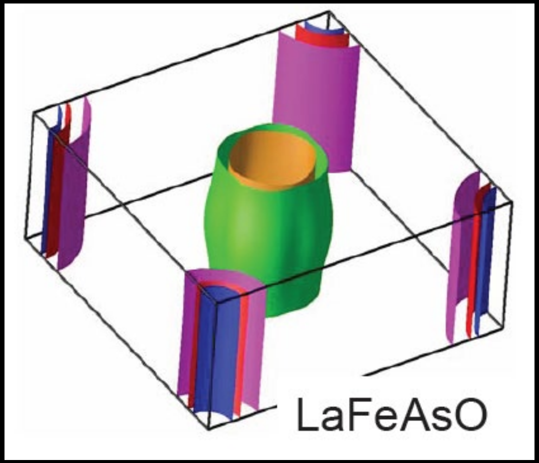
LaFePO Lebegue 2007 (T_c=6K)



LaFAs0 Cao et al2008 (T_c=26K)



Band structures for 2 materials nearly identical!
Hole pocket near Γ, electron pocket near M



2D!

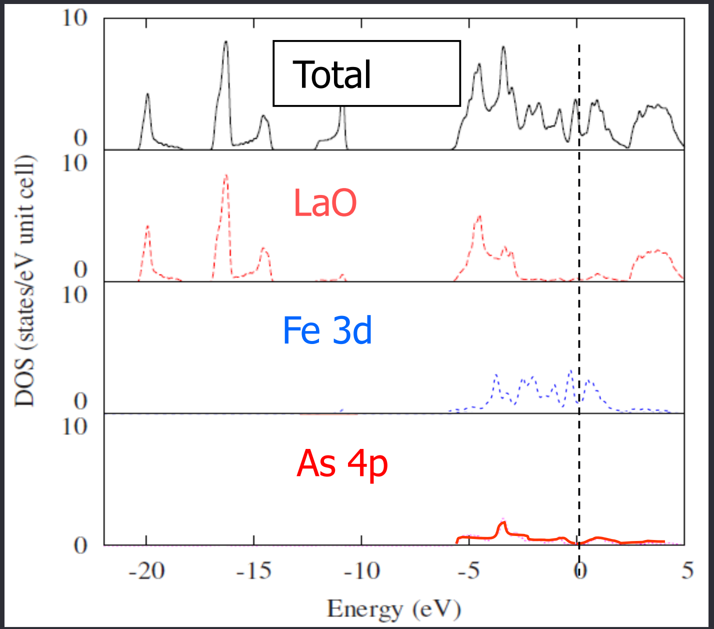
Kotliar et al, Cao et al: correlations can be important

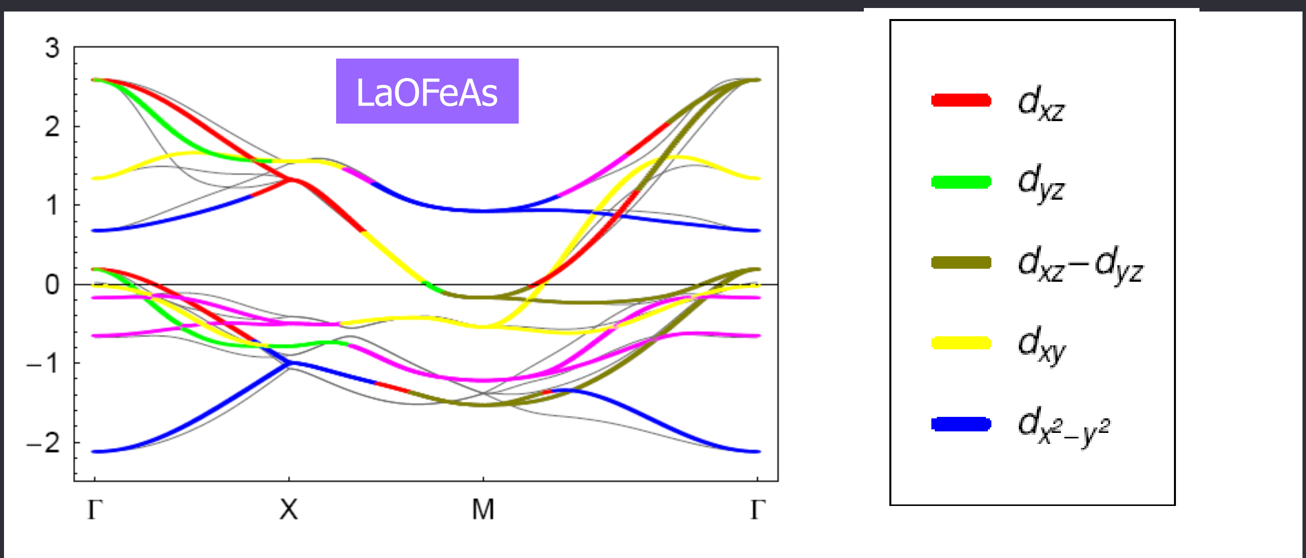
Multiorbital physics

DOS near Fermi due almost entirely to 5 Fe d-states

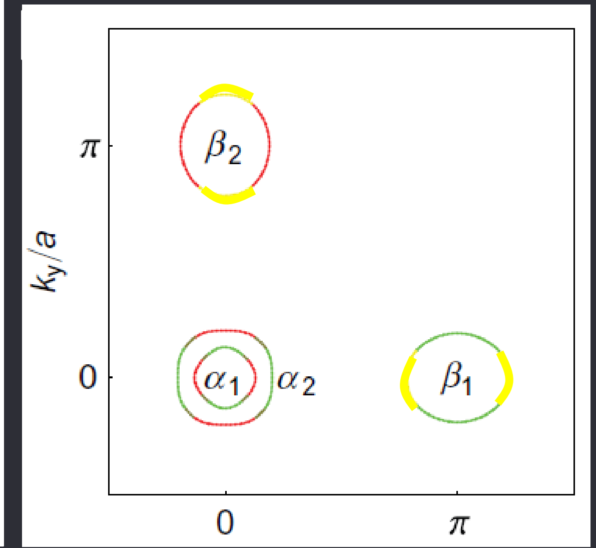
Complications: calculations will be harder

Novelty: surprising new aspects of multiorbital/ multiband physics



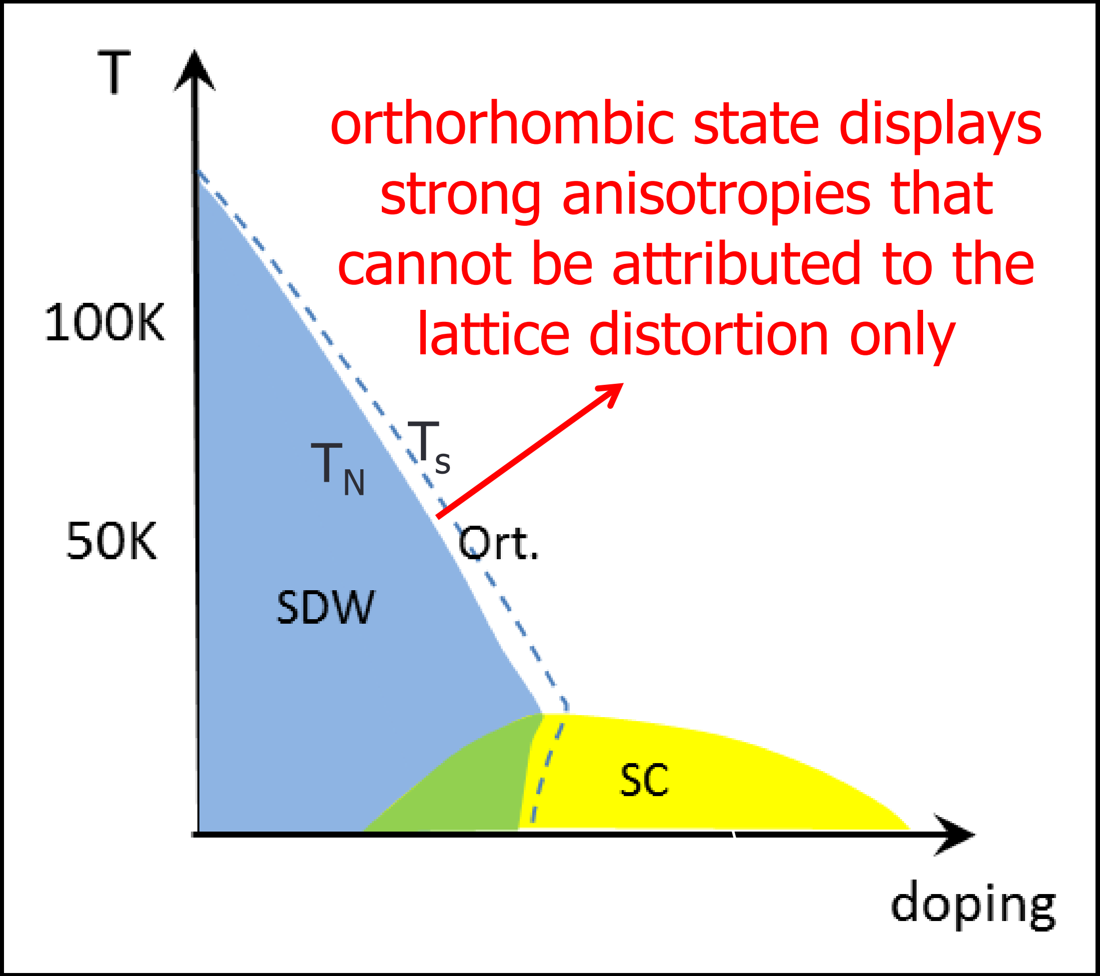


Band structure



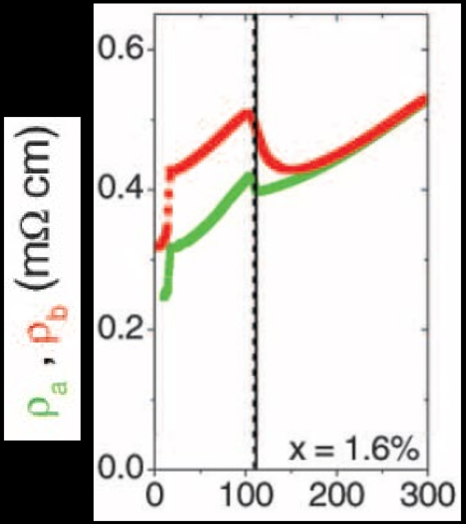
Fermi surface

Nematic behavior



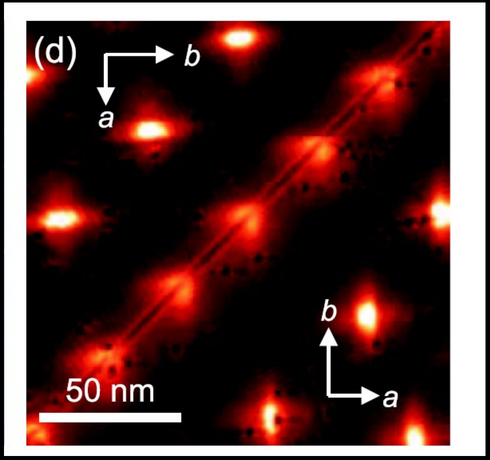
~0.3% change in a,b at T_s in Ba-122

Ba122 resistivity



Chu et al, Science (2010)

Tanatar et al, PRB (2010)

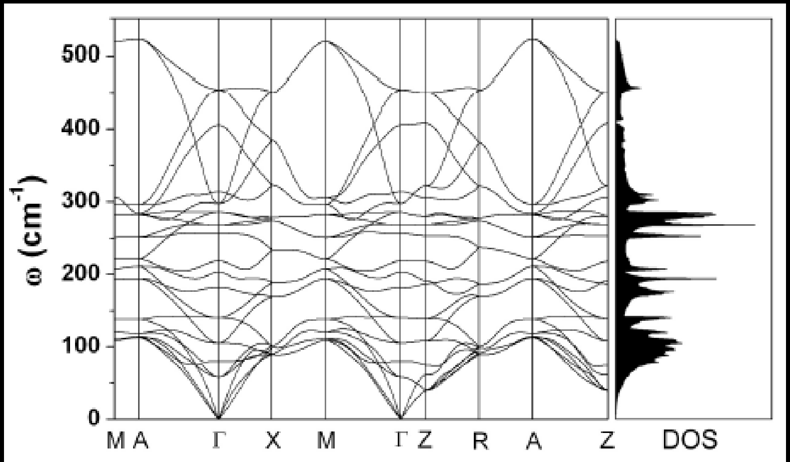


FeSe vortices near twin bdry

Watashige et al, Science (2010)

Superconductivity: e-ph interaction is too weak

Phonon spectrum, density of states



Singh & Du PRL 2008

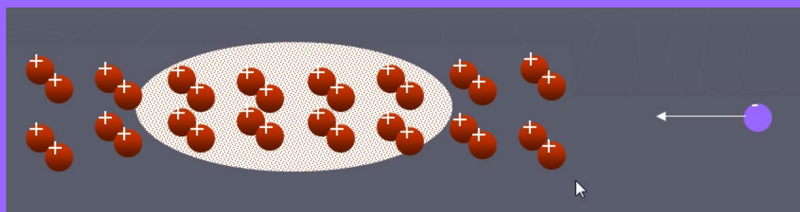
We have calculated *ab initio* the electron-phonon spectral function, $\alpha^2F(\omega)$, and coupling, λ, for the stoichiometric compound [9]. Some moderate coupling exists, mostly to As modes, but the total λ appears to be ~ 0.2, with $\omega_{log} \sim 250$ K, which can in no way explain $T_c \gtrsim 26$ K.

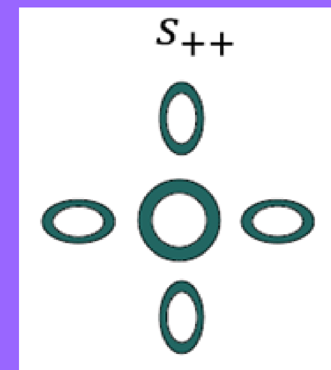
Mazin et al, PRL 2008, see also Mu et al CPL (2008), Boeri et al. PRL 2008

2 paradigms for superconductivity

according to how pairs choose to avoid Coulomb interaction

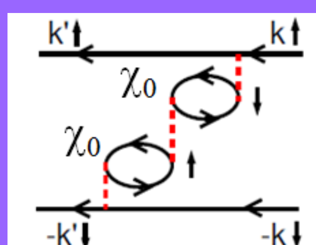
"conventional" : isotropic s-wave pair wave fctn, interaction retarded in time

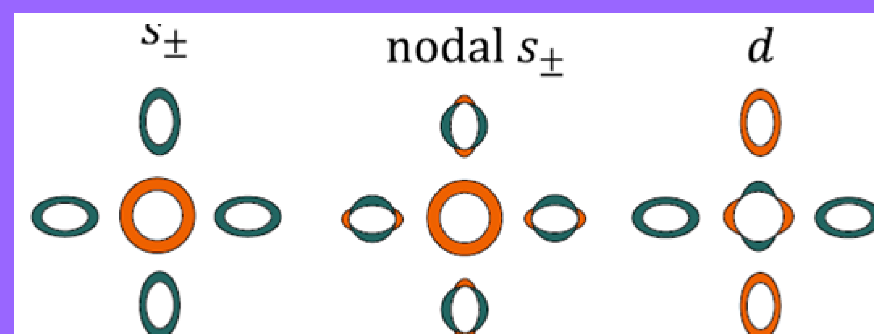




Overall effective interaction *attractive*

"unconventional": anisotropic or sign-changing pair wave fctn,





Overall effective interaction *repulsive*

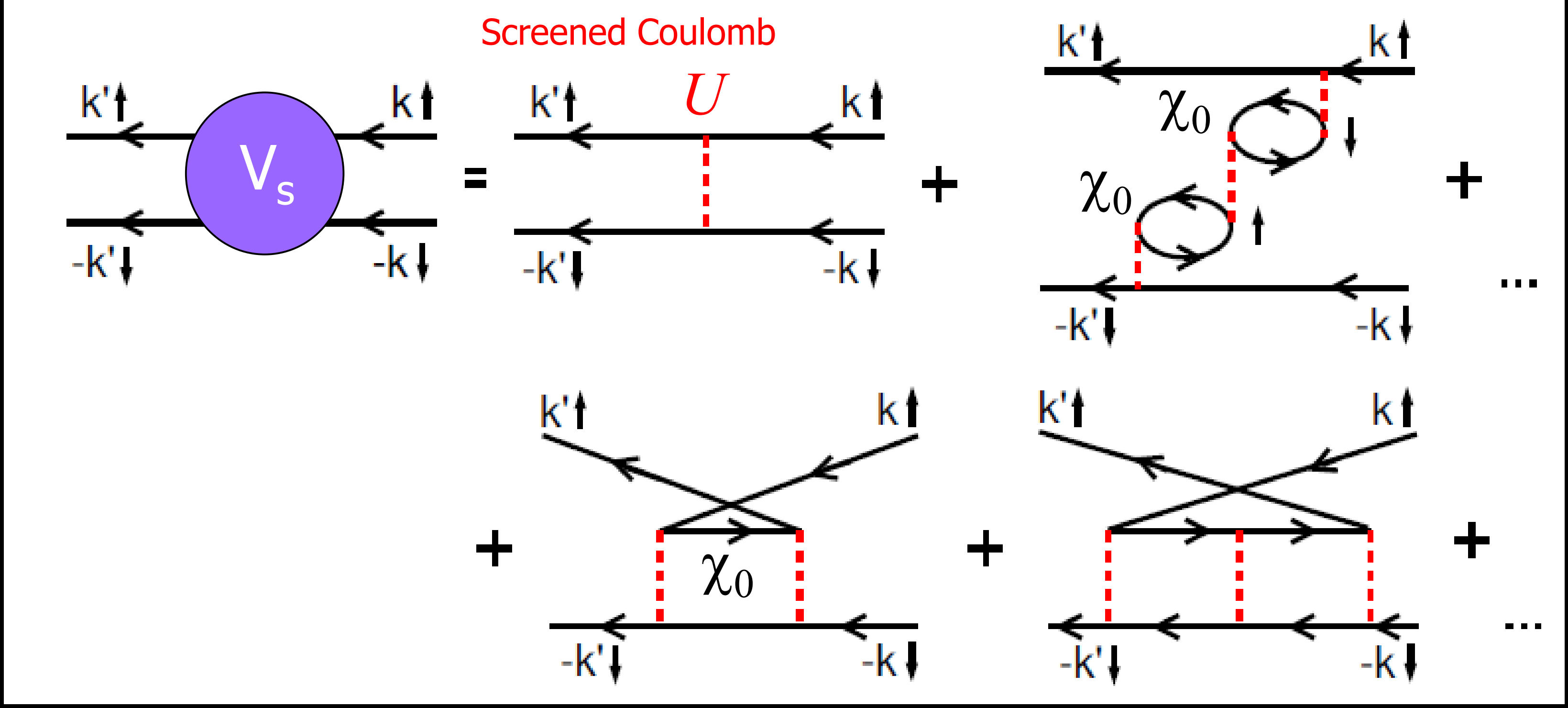
Spin fluctuation theories of pairing

Effective singlet interaction from spin fluctuations (Berk-Schrieffer 1966)

$$V_s(q,\omega) \cong \frac{3}{2}\,\frac{\bar{U}^2\chi_0(q,\omega)}{1-\bar{U}\chi_0(q,\omega)}$$

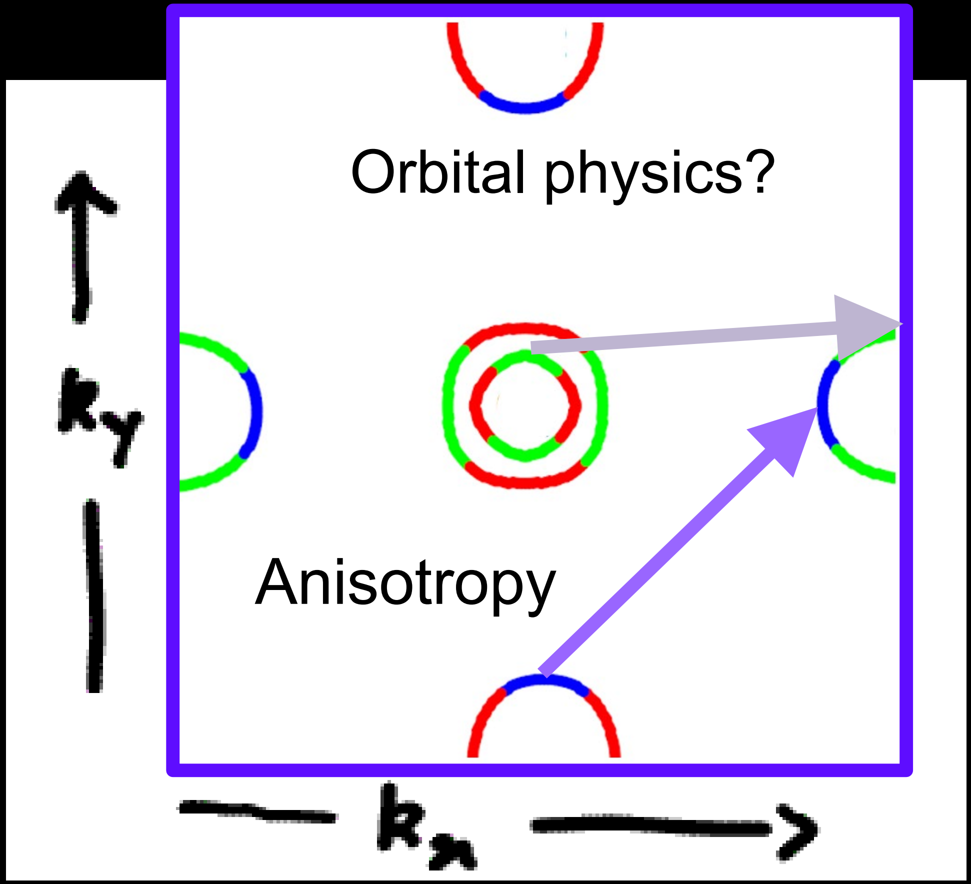
$$\chi_0(q,\omega) = \int \frac{d^3p}{(2\pi)^3}\,\frac{f(\varepsilon_{p+q})-f(\varepsilon_p)}{\omega-(\varepsilon_{p+q}-\varepsilon_p)+i\delta}$$

Generate attractive interaction from repulsion at large q on a lattice – e.g., d-wave in cuprates

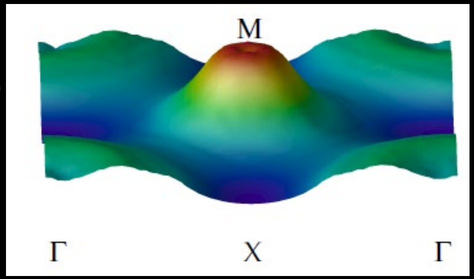


$s_{\pm}$ pairing in Fe-pnictides Mazin et al PRL 2008

electron-hole pocket pair scattering dominates



$\chi(q)$



also:

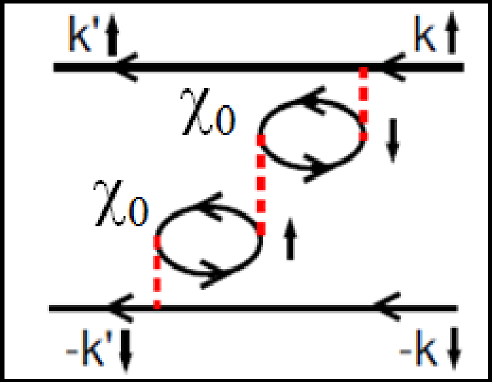
Graser et al 2009
Zhang et al 2009
Sknepnek et al 2009

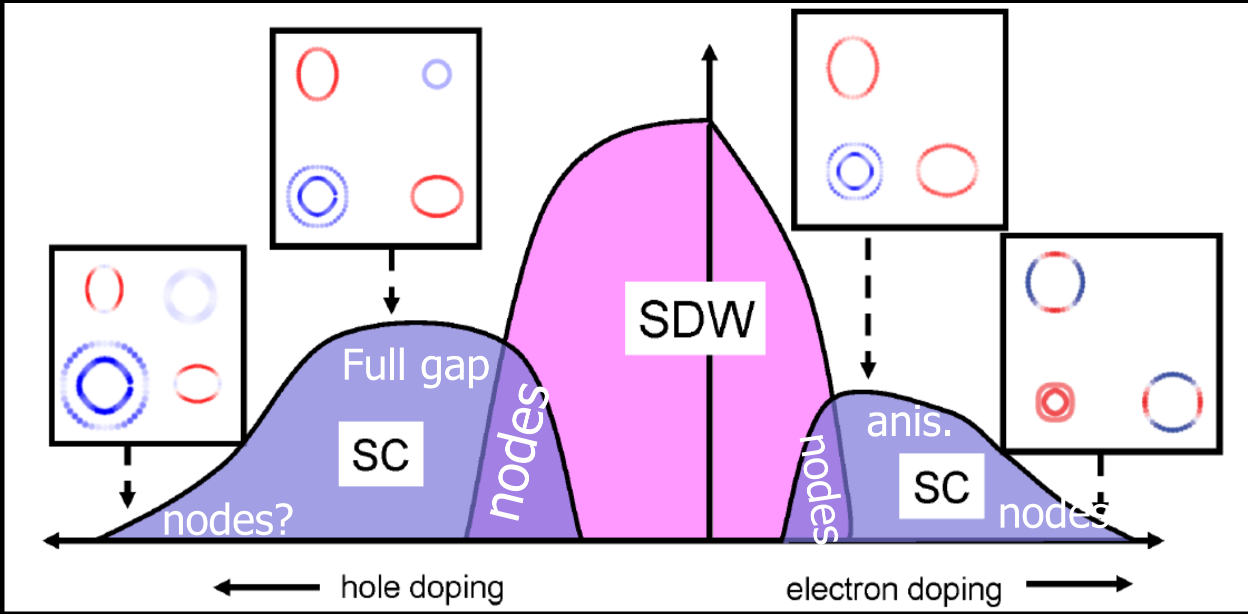
$$\Delta_p = -\sum_{p'} \frac{V(p-p')\Delta_{p'}}{2E_{p'}}$$

- nesting peaks interaction *V*(q) at $(\pi,0)$ in 1-Fe zone
- interaction is ~ constant over small pockets
- therefore sign-changing $s_{+/-}$ state solves gap eqn

Fe-pnictides: evolution of gap with doping from spin fluct. thy

PH, Korshunov and Mazin Rep. Prog. Phys. 2011
PH, Comptes Rendus Physique 2016





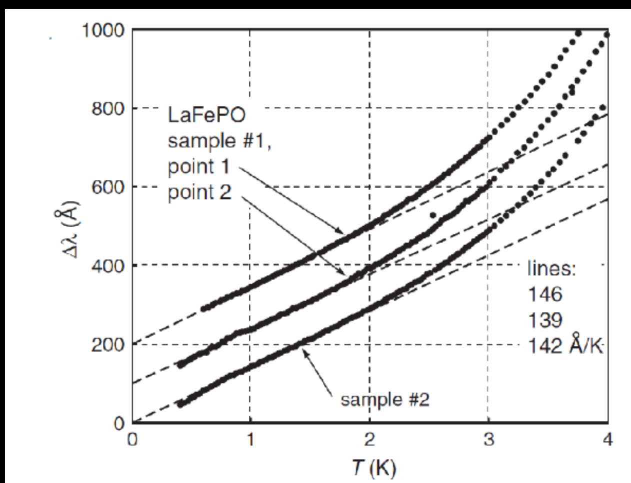
$$H_{int} = U\sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow}n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2})\sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma}n_{\mathbf{i}\nu\sigma'} - 2J\sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu}\cdot\vec{S}_{\mathbf{i}\nu} + J'\sum_{\mathbf{i},\mu<\nu,\sigma} c^\dagger_{\mathbf{i}\mu\sigma}c^\dagger_{\mathbf{i}\mu\bar\sigma}c_{\mathbf{i}\nu\bar\sigma}c_{\mathbf{i}\nu\sigma}$$

$$\Gamma_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}',\omega) = \left[\tfrac{3}{2}\bar U^s\chi_1^{\rm RPA}(\mathbf{k}-\mathbf{k}',\omega)\bar U^s + \tfrac{1}{2}\bar U^s - \tfrac{1}{2}\bar U^c\chi_0^{\rm RPA}(\mathbf{k}-\mathbf{k}',\omega)\bar U^c + \tfrac{1}{2}\bar U^c\right]_{\ell_3\ell_4\ell_1\ell_2}$$

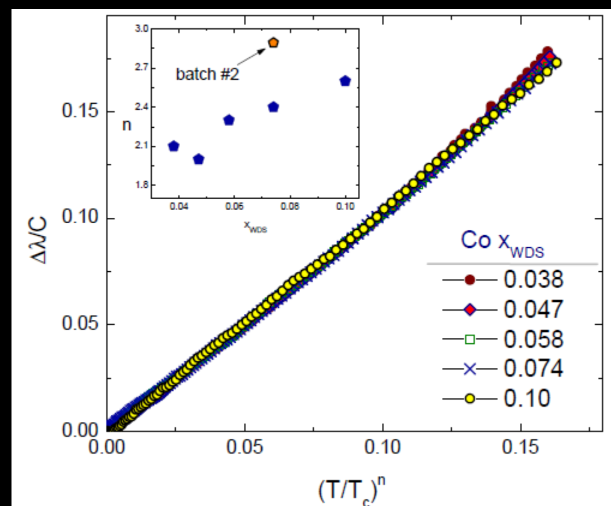
$$-\sum_j \oint_{C_j} \frac{dk'_\parallel}{2\pi}\frac{1}{2\pi v_F(k')}\Gamma_{ij}(k,k')g_\alpha(k') = \lambda_\alpha g_\alpha(k)$$

SC state: experimental "lack of universality" e.g., penetration depth experiments

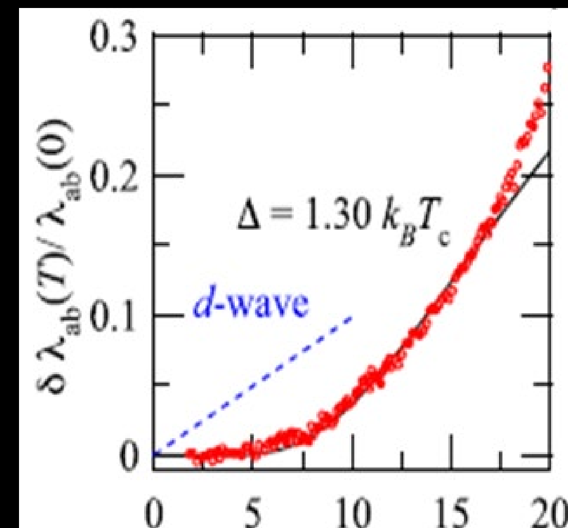
Hicks et al 2008
LaFePO T_c=6K



Prozorov, 2011
Co-doped Ba122 T_c=25K



Hashimoto et al 2009
K-doped Ba122 T_c=40K



$$\Delta\lambda \simeq \int d\omega\left(-\frac{\partial f}{\partial \omega}\right) N(\omega)$$

nodal SC

dirty: $N(\omega) \simeq N_0 + a\omega^2$

clean: $N(\omega) \simeq \omega$

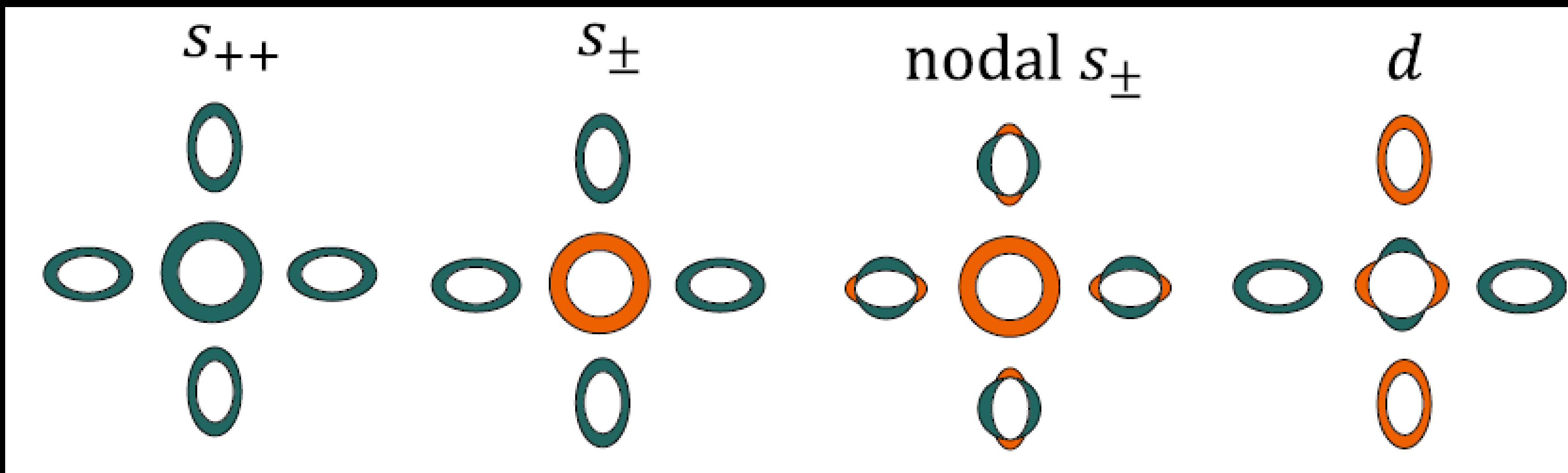
so $\Delta\lambda \simeq \begin{cases} T^2 & \textit{dirty} \\ T & \textit{clean} \end{cases}$

gapped SC

so $\Delta\lambda \simeq e^{-\Delta/T}$

SC gap symmetry and structure

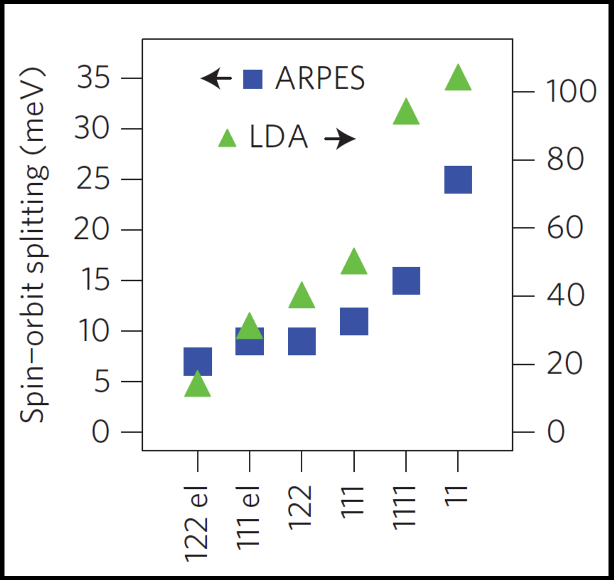
$\Delta(k)$ = "energy gap" or "order parameter" or "pair wave function"



A_{1g} B_{1g}

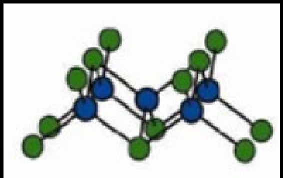
What's different between Fe-pnictides and Fe-chalcogenides?

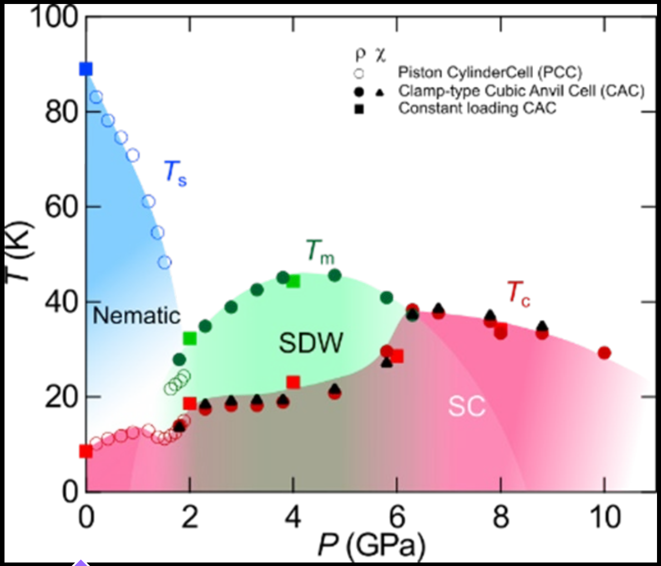
- Stronger electronic correlations Basov, Kotliar…
- Stronger spin-orbit coupling Borisenko Nat Phys 2015



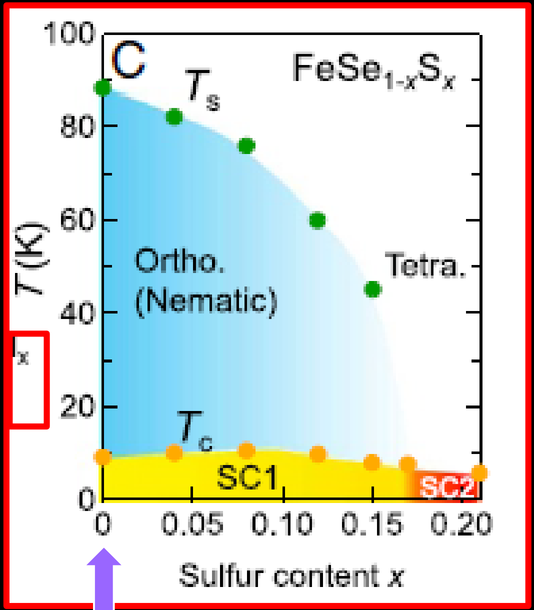
- "Intrinsic" electron doping, at least in some systems (not FeSe bulk)

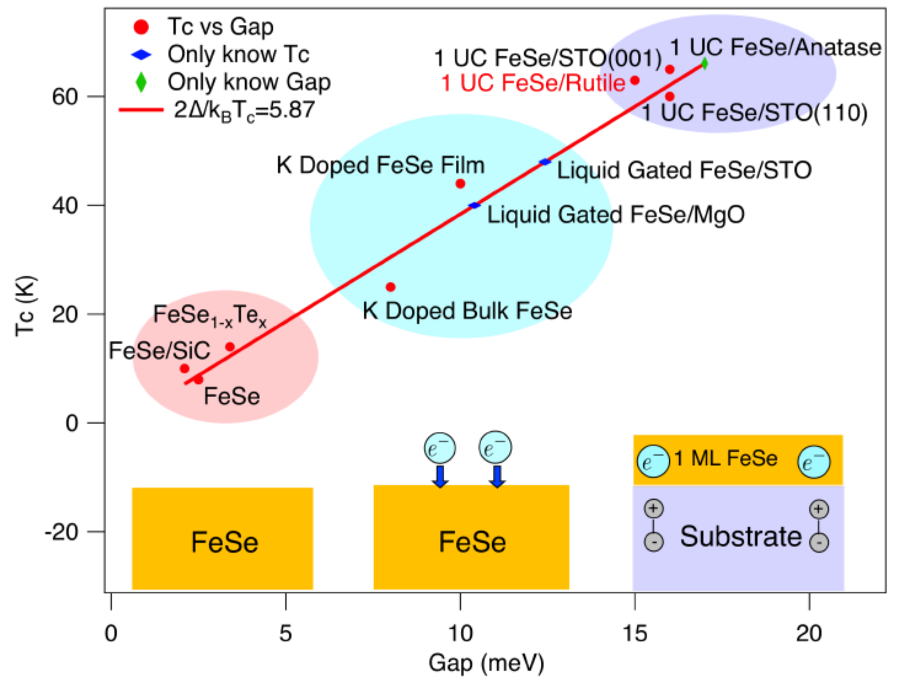
FeSe: low-Tc building block for high-Tc Fe-based SC





FeSe: nematic order without LR magnetic order, 8K superconductor



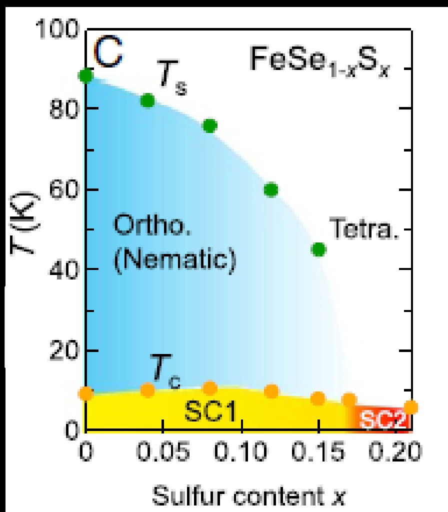


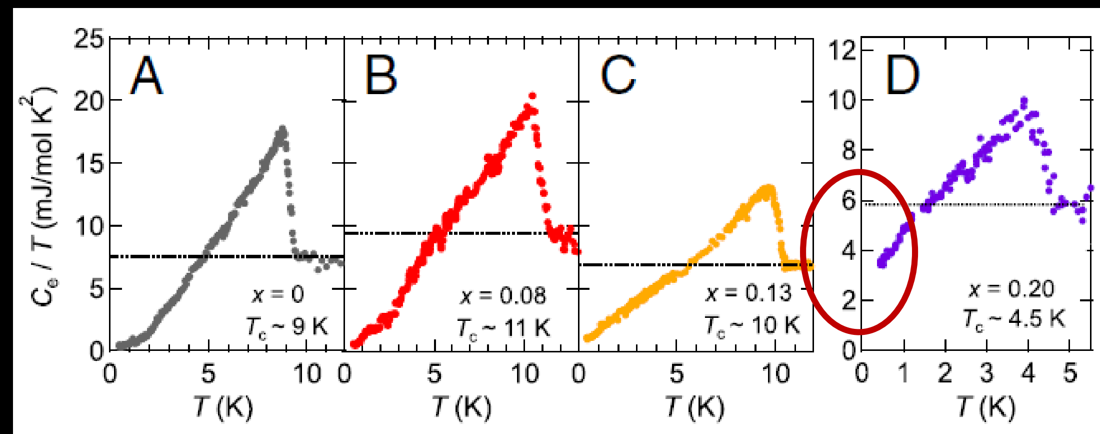
Possible topological ultranodal state in FeSe,S

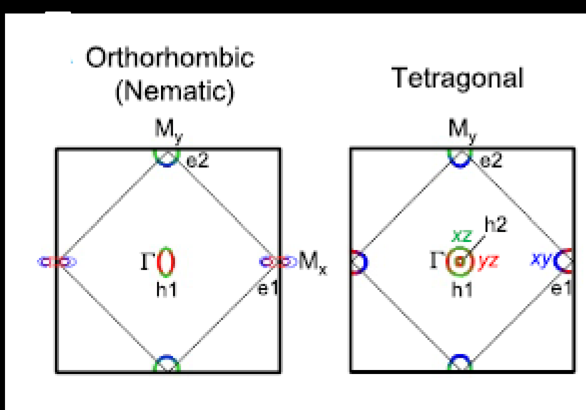
Abrupt change of the superconducting gap structure at the nematic critical point in $FeSe_{1-x}S_x$

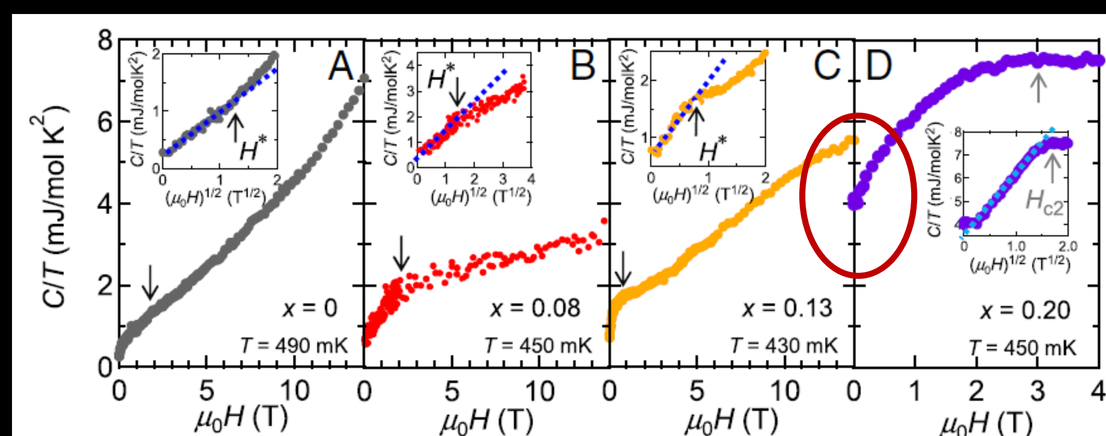
Yuki Sato[a], Shigeru Kasahara[a,1], Tomoya Taniguchi[a], Xiangzhuo Xing[a], Yuichi Kasahara[a], Yoshifumi Tokiwa[b], Youichi Yamakawa[c], Hiroshi Kontani[c], Takasada Shibauchi[d], and Yuji Matsuda[a,1]

PNAS 115, 1227 (2018)



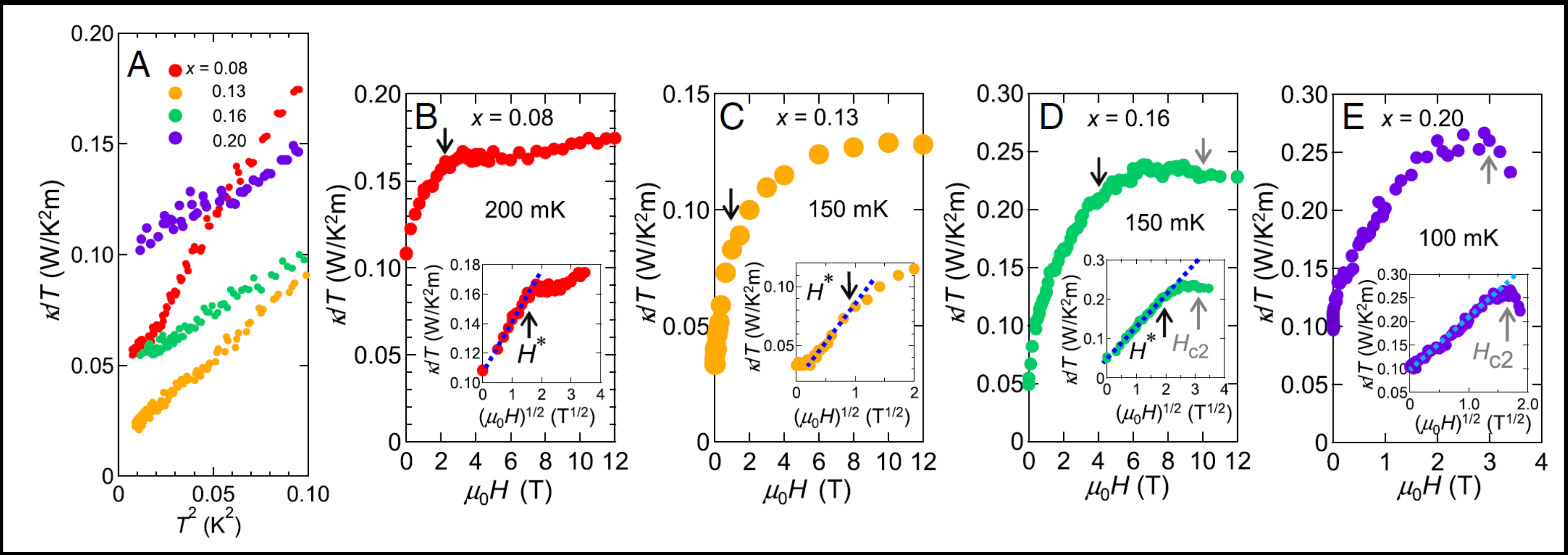






Thermal conductivity

Sato et al, PNAS 115, 1227 (2018)



Two distinct superconducting pairing states divided by the nematic end point in $FeSe_{1-x}S_x$

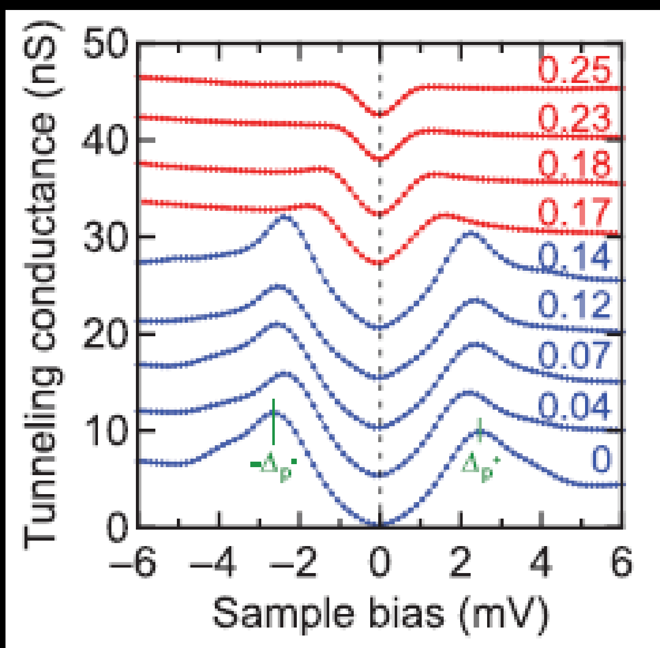
Tetsuo Hanaguri,[1]* Katsuya Iwaya,[1] Yuhki Kohsaka,[1] Tadashi Machida,[1] Tatsuya Watashige,[2†] Shigeru Kasahara,[2] Takasada Shibauchi,[3] Yuji Matsuda[2]

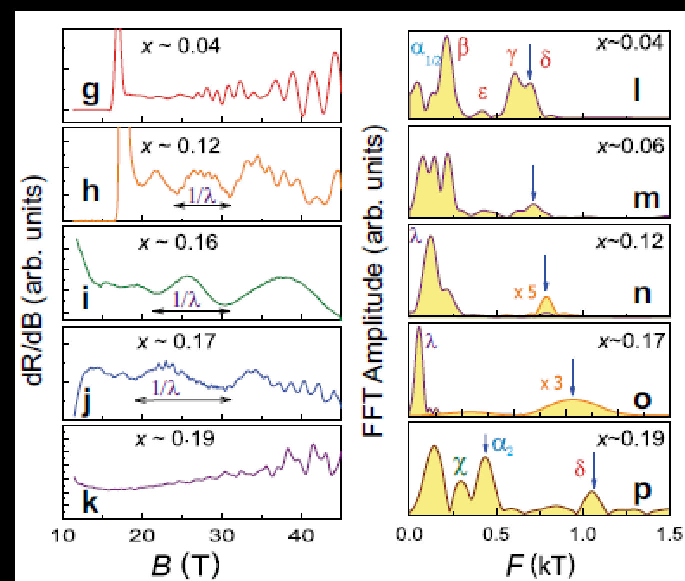
Science Advances 4, eaar6419 (2018):

SC state with nonzero zero-bias DOS!

NOT due to disorder in nodal SC state

Q. Osc.: Coldea et al npj-Quant. Mat. 2019





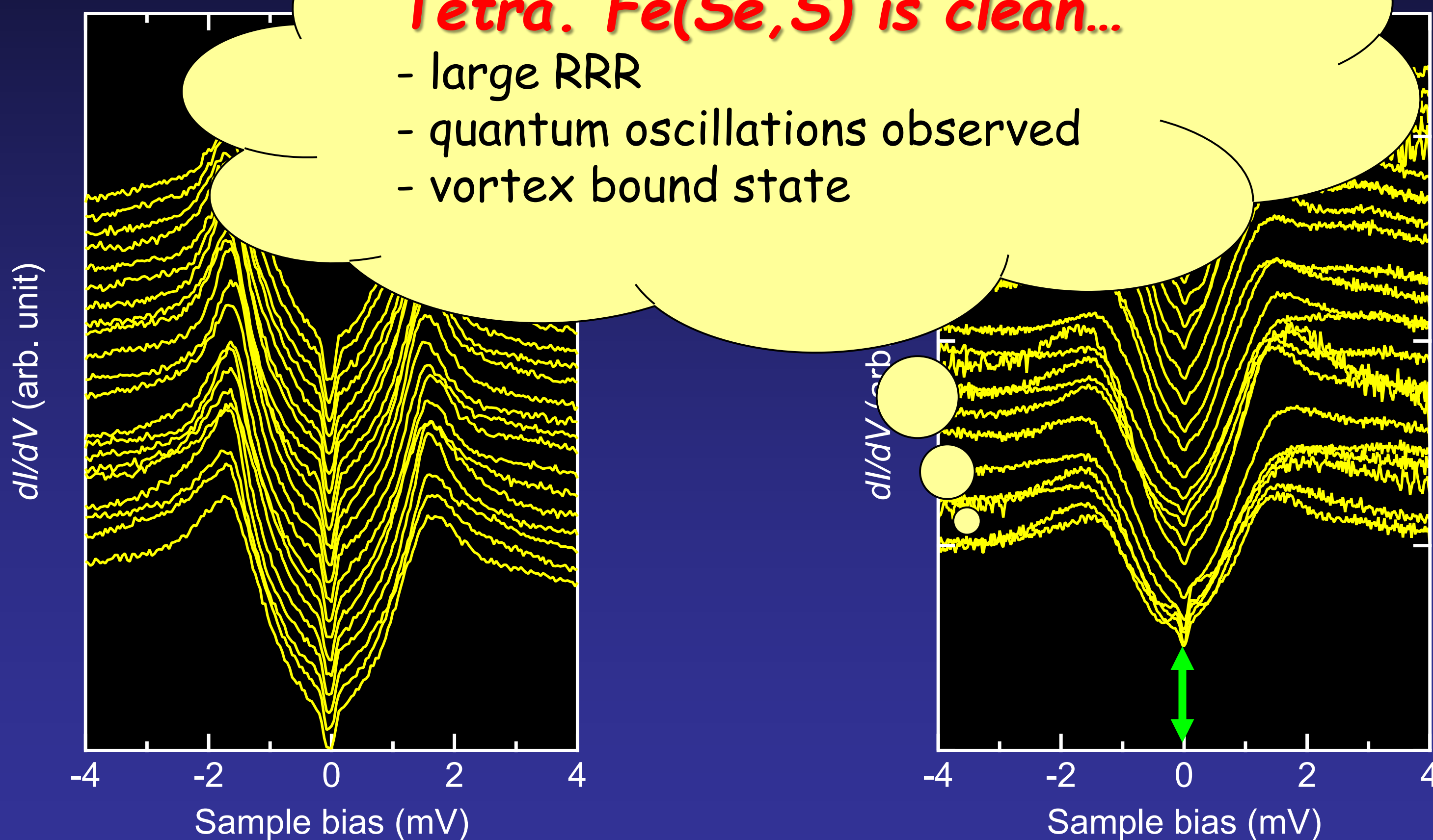
Conclusion from experiments: gap is more anisotropic outside nematic phase!

What is happening in SC at high S contents?

Ultra-high energy resolution spectroscopy below 90 mK

cf. T. Machida, Y. Kohsaka and T. Hanaguri, RSI **89**, 093707 (2018).

x = 0.17 jus



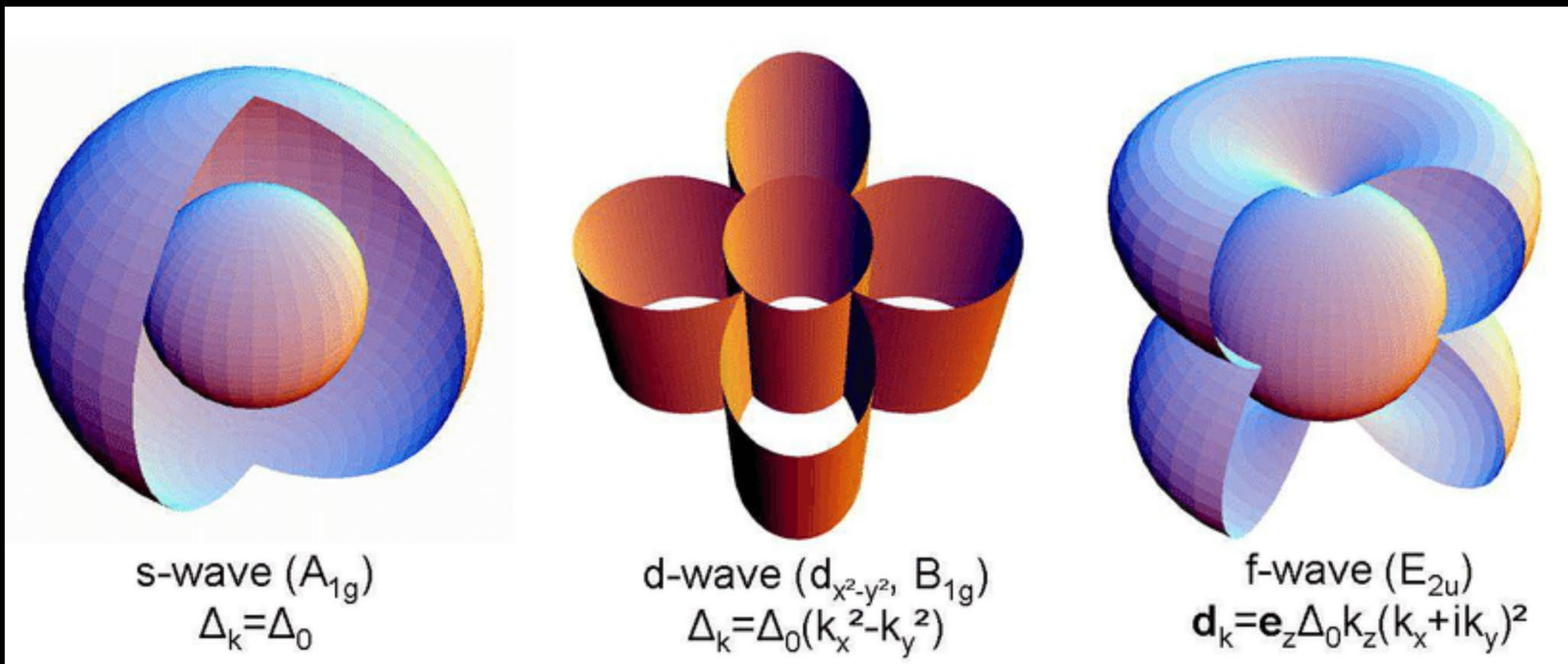
Tetra. Fe(Se,S) is clean…

- large RRR
- quantum oscillations observed
- vortex bound state

Large residual DOS at E_F may be intrinsic

Thanks to Tetsuo Hanaguri, RIKEN!

Gap nodal surfaces in unconventional superconductors

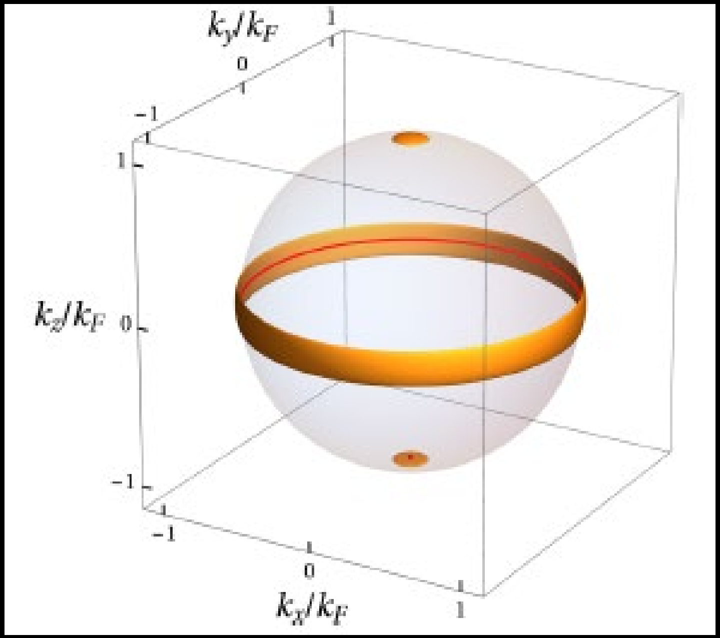


Another possibility?

Bogoliubov Fermi Surfaces in Superconductors with Broken Time-Reversal Symmetry

D. F. Agterberg,[1,*] P. M. R. Brydon,[2,†] and C. Timm[3,‡]
[1]*Department of Physics, University of Wisconsin, Milwaukee, Wisconsin 53201, USA*
[2]*Department of Physics, University of Otago, P.O. Box 56, Dunedin 9054, New Zealand*
[3]*Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany*

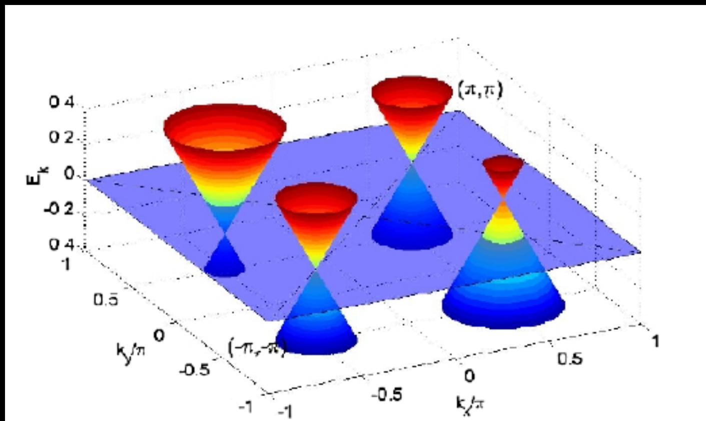
PRL 118, 127001 (2017)



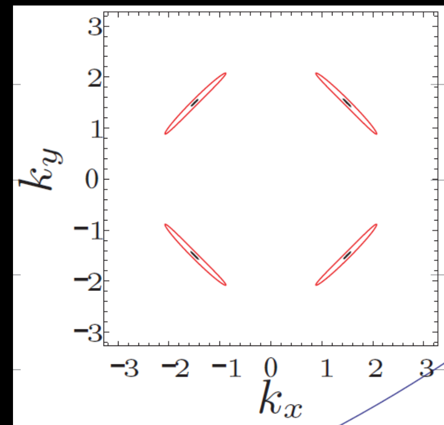
Ingredients:
- even-parity nodal superconducting state
- spontaneous time reversal symmetry breaking (TRSB)
- effective j=3/2 fermions

Other examples of Bogoliubov Fermi surfaces

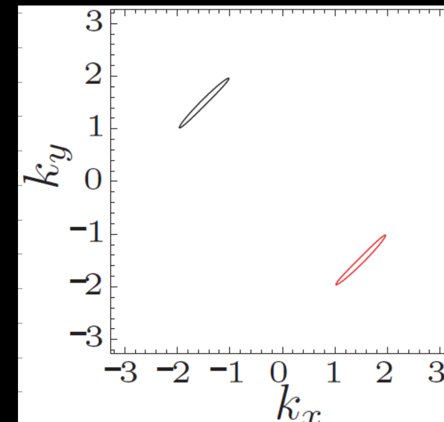
dSC with loop current order



d-wave SC in Zeeman field



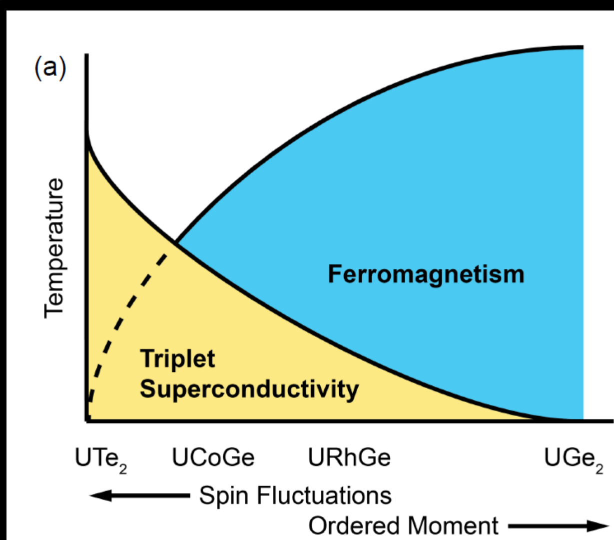
dSC with loop current order

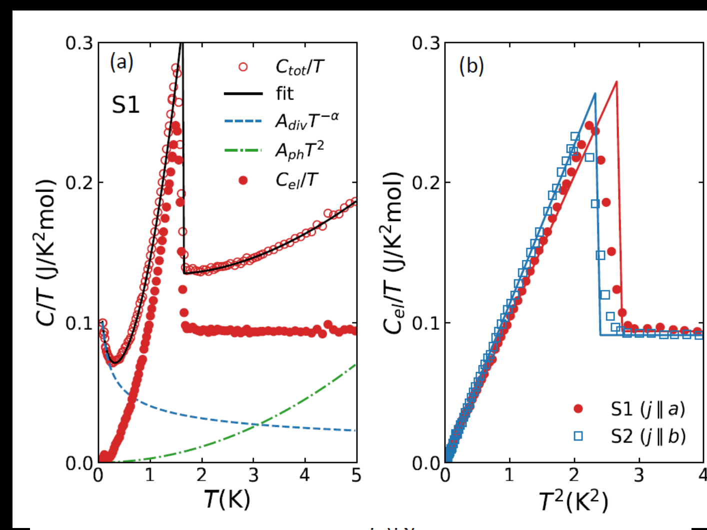


Berg et al PRL 2008

Wang-Vafek PRB 2013

?





UTe$_2$

Ran et al arXiv 1811.1180;

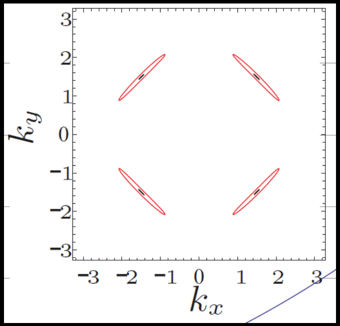
Metz et al 1908.01069

Evidence for possible nonunitary triplet pairing in centrosymmetric system

Examples of BFS

$$\hat{H} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \hat{H}(\mathbf{k}) \Psi_{\mathbf{k}} \qquad \Psi^\dagger_{\mathbf{k}} = \left(c^\dagger_{\mathbf{k}\uparrow}, c^\dagger_{\mathbf{k}\downarrow}, c_{-\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}\right)$$

1. d-wave SC in Zeeman field



$$\hat{H}(\mathbf{k}) = \Delta(\mathbf{k})\,(i\pi_y \otimes i\sigma_y) + \epsilon(\mathbf{k})(\pi_z \otimes \sigma_0) + h(\pi_z \otimes \sigma_z)$$

π and σ are Pauli matrices in Nambu, spin respectively

C,P preserved independently

$$\mathrm{Pf}(\mathbf{k}) = \epsilon(\mathbf{k})^2 + \Delta(\mathbf{k})^2 - h^2$$

$$\mathrm{Min}\{\mathrm{Pf}(\mathbf{k})\} = \Delta(\mathbf{k})^2 - h^2 \;\Rightarrow\; \pm,\, Z_2 \text{ inv}$$

2. Loop currents coexisting with d-wave order

$$\hat{H}(\mathbf{k}) = \Delta(\mathbf{k})\,(i\pi_y \otimes i\sigma_y) + \epsilon(\mathbf{k})(\pi_z \otimes \sigma_0) + J(\mathbf{k})(\pi_z \otimes \sigma_z)$$

$$J(\boldsymbol{k}) = J(\sin k_x - \sin k_y + \sin(k_y - k_x))$$

breaks C,P but preserves CP

$$\mathrm{Min}\{\mathrm{Pf}(\mathbf{k})\} = \Delta(\mathbf{k})^2 - J(\mathbf{k})^2$$

Topological Ultranodal pair states in iron-based superconductors

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$\vec{\sigma}$ spin space

$\vec{\tau}$ band space

$$H_\Delta(\mathbf{k}) = \Delta_i(\mathbf{k})\tau_0 \otimes i\sigma_y + \Delta_0\, i\tau_y \otimes \sigma_0 + \delta\, i\tau_y \otimes \sigma_z$$

Intraband
spin singlet

Interband
spin triplet

Interband
spin triplet
TRSB

SOC

Agterberg
et al.

H is CP-symmetric matrix ⇒ Det=Pf²

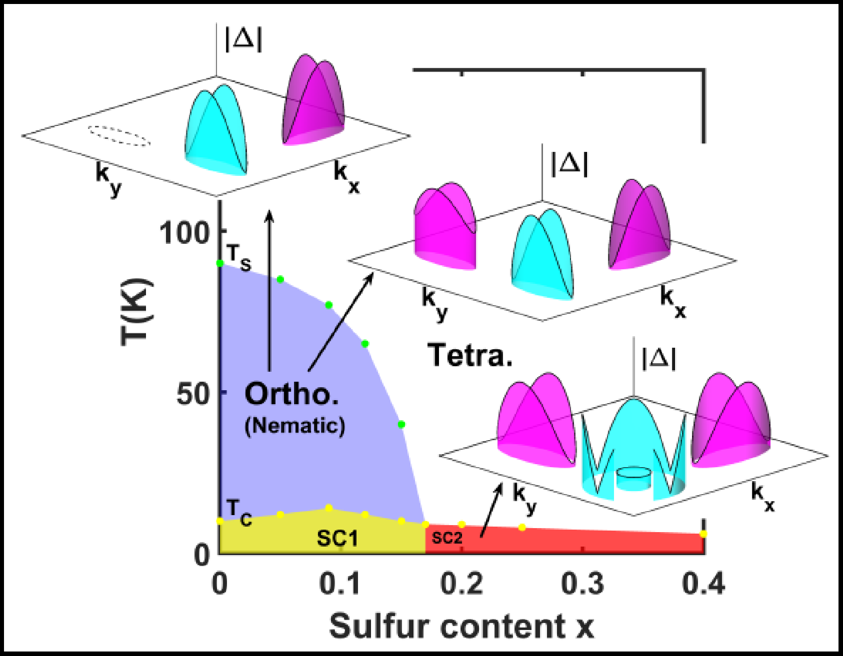
Topological transition to an ultranodal SC state when Pf changes sign!

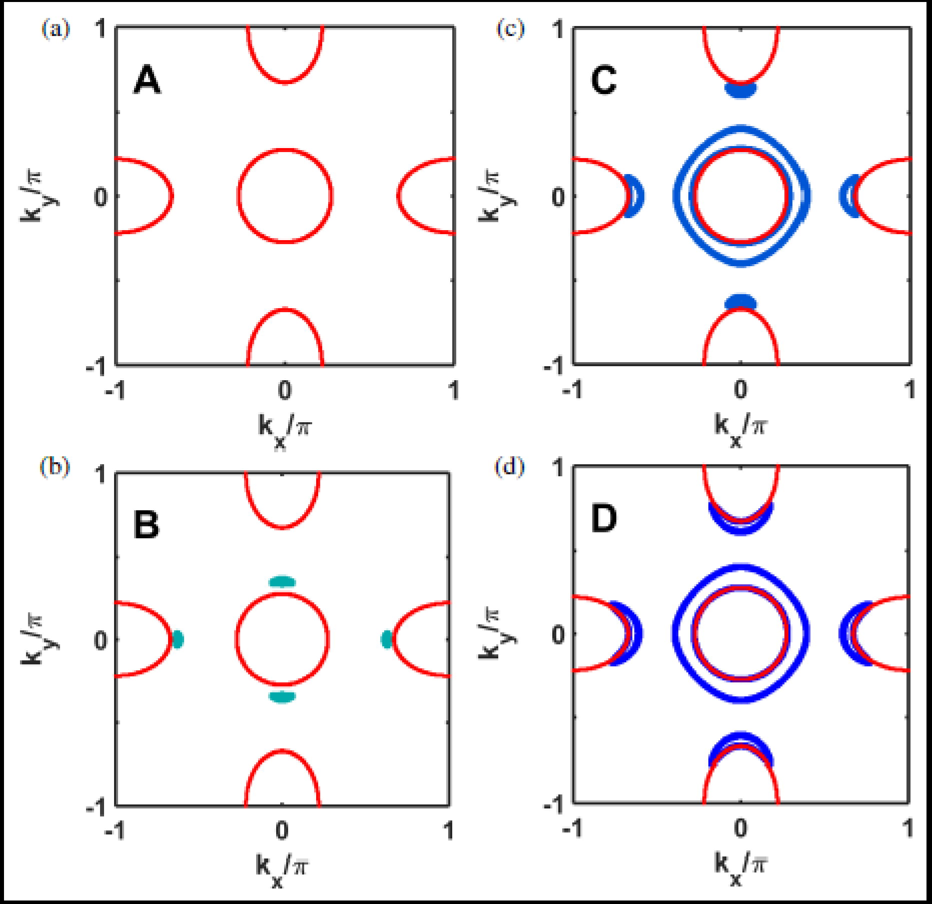
$$\mathrm{Min[Pf]} = \begin{cases} \delta^2\left(|\Delta_1(\mathbf{k})||\Delta_2(\mathbf{k})| - \Delta_0^2\right) & \text{if } \Delta_1(\mathbf{k})\Delta_2(\mathbf{k}) > 0 \\ \Delta_0^2\left(|\Delta_1(\mathbf{k})||\Delta_2(\mathbf{k})| - \delta^2\right) & \text{if } \Delta_1(\mathbf{k})\Delta_2(\mathbf{k}) < 0. \end{cases}$$

Ansatz for intraband gap evolution in $FeSe_{(1-x)}S_x$

Conventional → *ultranodal* Z_2 transition

$$\boxed{\Delta_s = \Delta_j(\mathrm{k}) = \Delta_{ja}(\mathrm{k}) + \Delta_j}$$



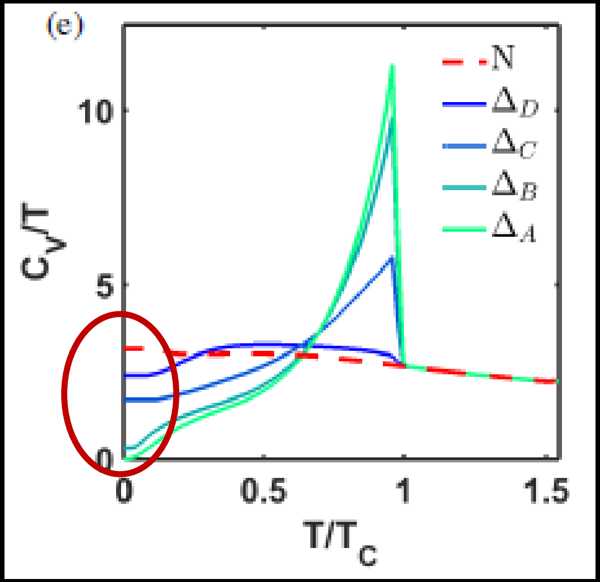


Anisotropic components held fixed, isotropic ones decreasd with x (scenario proposed by Tokyo-Kyoto collaboration)

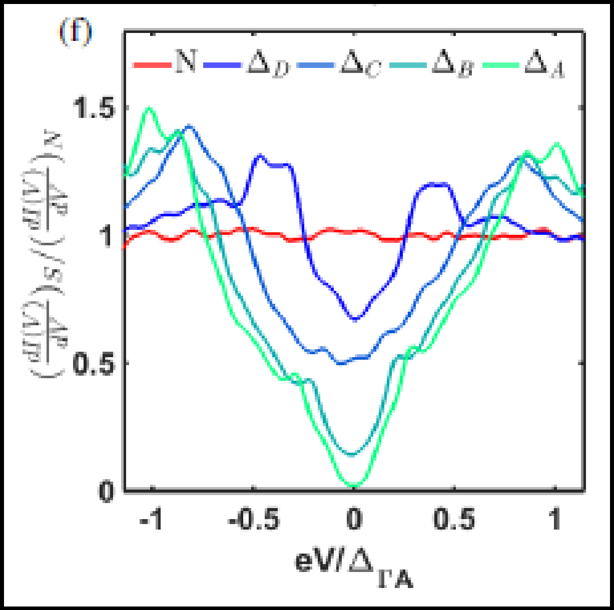
Comparison with experiment on $FeSe_{(1-x)}S_x$

Setty et al arXiv: 1903.00481

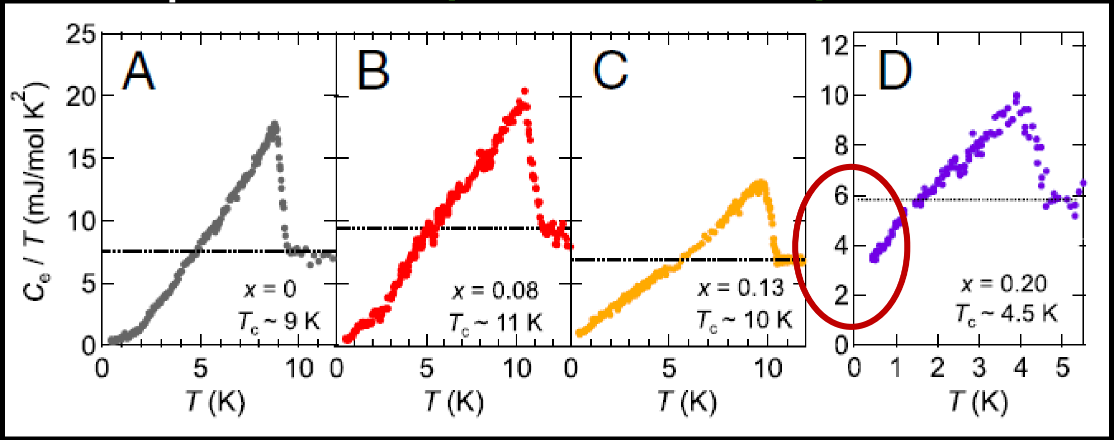
Sp. heat: theory



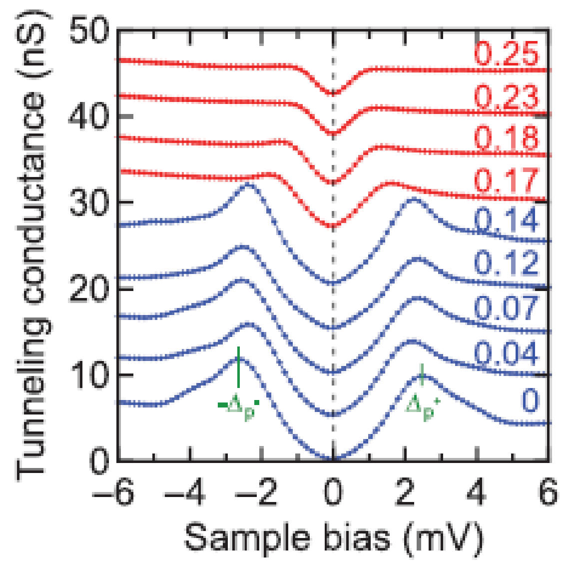
STM: theory



experiment (Sato et al 2018)

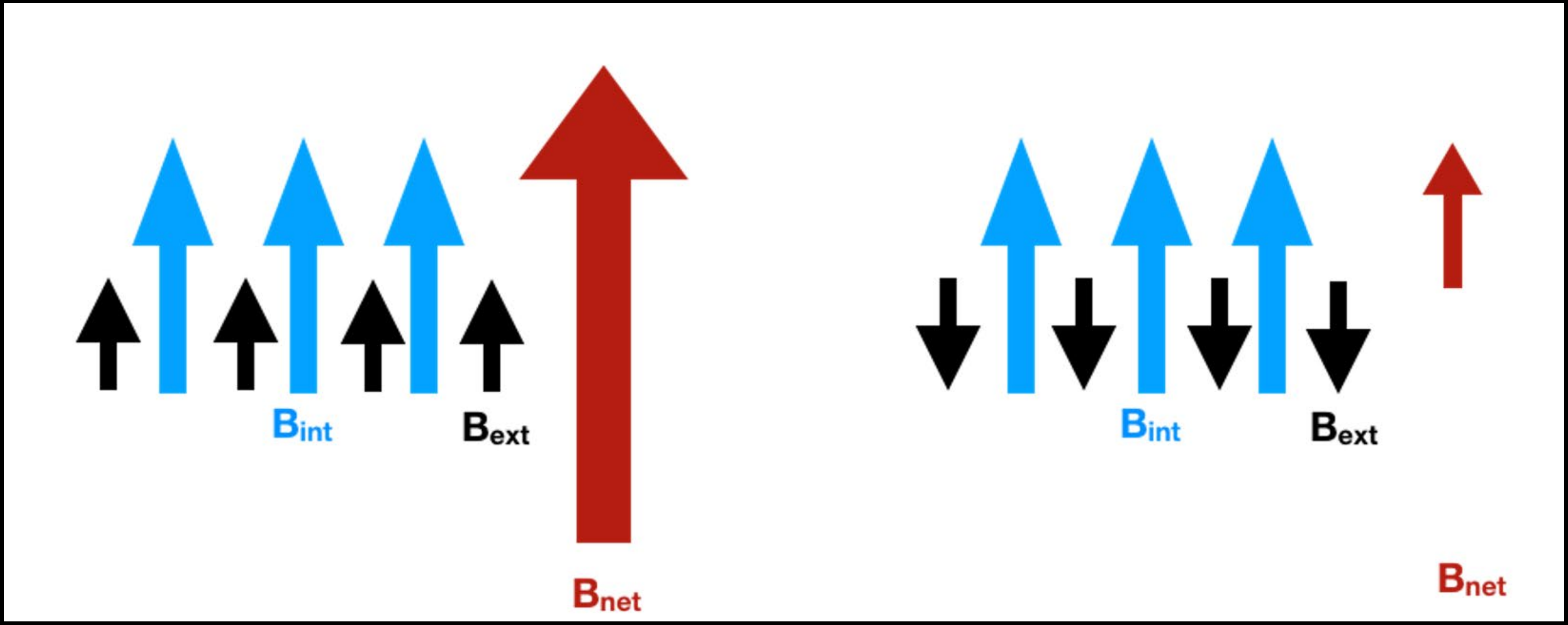


expt. (Hanaguri et al 2019)



Is there a "smoking gun" for the ultranodal state?

Consequences of time reversal symmetry breaking by "internal magnetic field"

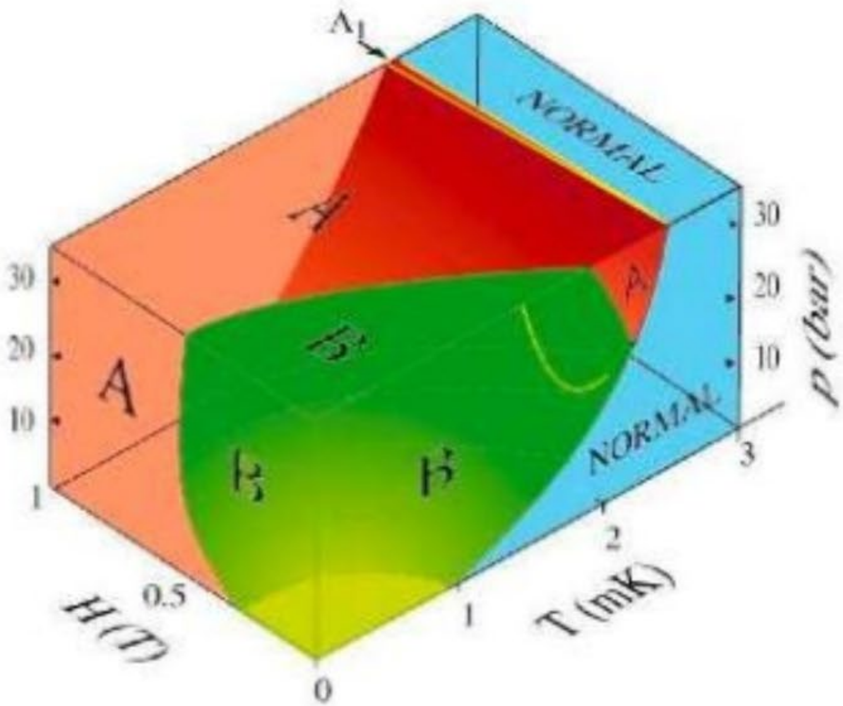


Nonunitary superconducting state $\Delta_{\uparrow\uparrow} \neq \Delta_{\downarrow\downarrow}$

Non-unitary pairing

Spin-up superfluid coexisting with spin-down Fermi liquid.

$$\hat{\Delta} = \begin{pmatrix} \Delta_{\uparrow\uparrow} & 0 \\ 0 & 0 \end{pmatrix} \text{or} \begin{pmatrix} 0 & 0 \\ 0 & \Delta_{\downarrow\downarrow} \end{pmatrix}$$



C.f.

The A1 phase of liquid ^{3}He.

- Do we know examples where this happens spontaneously in zero field?
- Do we understand physics that could cause this?

NO

Out of plane field

Quadratic

Linear

$$\mathrm{Pf}\left(\delta,\Delta_s,\Delta_0,h,\epsilon_1,\epsilon_2\right)=\mathrm{Pf}_2\left(\delta,\Delta_s,\Delta_0,h^2,\epsilon_1,\epsilon_2\right)-h\delta\Delta_0(\epsilon_1+\epsilon_2)$$

Small fields

$$\mathrm{Pf}\left(\delta,\Delta_s,\Delta_0,h,\epsilon_1,\epsilon_2\right)\simeq\mathrm{Pf}_0\left(\delta,\Delta_s,\Delta_0,\epsilon_1,\epsilon_2\right)-h\delta\Delta_0(\epsilon_1+\epsilon_2)$$

Near criticality

$$\mathrm{Min}[\mathrm{Pf}_0]\left(\delta,\Delta_s,\Delta_0,h\right)\simeq 0$$

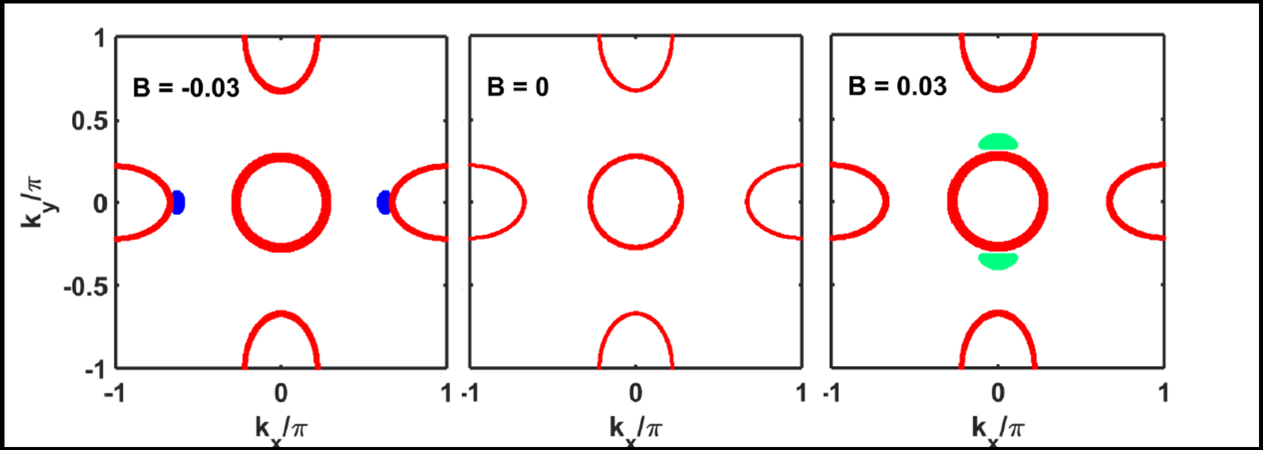
Determines Minimum

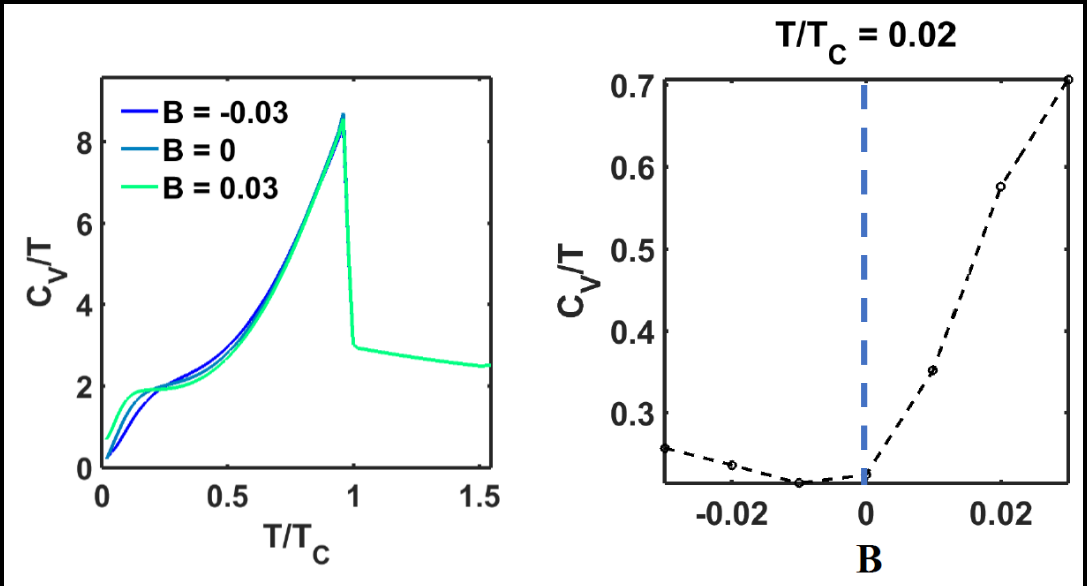
Pfaffian minimum determined by the relative sign of *h* and δ

In-plane field: only h^2 term $\Rightarrow$ only shift of transition

Bogoliubov Fermi surfaces shrink/grow with out-of-plane field

Prediction (after subtraction of Volovik term):
C(T→0)/T depends on direction of field





Stability of ultranodal state

$$\mathbf{j}^P(\mathbf{q}) = -\frac{e}{2}\sum_{\mathbf{k}}(\mathbf{k}+\frac{\mathbf{q}}{2})\psi^\dagger_{\mathbf{k}}\begin{pmatrix}\frac{1}{m_1} & \\ & \frac{1}{m_2}\end{pmatrix}\psi_{\mathbf{k}+\mathbf{q}}$$

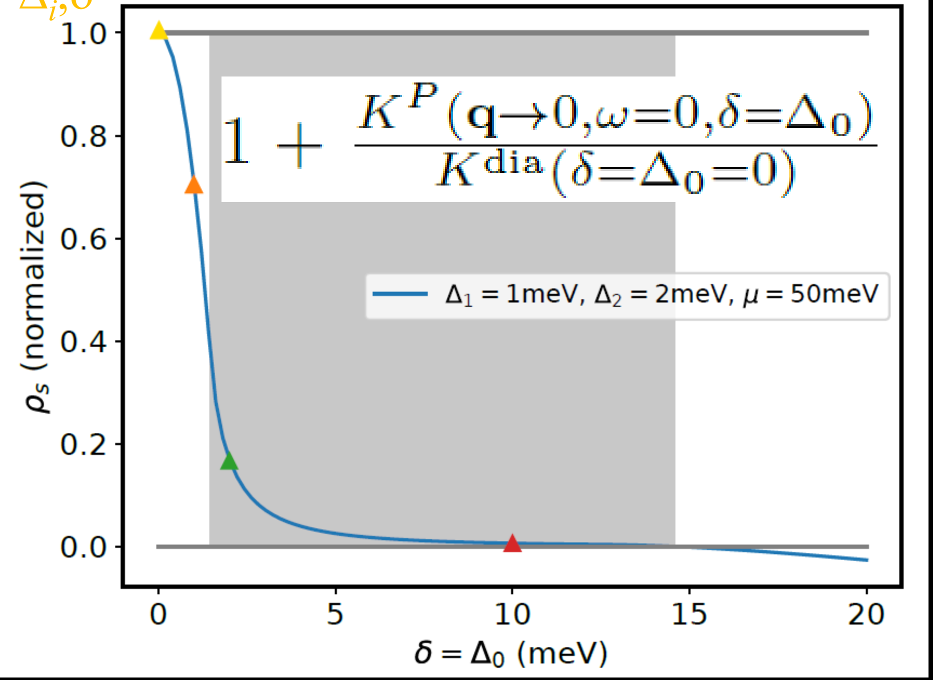
$$K^{\mathrm{dia}} = \frac{4\pi e^2}{c^2}\sum_\alpha \frac{n_\alpha}{|m_\alpha|}$$

$$J_i(\mathbf{q},\omega) = -\frac{c}{4\pi}K_{ij}(\mathbf{q},\omega)A_j(\mathbf{q},\omega),$$
$$K = K^P + K^{\mathrm{dia}},$$

Tendency to negative Meissner effect, as in odd-frequency pairing, but:

a) Large stable topological region
b) Stability enhanced by intraband gap anisotropy

Model with *isotropic* intra, interband gaps Δ_i,δ



Conclusions

- Novel even parity triplet interband pair states may be realized in presence of spin orbit coupling
- Combination TRSB interband triplet, anisotropic intraband singlet pairing can lead to "ultranodal" state, explain nonzero residual DOS in $FeSe_{1-x}S_x$. Bogoliubov Fermi surface is topological, robust against perturbations that preserve particle-hole & inversion symmetries
- Microscopic mechanism for nonunitary pairing missing. Needed: theory treating spin-fluctuation pair states & exotic (interband) states on equal footing!
- Einstein: "perhaps"