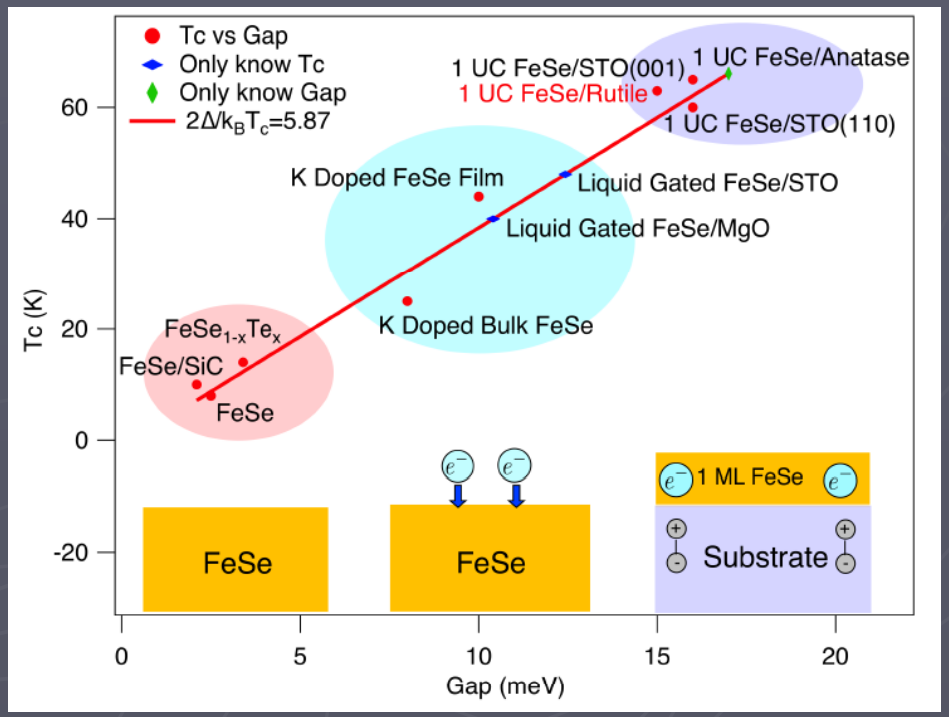
Phenomenology of iron selenide - based Superconductors

P. Hirschfeld, U. Florida



PJH, Comptes Rendus Physique 17, 197 (2016)
(Special focus issue on Fe-based superconductivity)
S. Mukerjee et al., PRL 2015; A. Kreisel et al, PRB 2015
X. Chen et al PRB 2015; A. Linscheid et al. arXiv:1603.03739
S. Teknowijoyo et al, arXiv:1605.04170

Collaborators

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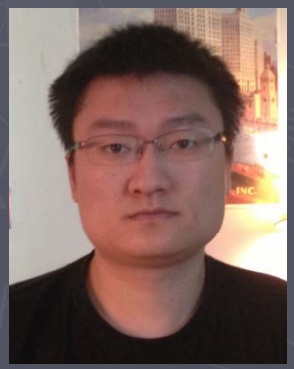
Andy Linscheid



Xiao Chen

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(ORNL)

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(U. Tennessee)

Niels Bohr Inst., Cph

Brian Andersen

Maria N. Gastiasoro

Andreas Kreisel

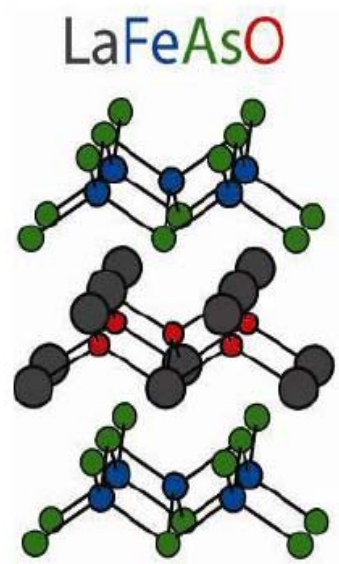
Astrid Roemer

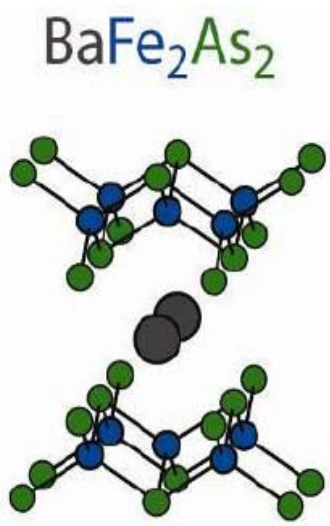
Outline

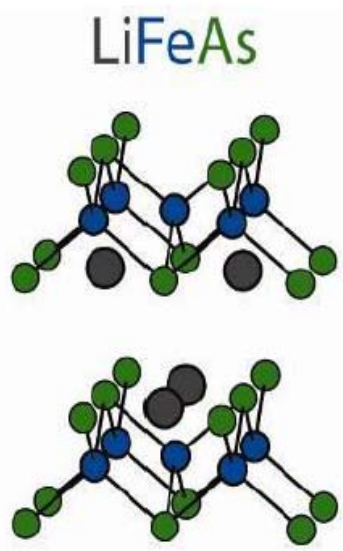
- Lightning review of Fe-based SC concepts
- Phenomenology of bulk FeSe
- Role of disorder in FeSC: general
- Electron irradiation of FeSe
  - Pair strengthening by impurities
  - Competition of nematic order & SC + disorder
- FeSe monolayers and intercalates: role of incipient bands
- Conclusions & open questions

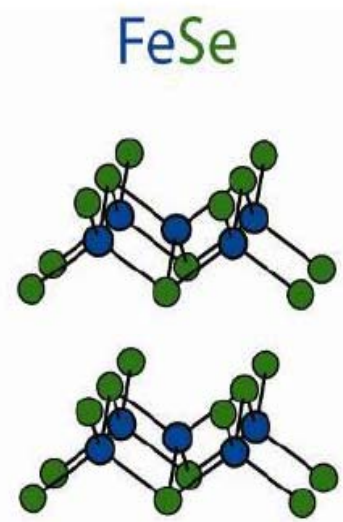
Iron-based superconductors

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

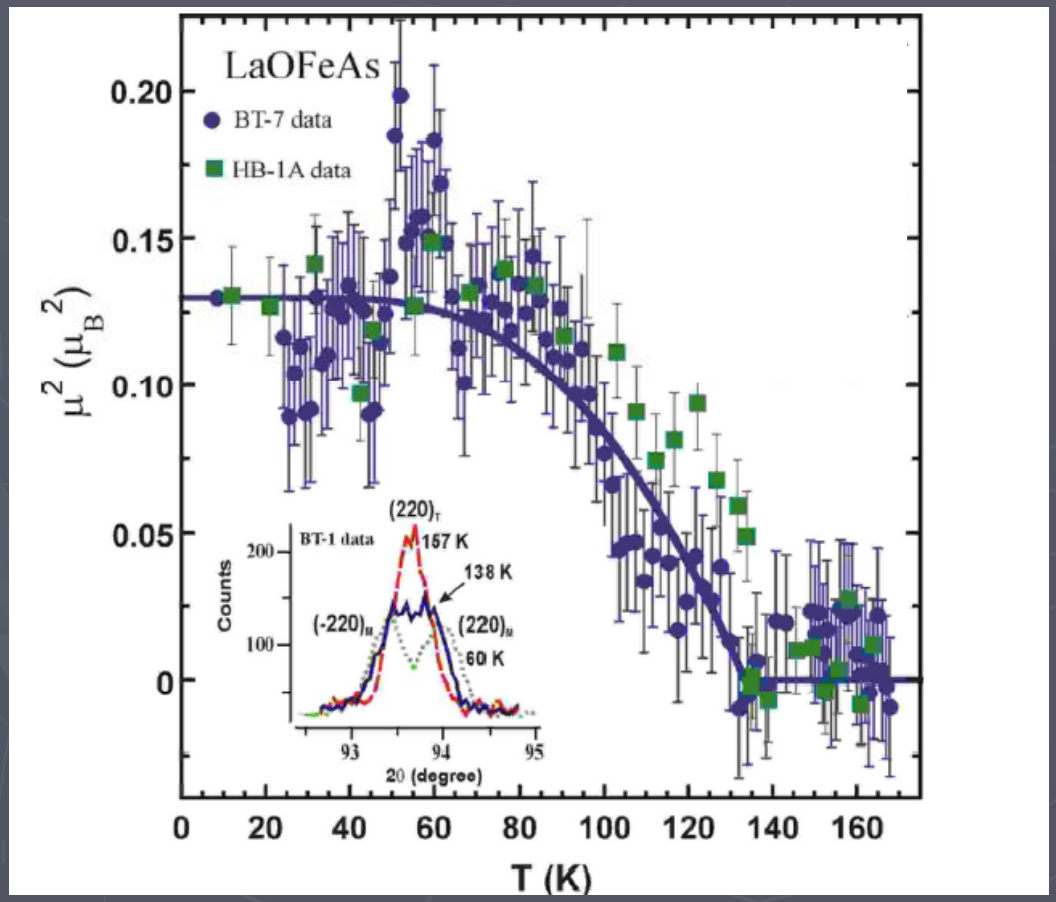
T_c=8K

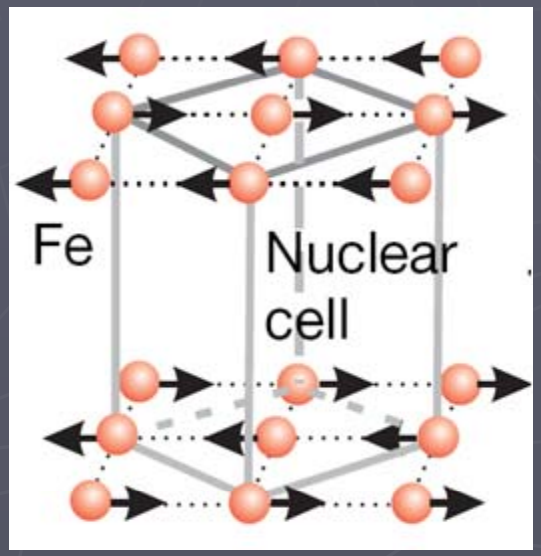
Hsu et al
PNAS 2008

No arsenic ☺!

Magnetic order in most (not all) parent compounds

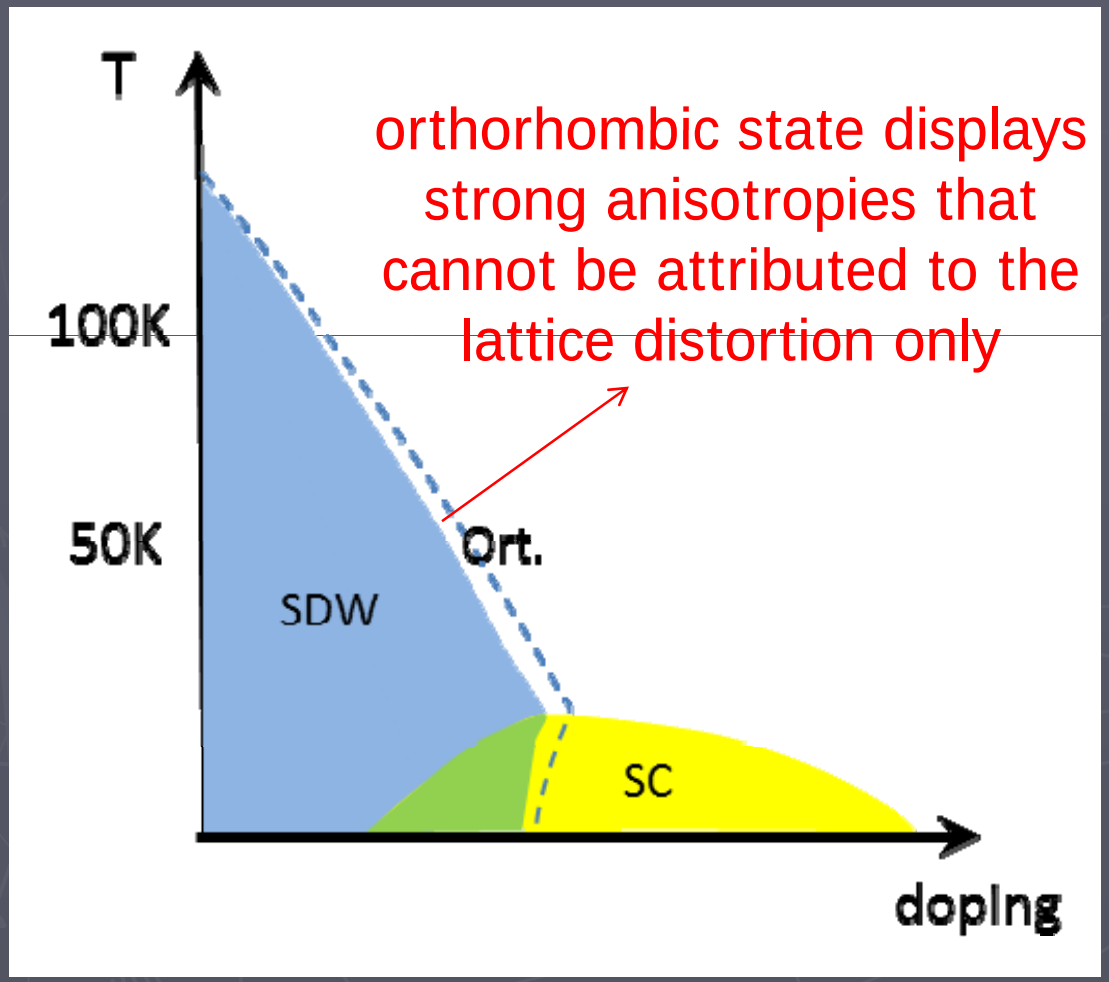
de la Cruz et al Nature 453, 899 (2008)



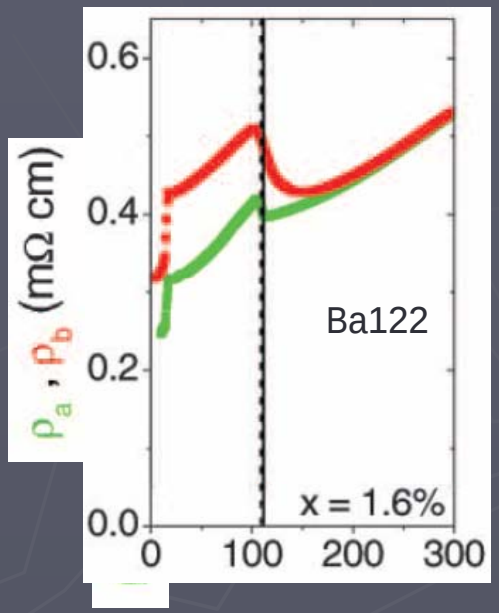


Stripe like order w q=(π,0)

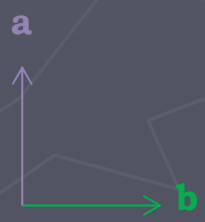
Nematic behavior

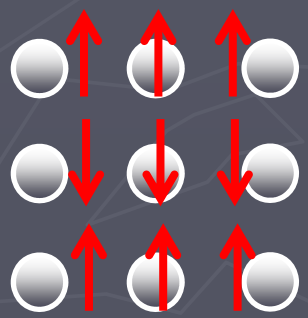


- resistivity



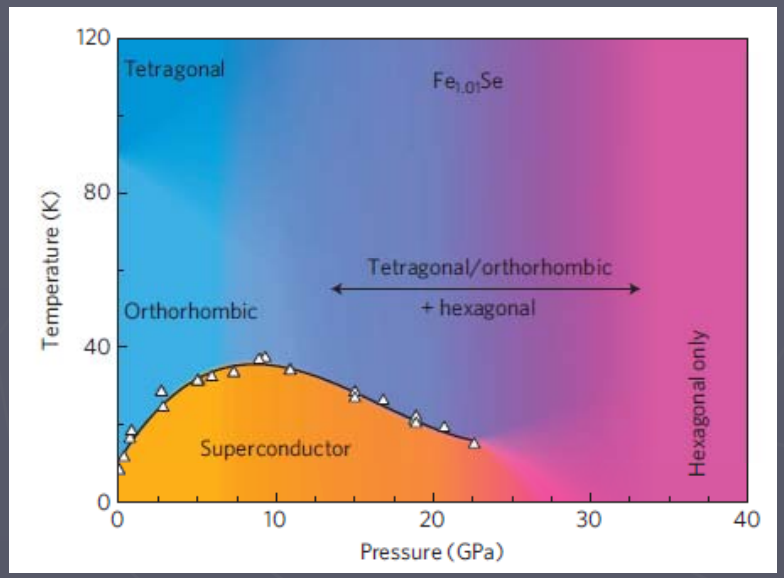
Chu et al, Science (2010)
Tanatar et al, PRB (2010)



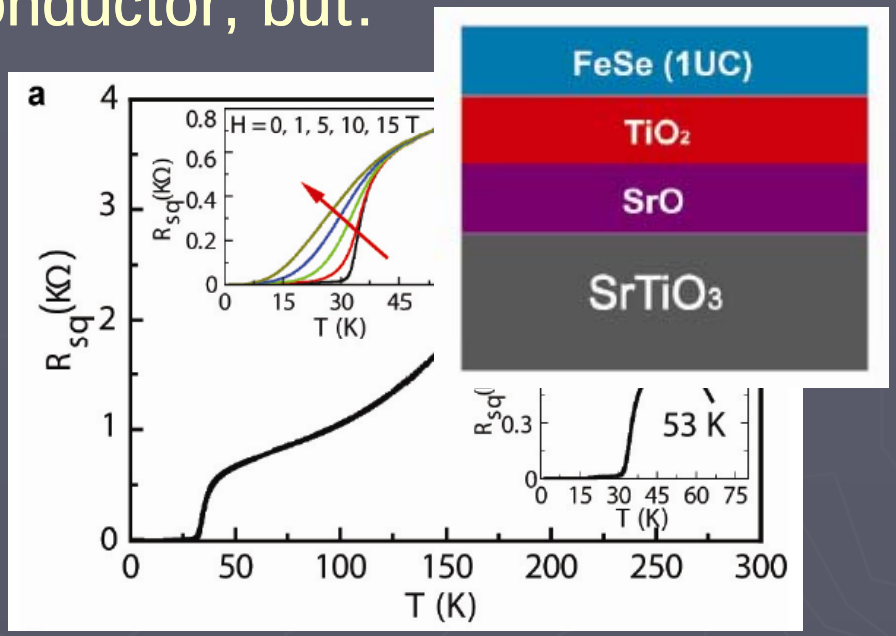


~0.3% change in a,b at T_s in Ba-122

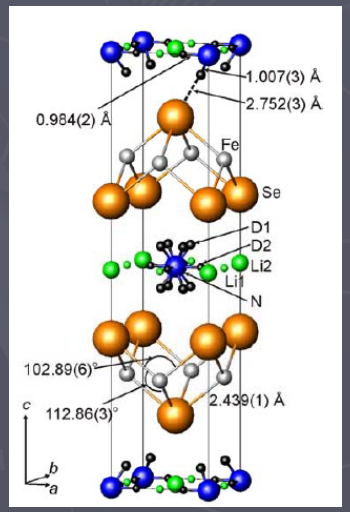
FeSe: nonmagnetic 8K superconductor, but:

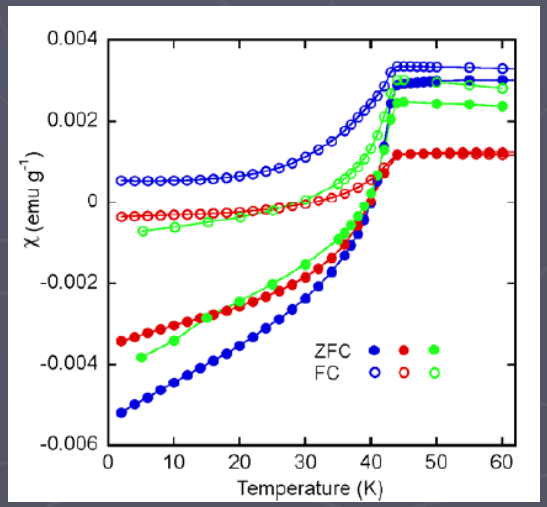


Medvedev et al 2010: Tc→37K under pressure



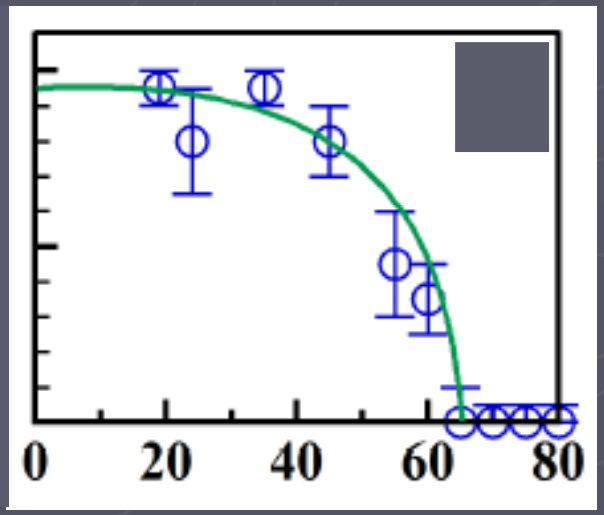
Wang et al. Chin. Phys. Lett. 2012
1 layer Tc→35K under tensile strain





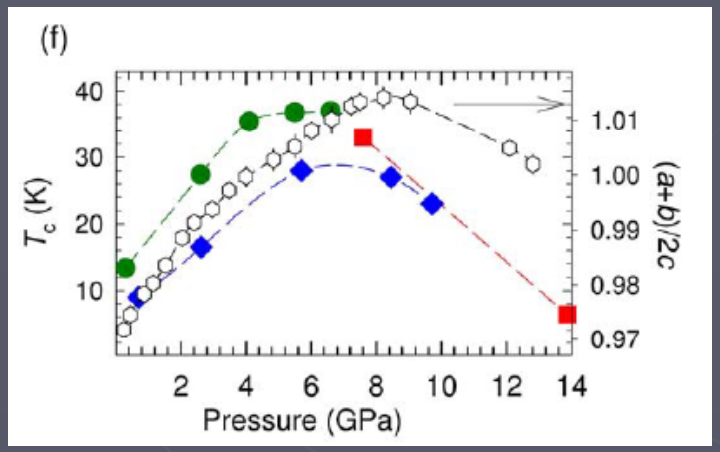
Burrard-Lucas et al 2012
Tc→43K molecular intercalation

ARPES gap

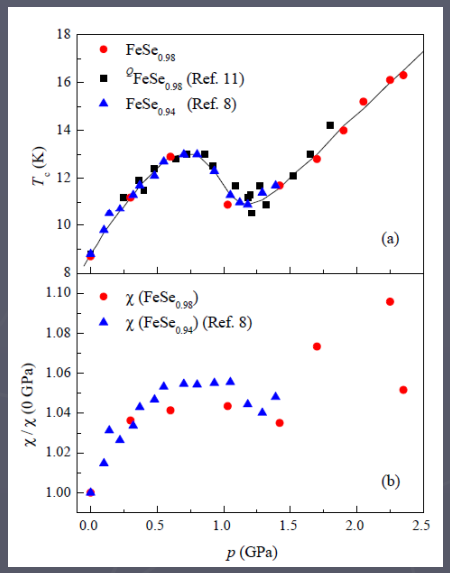


S. He et al aXv::1207.6823

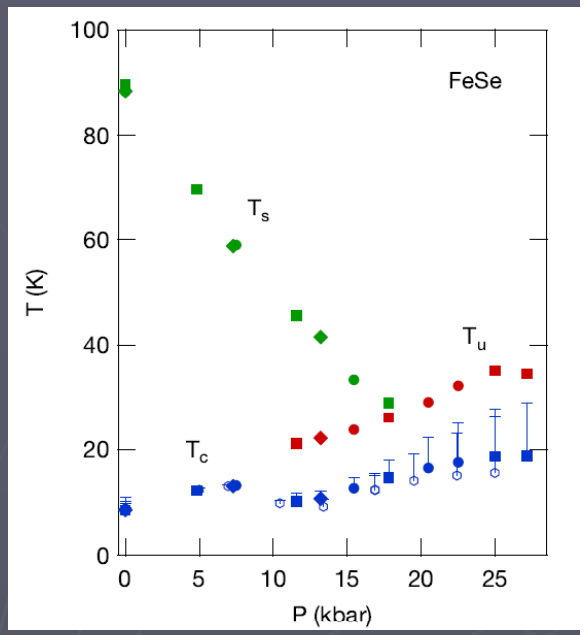
Phase diagram of bulk FeSe (pressure)
NB: no long range magnetic order at ambient P



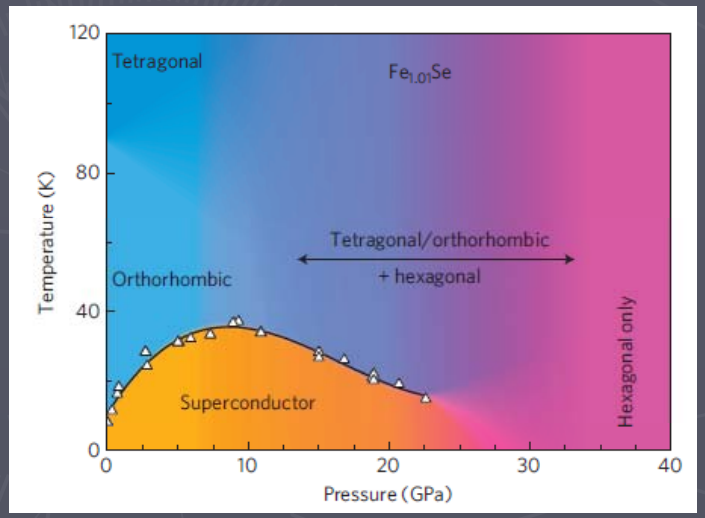
Margadona et al 2010



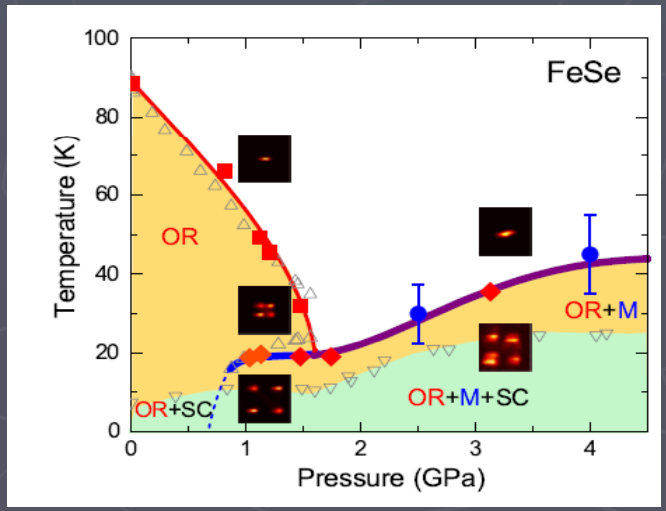
Bendele et al 2012:
magnetic state at low P



Terashima et al JPSJ 2015



Medvedev et al 2010

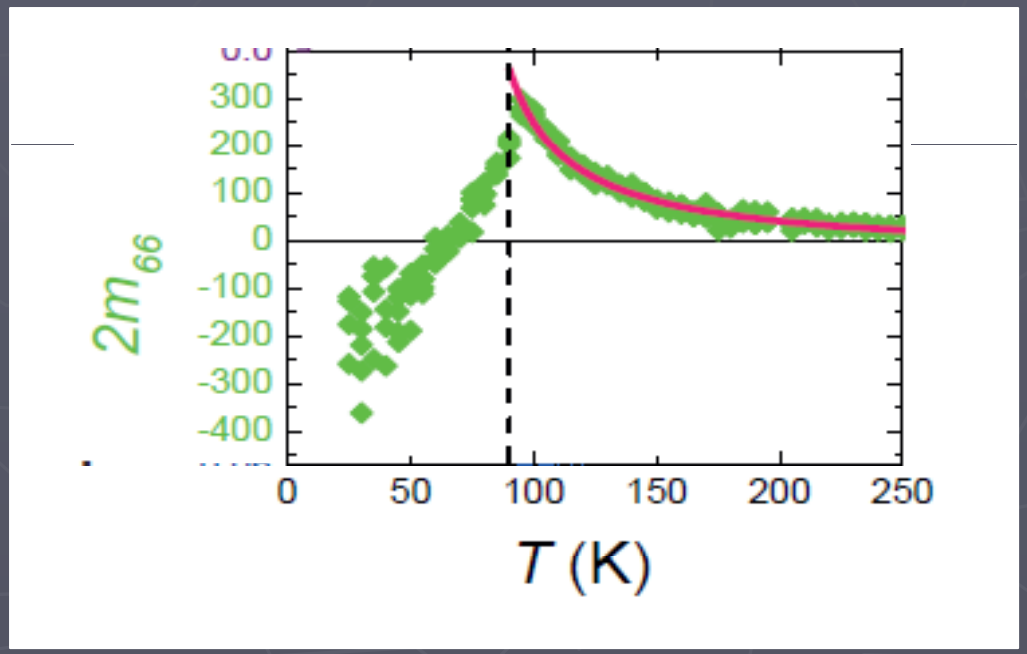


magnetism is stripelike

K. Kothapalli et al. arXiv:1603.04135

Signatures of electronic nematicity in FeSe
I. transport

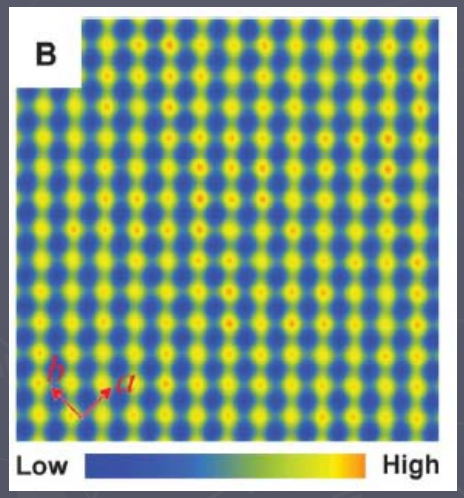
magnetoelastic coefficent



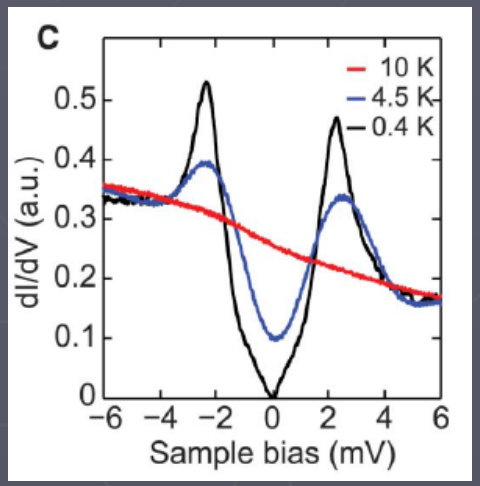
Watson et al. PRB 2015

Signatures of electronic nematicity in FeSe
II. STM in SC state

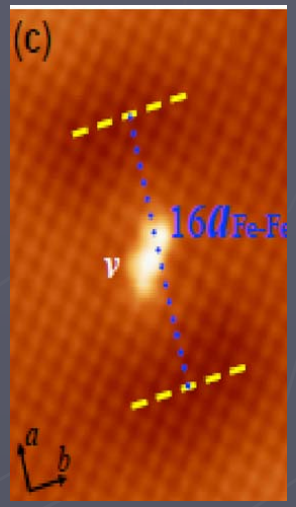
CL Song et al, Science 2011, PRL 2012



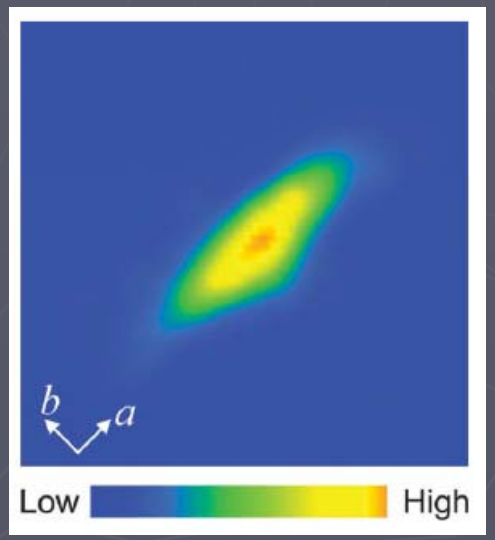
topography



spectrum



defect



vortex

gap nodes or deep minima!

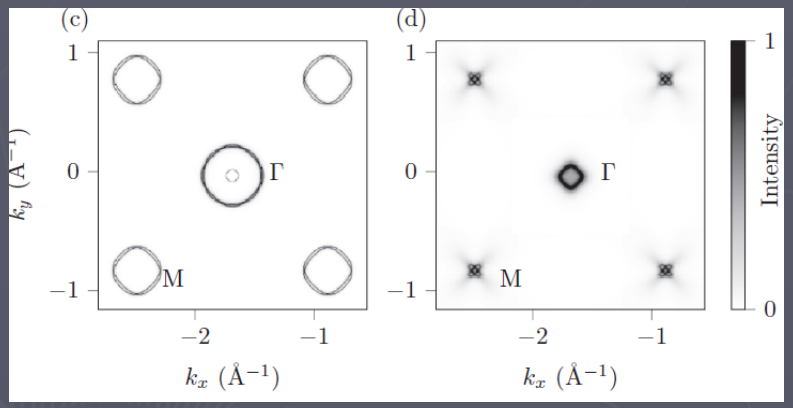
a and b are only ~0.1% different! But strong C_4 symmetry breaking in SC state.

Signatures of electronic nematicity in FeSe
III. ARPES: orbital ordering

strong band renormalization

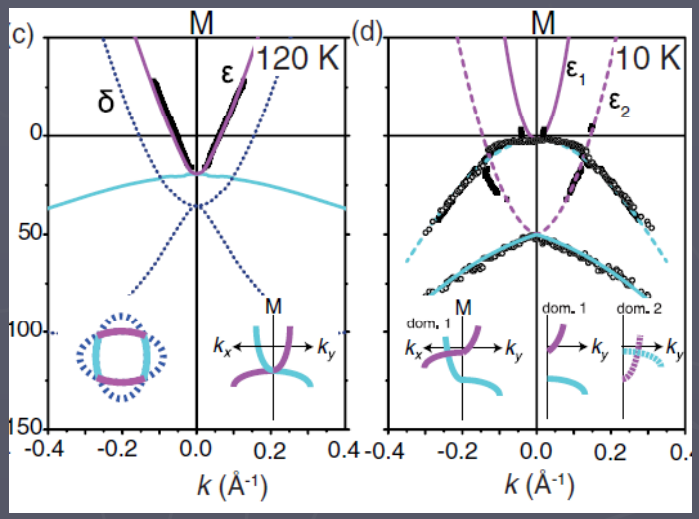
DFT

Measured



Maletz, et al. PRB 89, 220506 (2014)

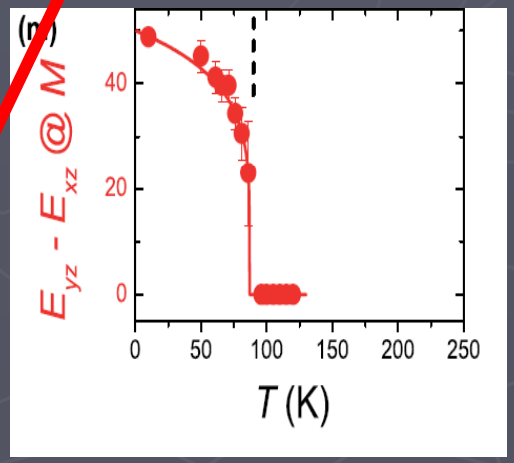
Watson et al., PRB 91, 155106 (2015)

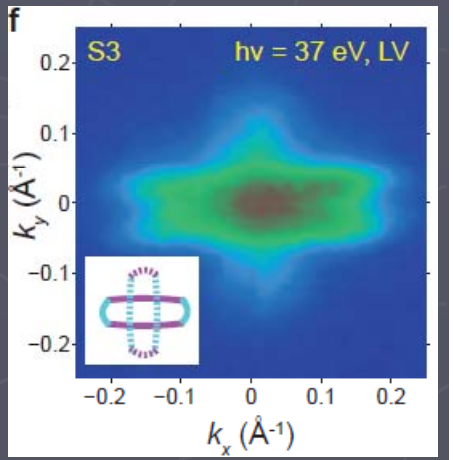


"Fermi energies" of order ~5meV
BEC/BCS crossover phenomena?

Caveat: alternate interpretations!

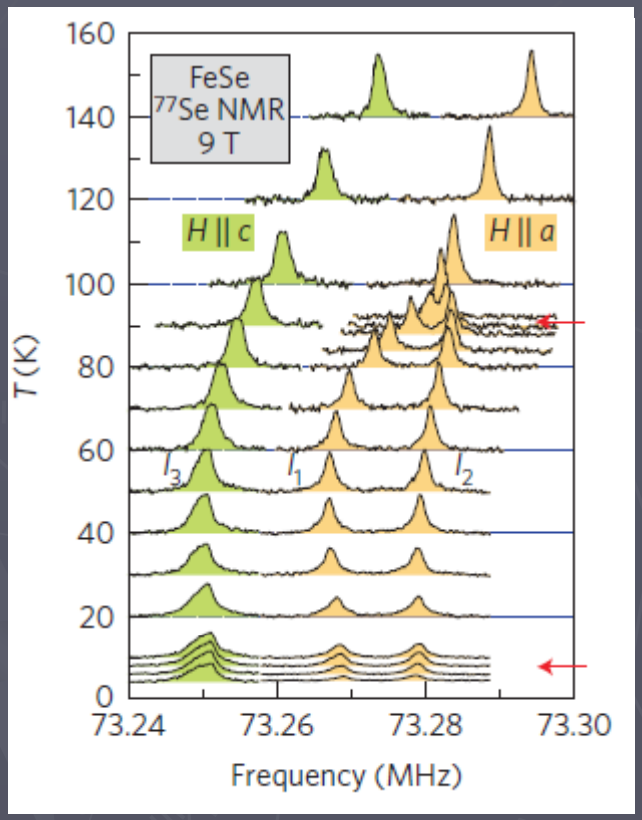
Watson et al, arXiv:1603.04545
Fanfarillo et al, arXiv:1605.02482
Fedorov et al, arXiv:1606.03022

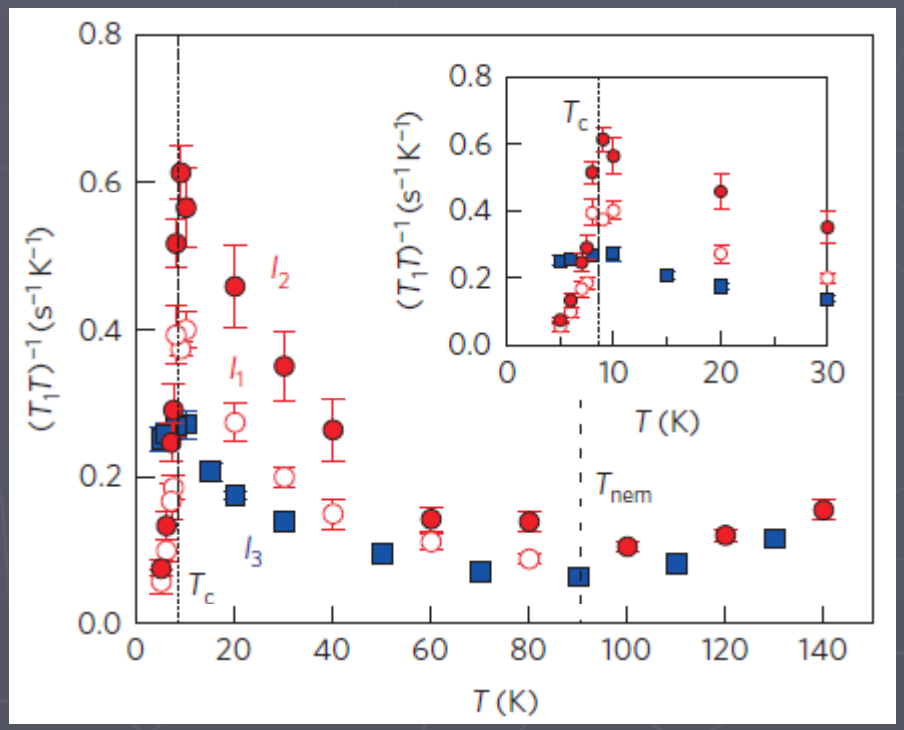




Signatures of electronic nematicity in FeSe
IV. NMR

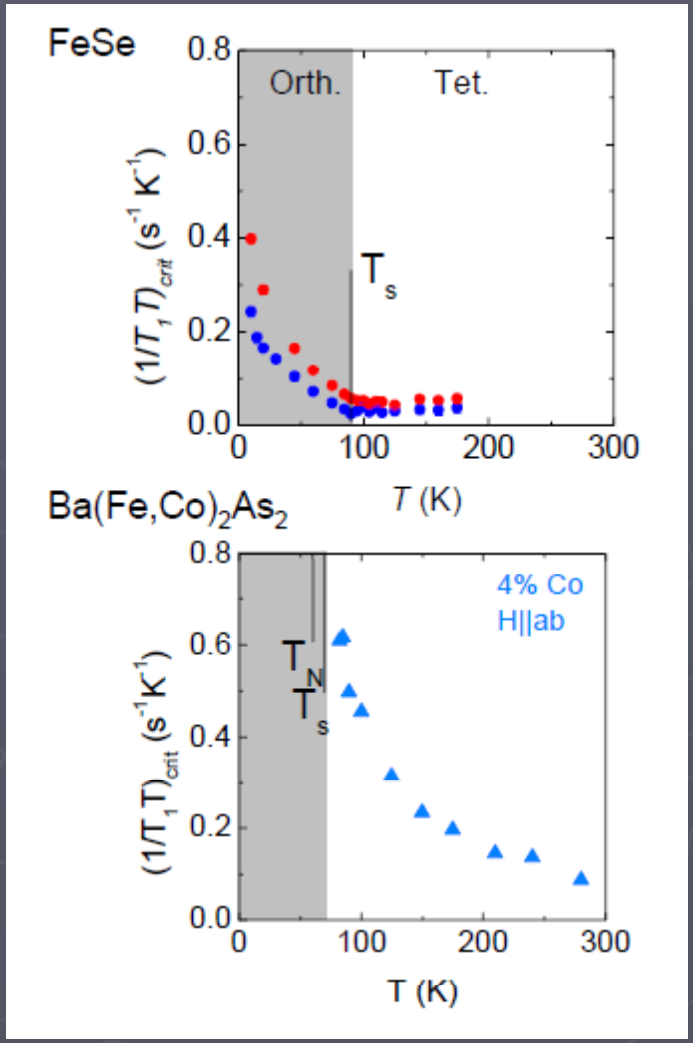
Nematic state promotes anisotropic spin fluctuations





Baek et al, Nat Comm 2014

But note difference from pnictides



FeSe Spin fluctuations seem to wait until orthorhombic transition happens

Three different types of order which break x/y symmetry

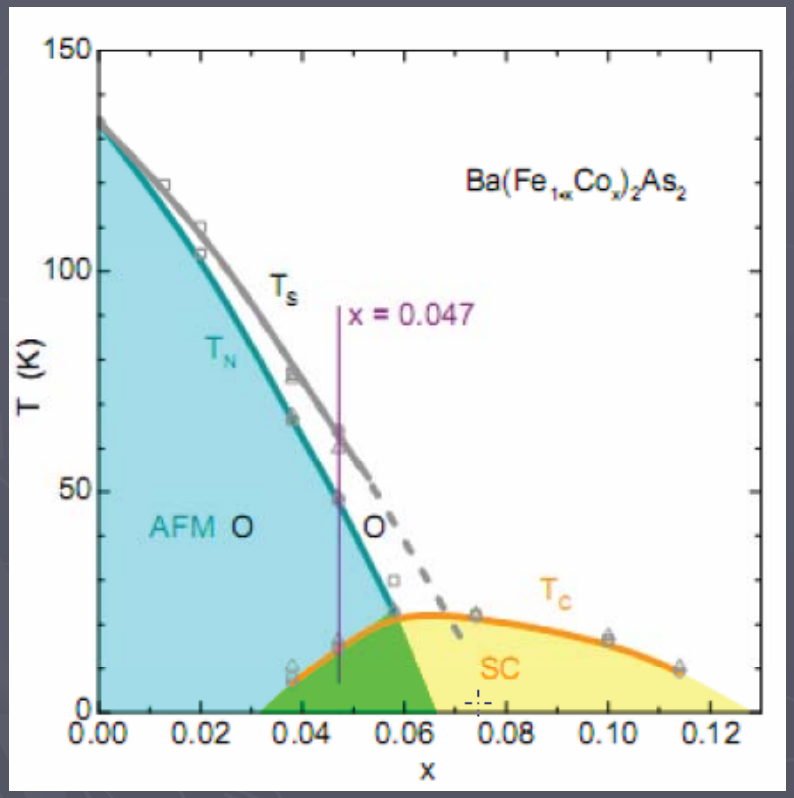
- stripe spin order (neutrons)
- structural order $a_x \neq a_y$ (X-ray diffraction)
- orbital order - dxz and dyz orbitals occupied differently (ARPES)

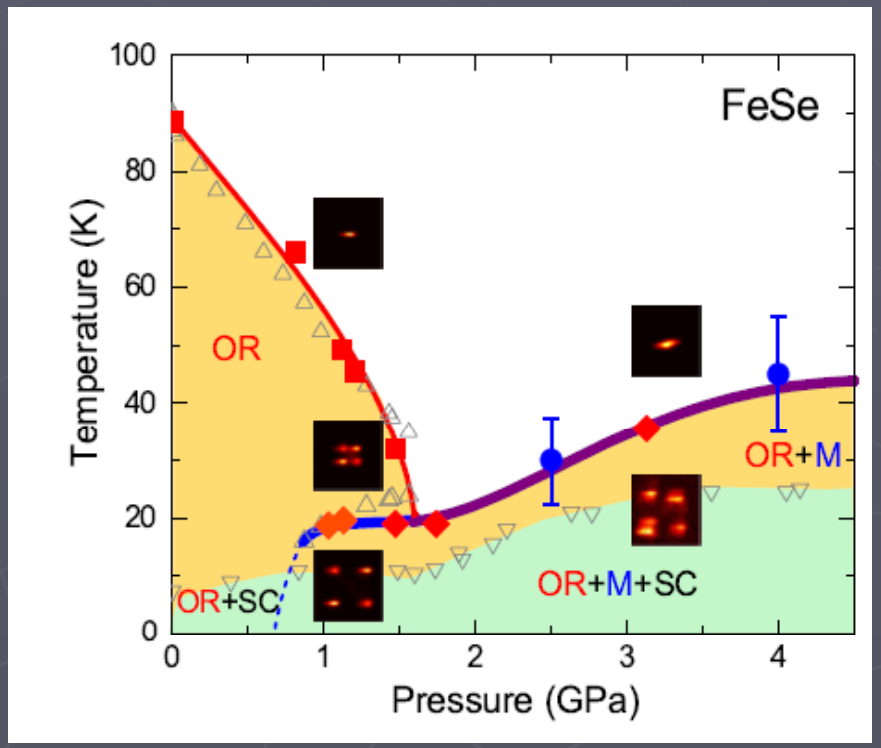
which one is the driving force?

?

Courtesy of A. Chubukov

Why is FeSe nematic, not magnetic at ambient pressure?

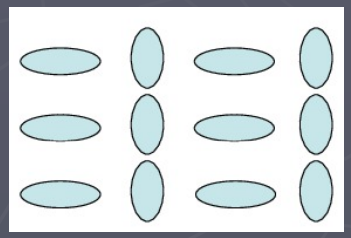




The theorists weigh in...

1) Paramagnet

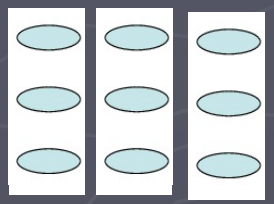
- strong competition between low-lying staggered colinear magnetic states
  J. Glasbrenner et al Nat. Phys. 2015
- quantum fluctuations of spin-1 local moments with strongly frustrated exchange interactions
  F. Wang et al. Nat. Phys. 2015
- strong competition between magnetism and charge order due to small Fermi surface A. Chubukov et al PRB 2015



2) Hidden magnetic order

- antiferro-quadrupolar order
  R. Yu and Q. Si, PRL 2015
  W-J Hu et al, arXiv: 2016
- ferro-quadrupolar order
  Z. Wang et al, arXiv: 2016

$$Q_i^{\alpha\beta} = S_i^\alpha S_i^\beta + S_i^\beta S_i^\alpha$$



3) Orbital order induced by weak spin fluctuations

Yamakawa et al. arXiv 2015

Pragmatic approach: tb band engineering

How to model fascinating low-energy phenomena if DFT gives manifestly incorrect results?

- use electronic structure that fits experimental results from ARPES and quantum oscillations

(Watson et al 2015)

$$H = H_{\mathrm{TB}} + H_{\mathrm{OO}},$$

$$H_{\mathrm{TB}} = \sum_{\mathbf{k},\mu,\nu,\sigma} t_{\mu\nu}(\mathbf{k}) c^{\dagger}_{\mu\sigma}(\mathbf{k}) c_{\nu\sigma}(\mathbf{k}),$$

$$H_{\mathrm{OO}} = \Delta_s(T) \sum_{\mathbf{k}\sigma} [n_{xz\sigma}(\mathbf{k}) - n_{yz\sigma}(\mathbf{k})].$$

orbital order:
site-centered or
bond-centered

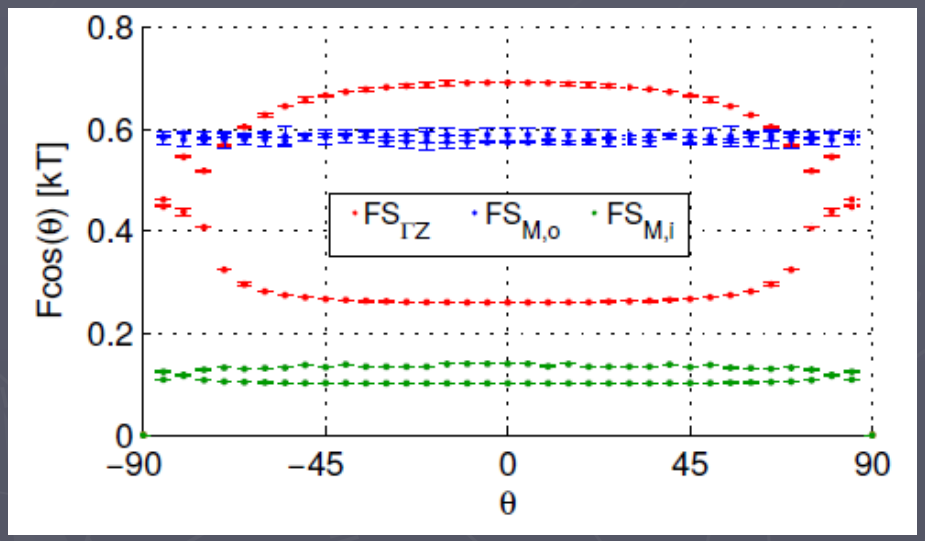
- calculate NMR response
- calculate superconducting gap

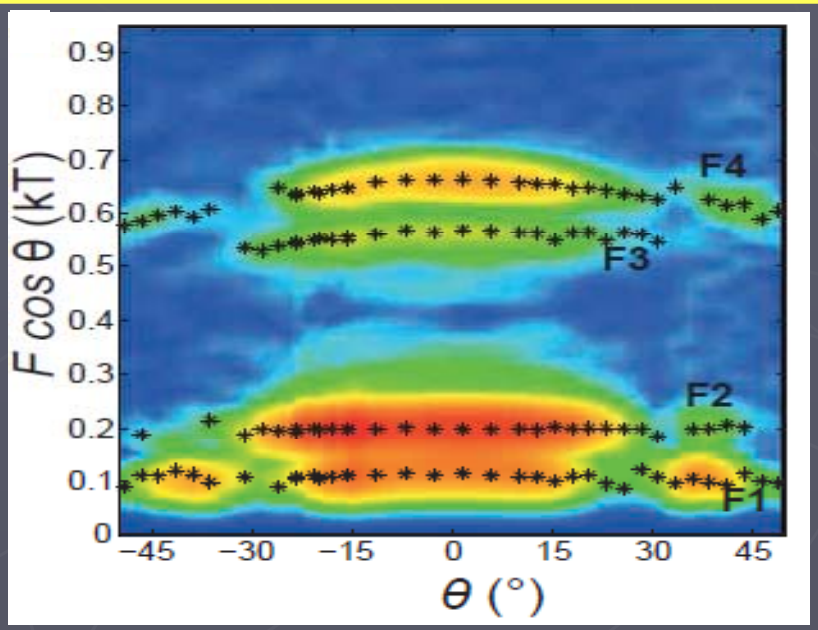
S. Mukherjee, A. Kreisel, P.J.H., B. M. Andersen, Phys. Rev. Lett. 115, 026402 (2015)

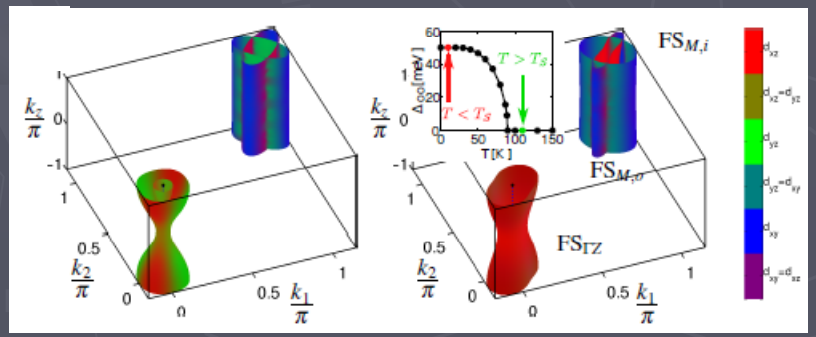
Minimal 10 orbital Tight Binding Model: Eschrig *et. al** bands + renormalization

$$H_{TB} = \sum_{\mathbf{k},\mu,\nu,\sigma} t_{\mu\nu}(\mathbf{k}) c^{\dagger}_{\mu\sigma}(\mathbf{k}) c_{\nu\sigma}(\mathbf{k}) + \Delta_{OO}(T) \sum_{\mathbf{k}\sigma} (n_{xz\sigma}(\mathbf{k}) - n_{yz\sigma}(\mathbf{k}))$$

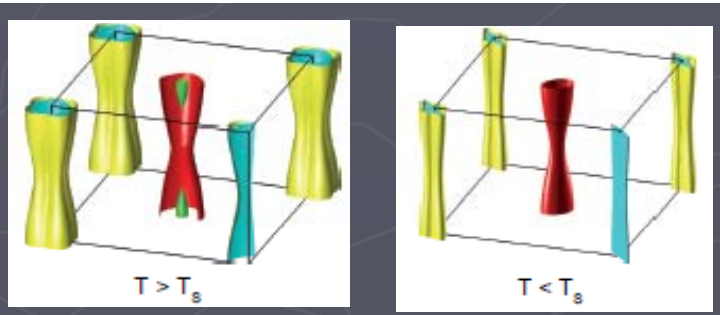
or other forms...







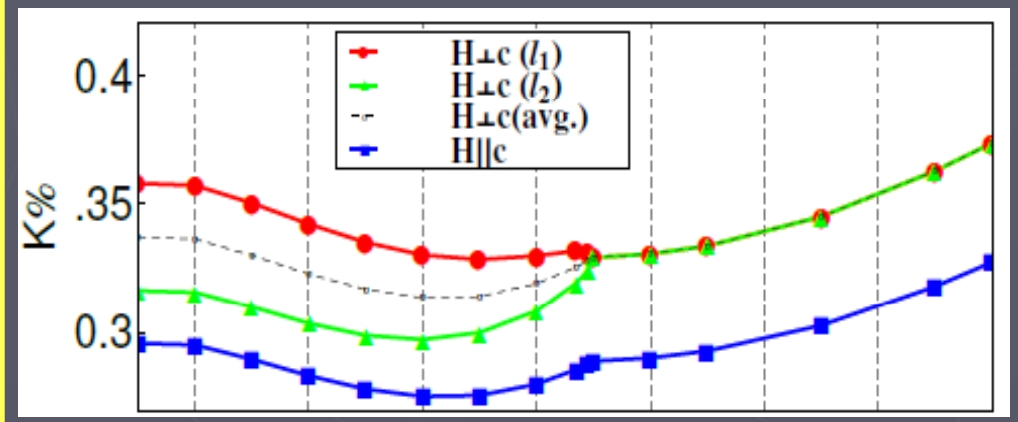
S. Mukherjee et. al, PRL 2015



Watson et. al, PRB 2015

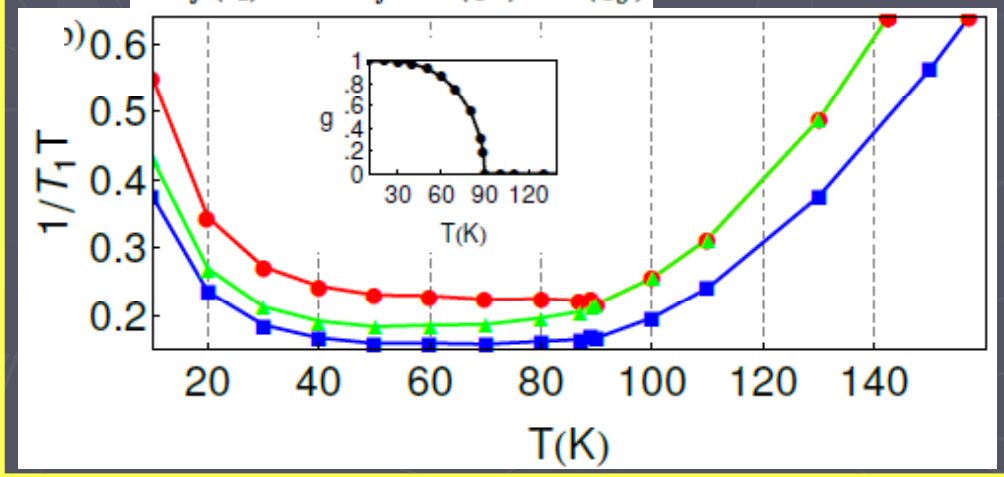
NMR: Knight Shift and Spin Lattice Relaxation Rate

$$K = A_{hf}\chi_{RPA}(\mathbf{q} = 0) + K_{\text{chem}}$$

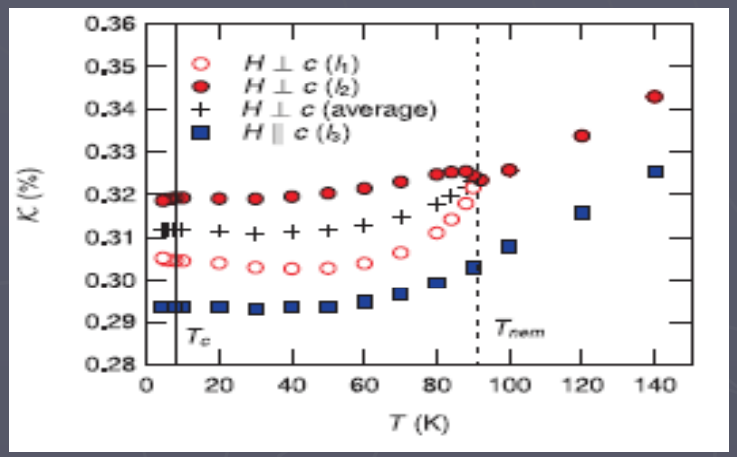


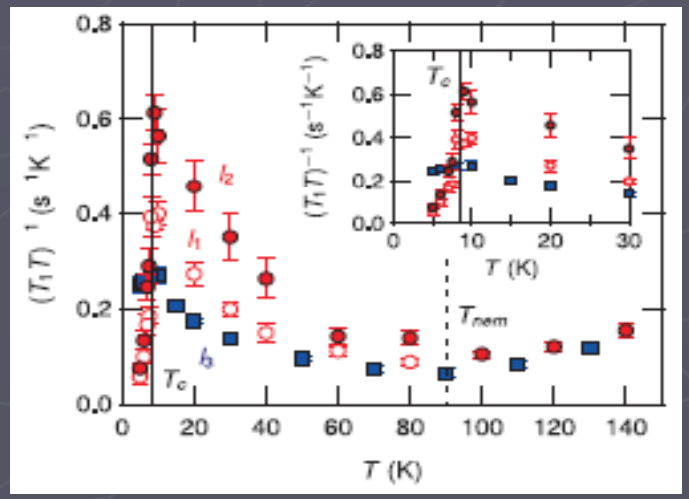
$$\frac{1}{T_1T} \propto \lim_{\omega\to 0}\sum_{\mathbf{q}} |A_{hf}(\mathbf{q})|^2 \frac{\mathrm{Im}[\chi_{RPA}(\mathbf{q},\omega)]}{\omega}$$

$$A_{hf}(\mathbf{q}) = A_{hf}\cos(q_x)\cos(q_y)$$



Baek et al. Nat. Mater. 2014

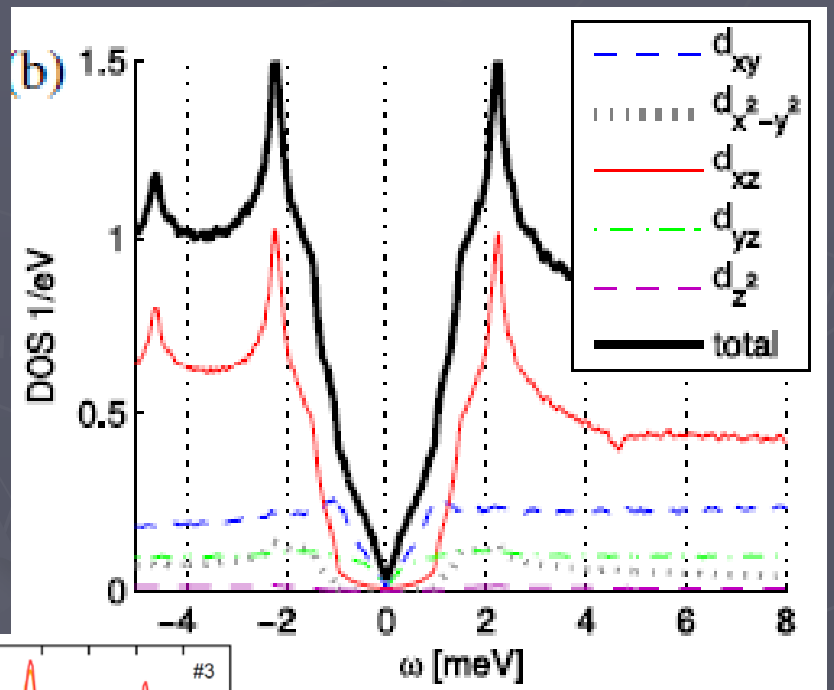


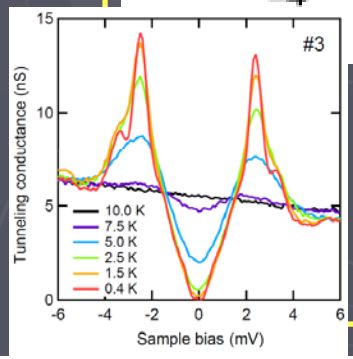


Superconducting State

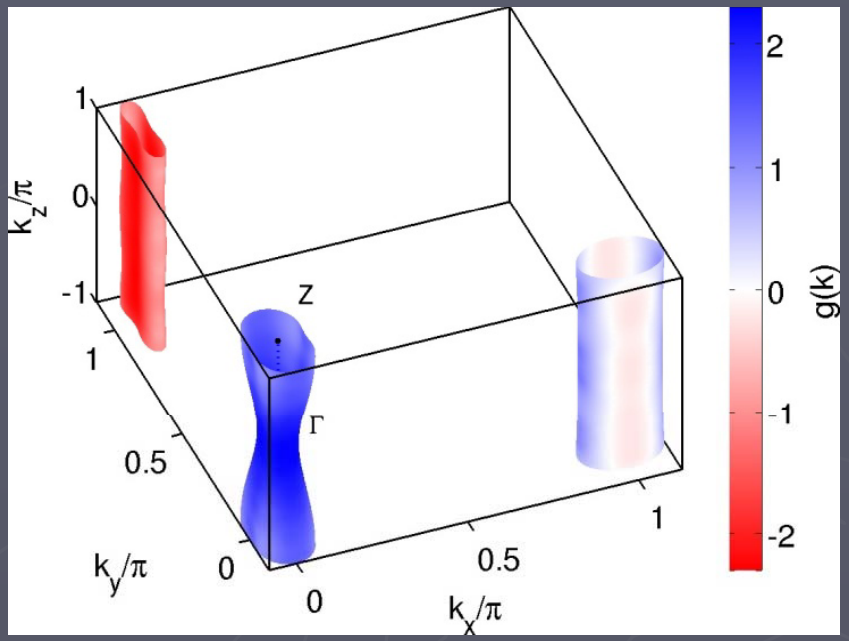
Linearized gap Equation

$$-\frac{1}{V_G}\sum_j \int_{\mathrm{FS}_j} dS'\,\Gamma(\mathbf{k},\mathbf{k}')\frac{g_\alpha(\mathbf{k}')}{|v_{\mathrm{F}j}(\mathbf{k}')|} = \lambda_\alpha g_\alpha(\mathbf{k})$$

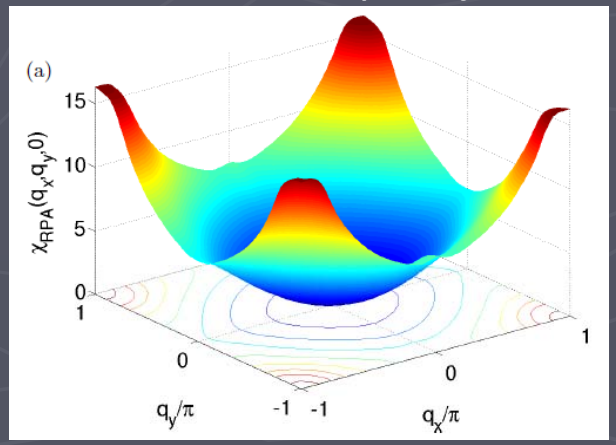




Kasahara et al. 2014



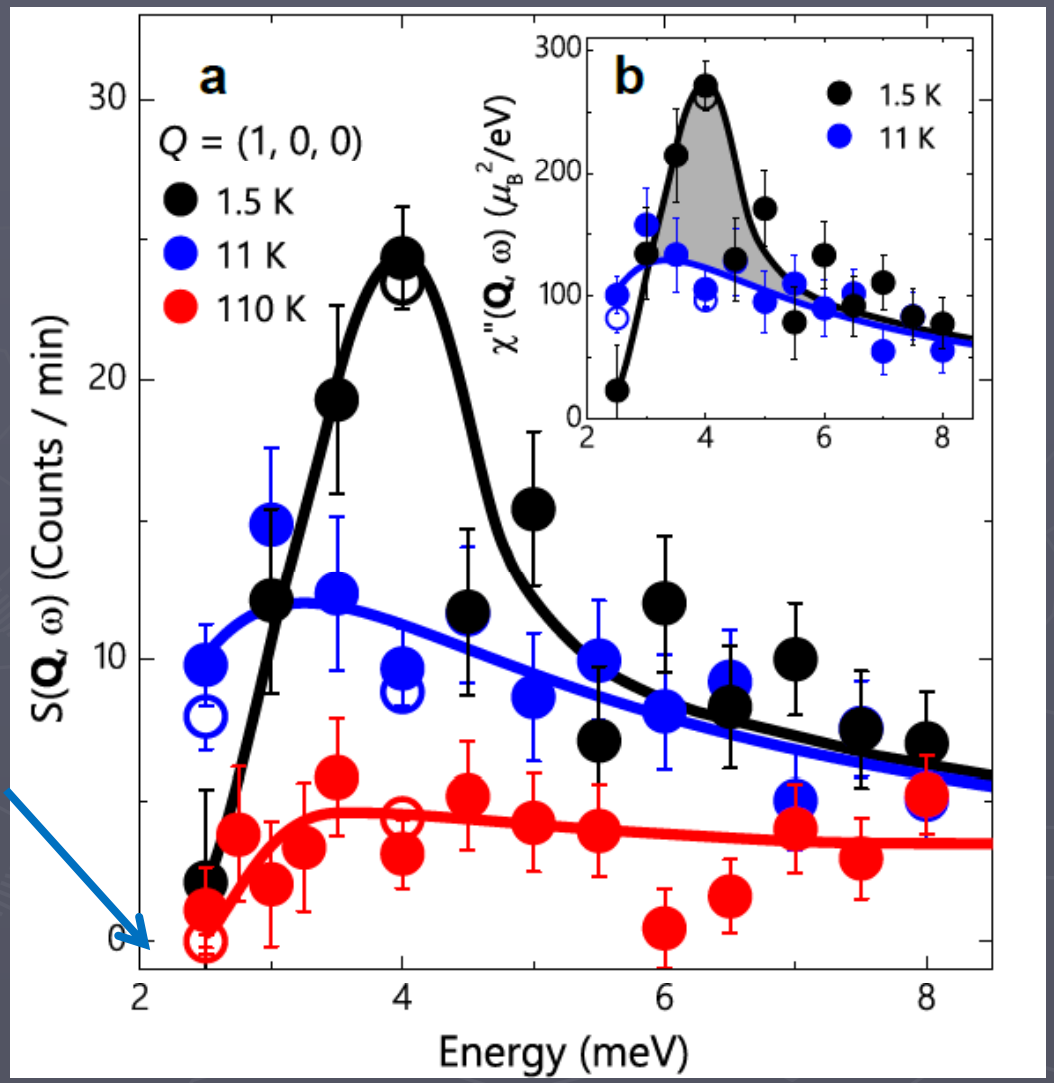
RPA Susceptibility



Note π,π peaks!

Low-T spin resonance near $\pi,0$

Wang et al Nat. Mat.15, 15 (2016)

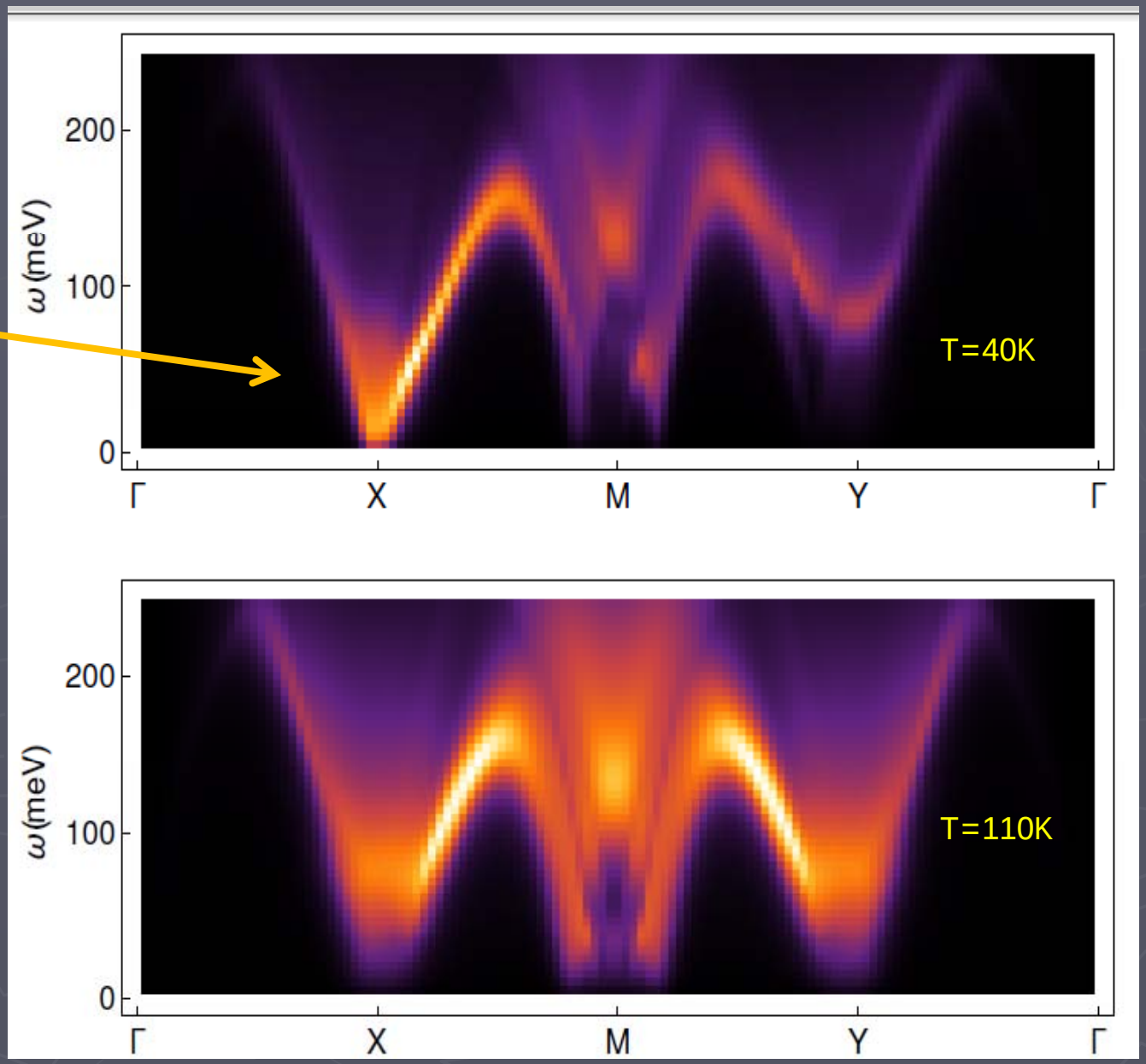


Spin gap?

Theory: spin excitations in RPA U=2.1eV J=0.25U

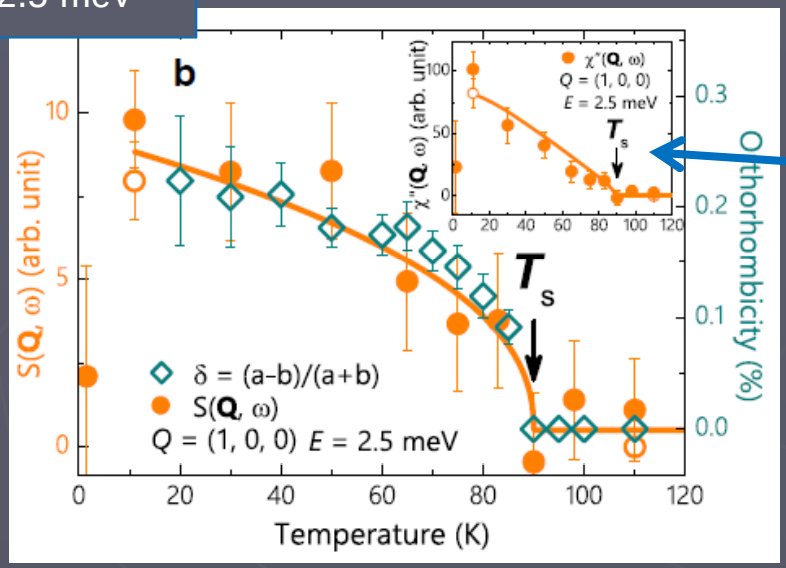
$\chi''(q,\omega)$

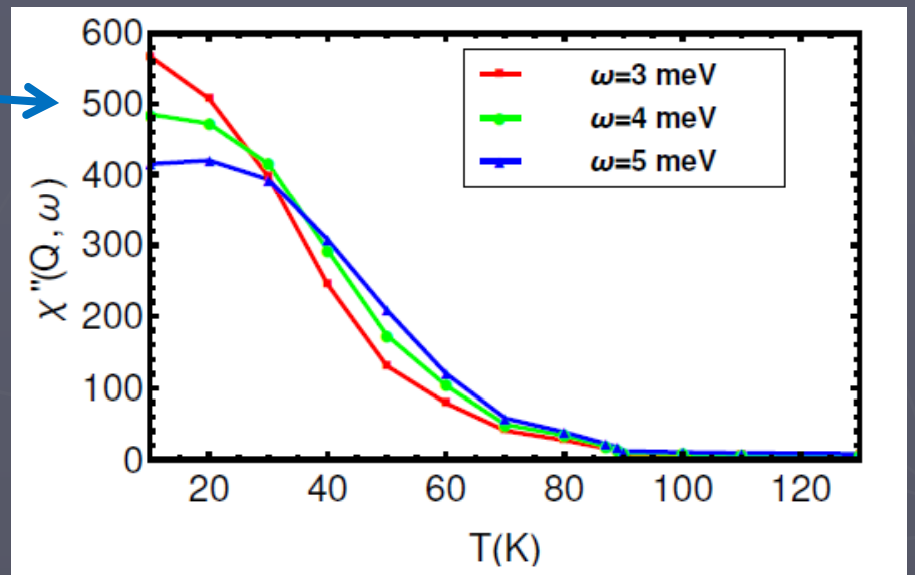
$(\pi,0)$ fluctuations moved to low ω in orb. ord. state

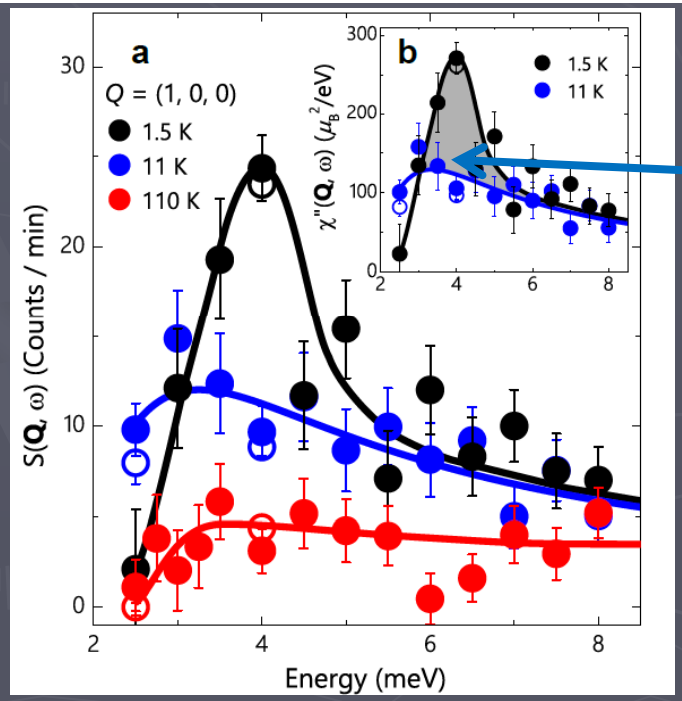


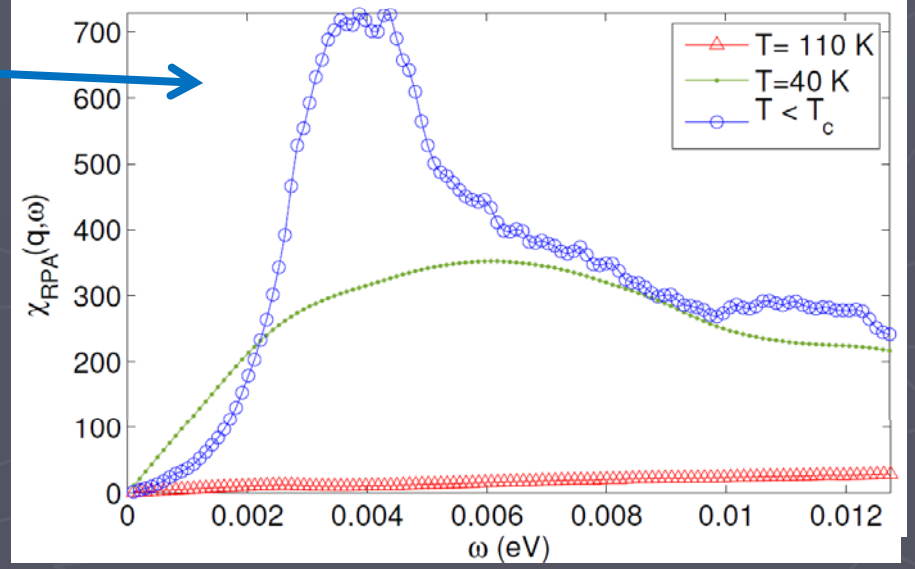
Energy and T-dependence of (π,0) fluctuations

2.5 meV

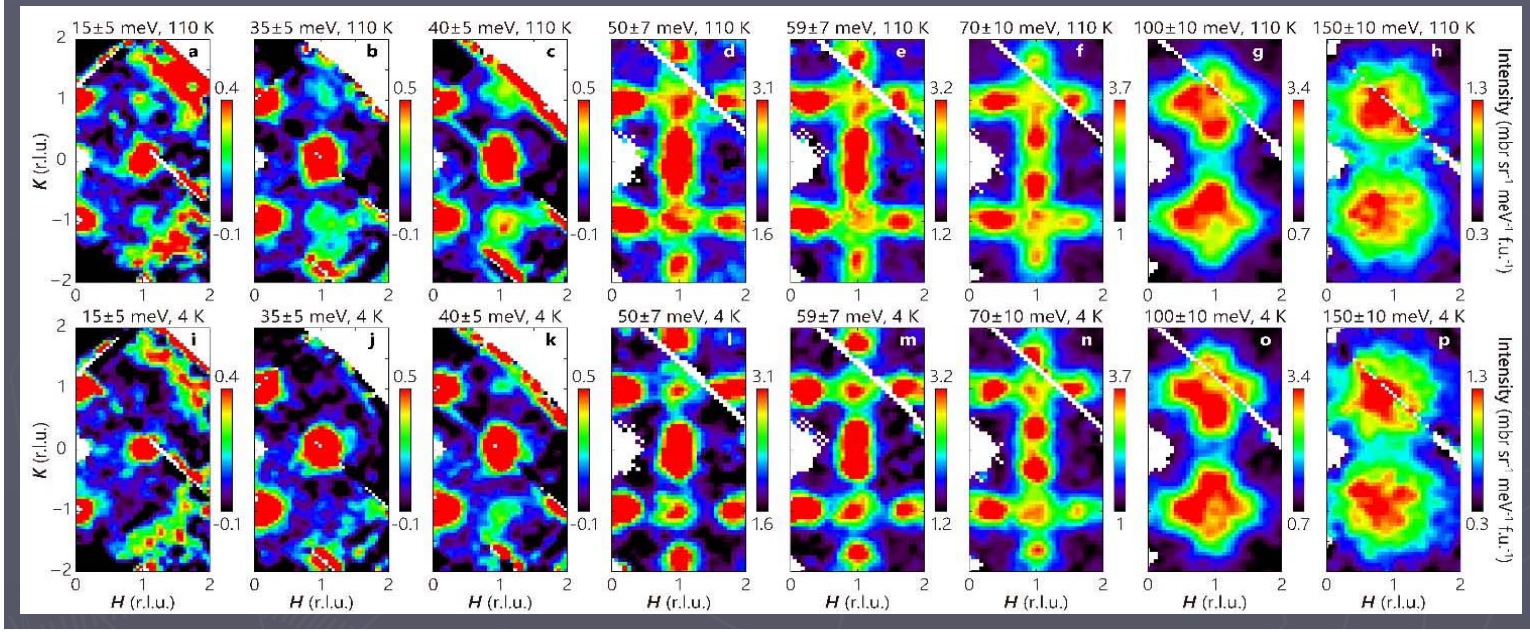




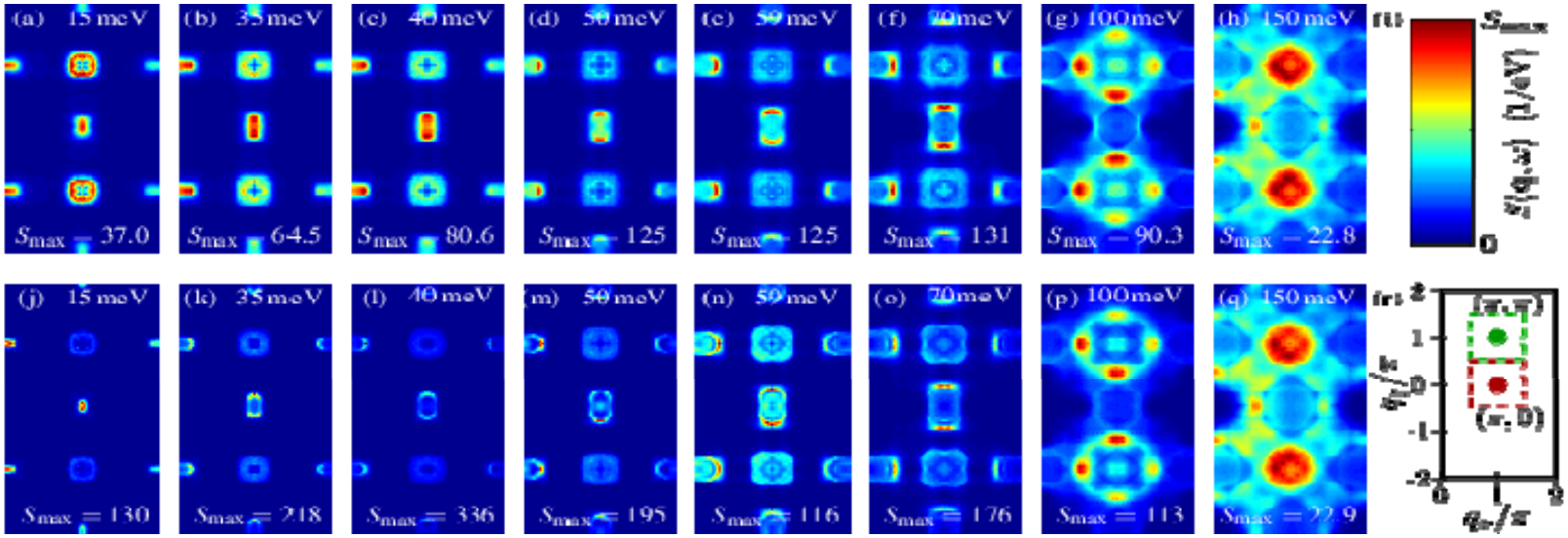




INS: detailed comparison S(q,ω)



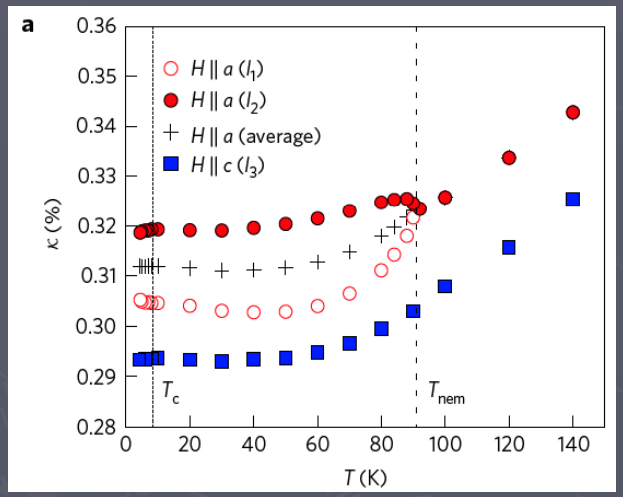
Wang et al 2016 (expt)

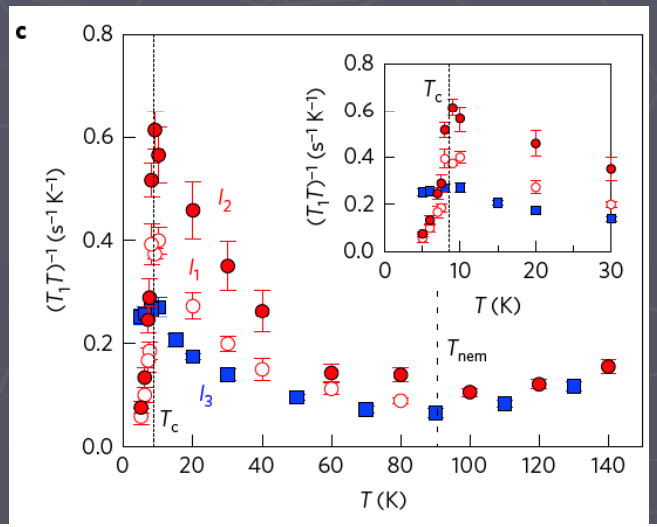


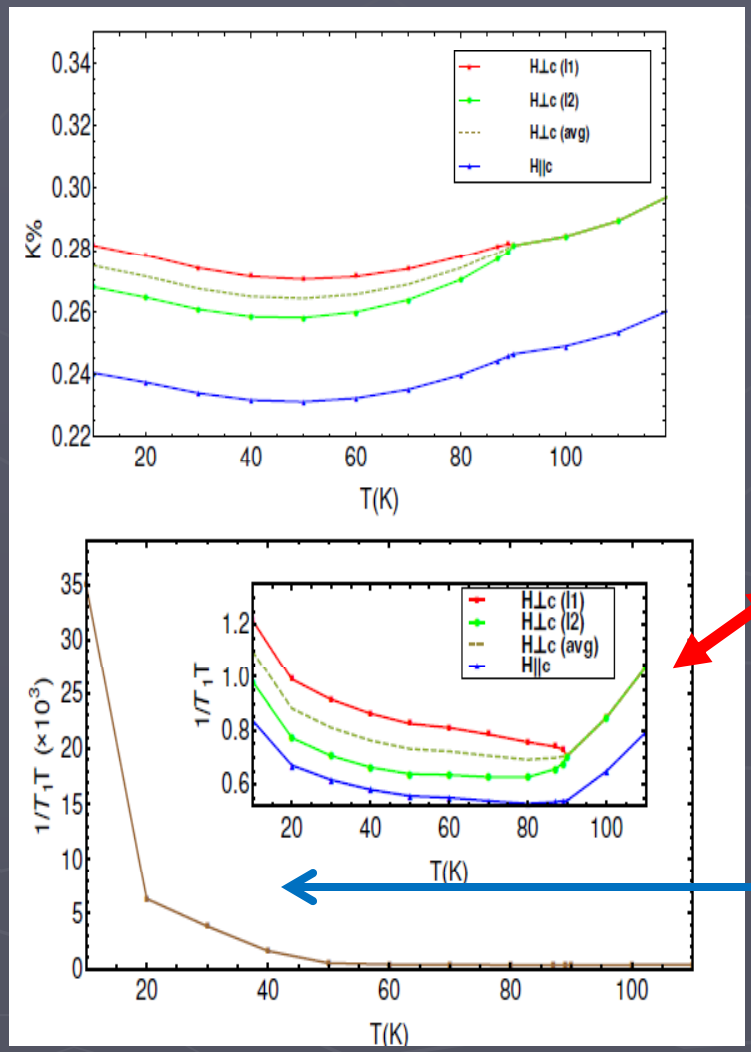
Kreisel et al 2016 (thy)

Low energy (π,0) fluctuations turning on at T_s consistent with NMR

Baek, et al. Nat. Mater. (2015)







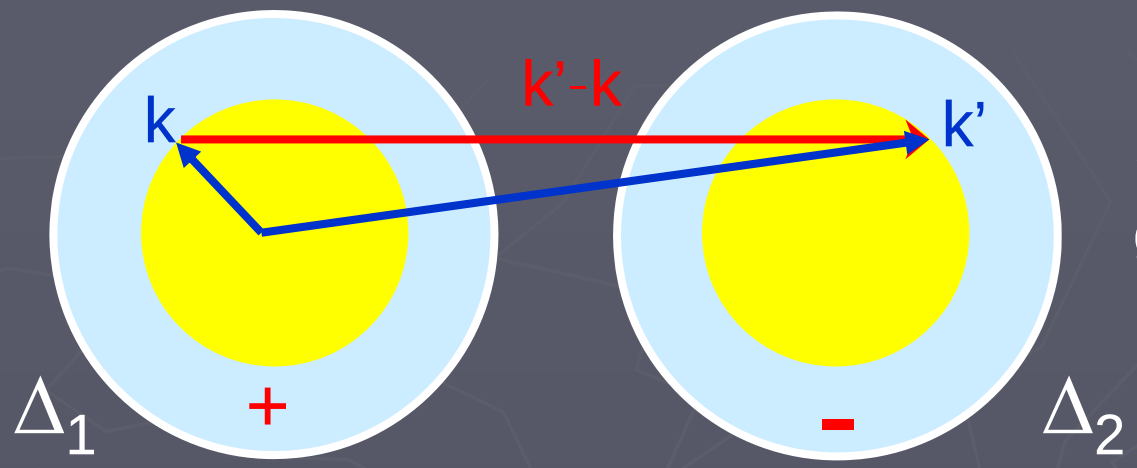
Combination of enhanced π,0 and suppressed π,π fluctuations as T→0

Without form factor

Disorder in multiband SC

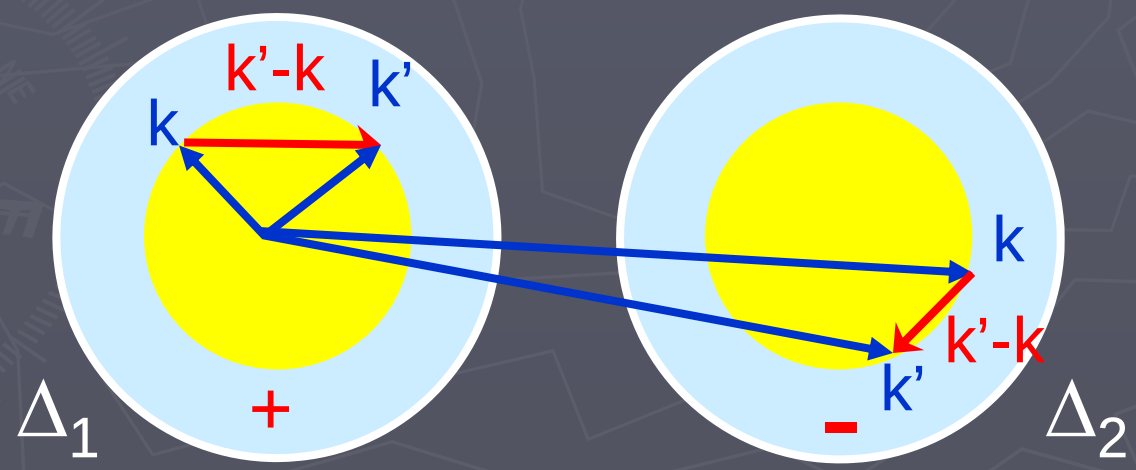
Inter- and intraband impurity scattering in 2-band $s_{+/-}$ system

Inter-



mixes + and –
gaps, breaks pairs

Intra-

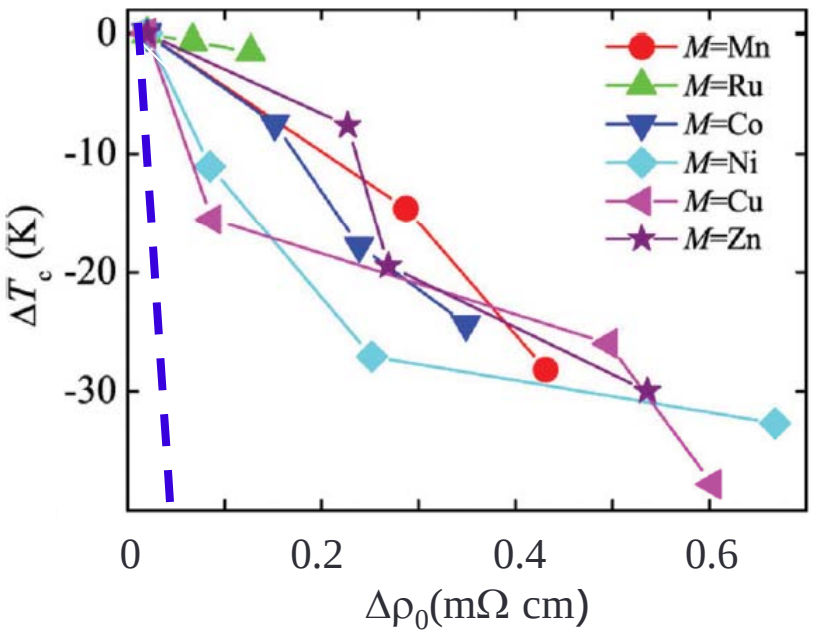


no mixing of +/-
no pairbreaking

H. Kontani, M2S 2012

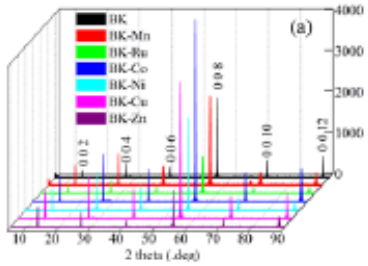
impurity effect in single crystal $(Ba,K)Fe_2As_2$

J.Li et al. PRB 85, 214509 (2012).



✓Vegard's law: good crystal

✓X-ray



other experiments:

1111 systems: Sato et al, JPSJ('08)
Ba122: Paglione et al, arXiv('12)
irradiation: Nakajima et al, PRB ('10)

Experiment:
T_c vanishes when
$\rho_{imp} > 500\mu\Omega cm$
$[l_{imp} \sim 3\,Å]$

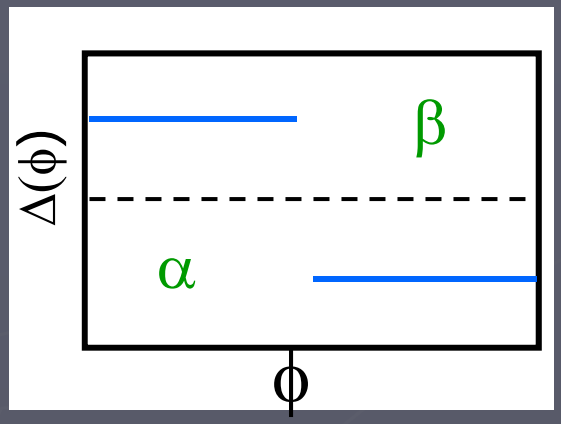
⇔

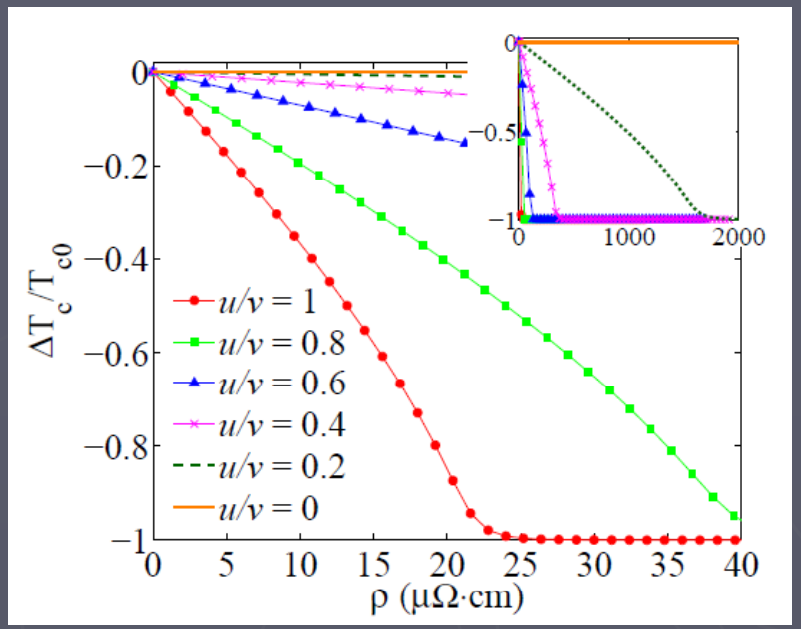
Theory:
$S\pm$ wave state
disappears when
$\rho_{imp} = 20\sim40\mu\Omega cm$

local impurity
on Fe-sites

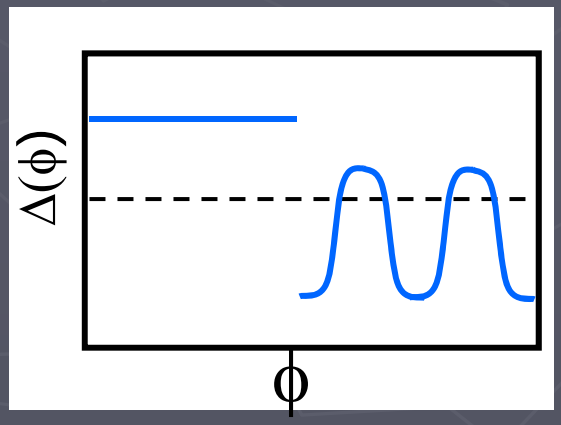
Theory (t-matrix)

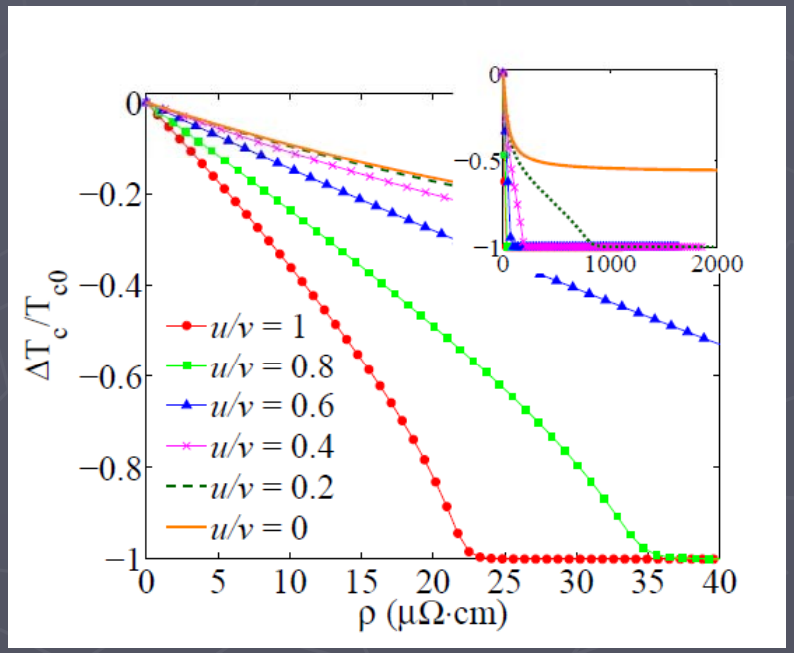
Wang et al PRB 2012





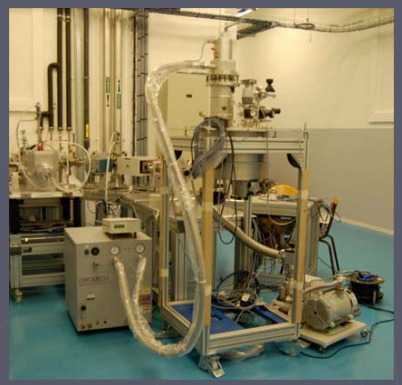
u = inter band impurity potential
v =intra band impurity potential





Critical $\Delta\rho_0$'s range from 20μΩ–cm to mΩ-cm!

Electron irradiation at LSI (Irradiated Solids Lab)--Paris

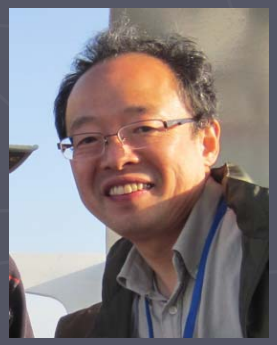


Pelletron
Facility
At LSI

http://emir.in2p3.fr/LSI

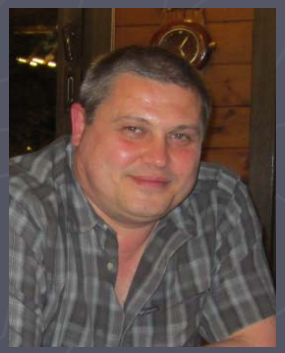
http://www.lsi.polytechnique.fr/accueil/equipements/accelerateur-sirius/

Shibauchi



Matsuda

Rullier-Albenque



Prozorov

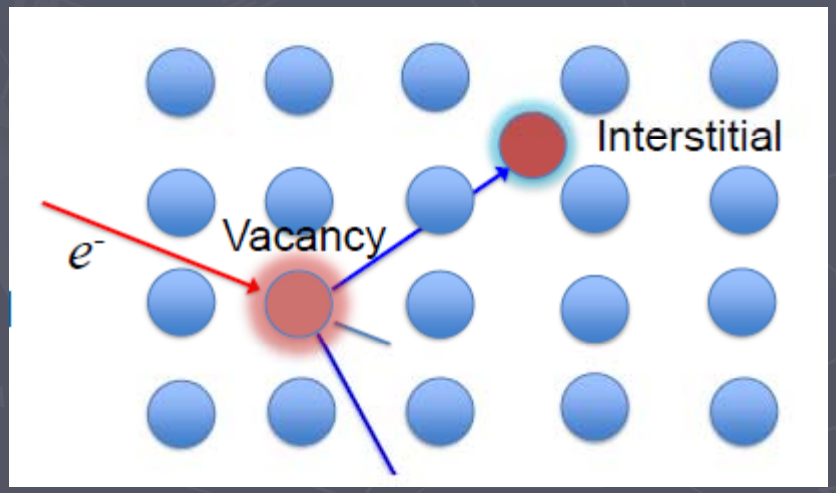
also: K. van der Beek, M. Konczykowski

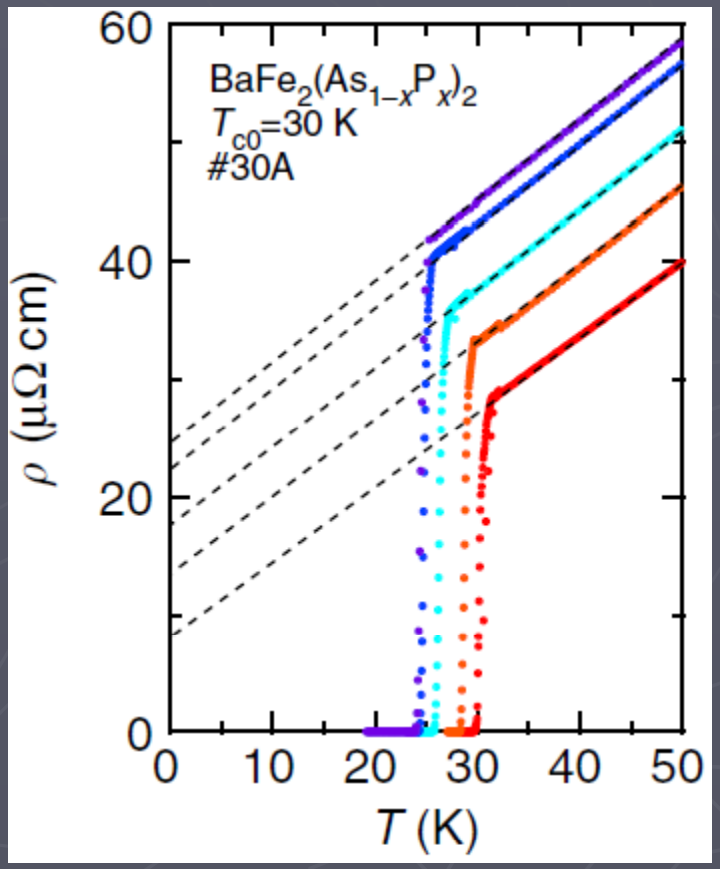
Thanks: K. van der Beek

Low-E e^- irradiation produces pt.-like defects (Frenkel pairs)

Advantages of e- irradiation

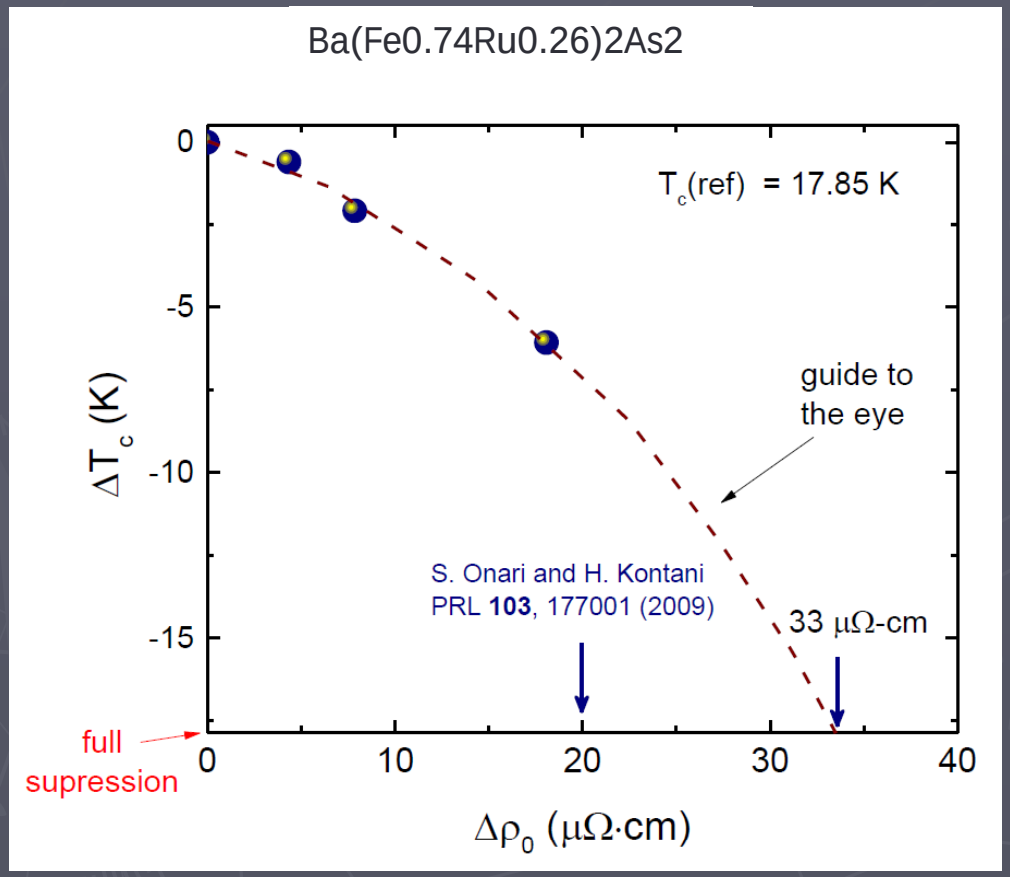
- In metals, no change of carrier density
- Homogeneous point defects can be introduced
- Defects can be added on the same sample

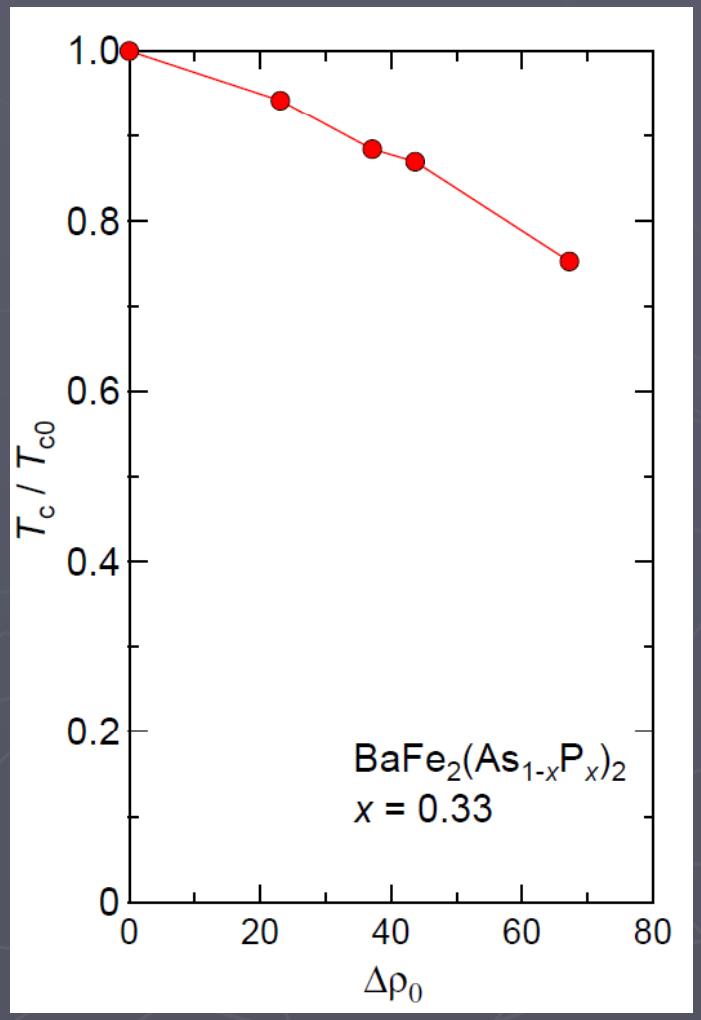




Y. Mizukami et al., Nat. Comm 2014

e- irradiation expts in Fe-pnictides: “fast” T_c suppression – evidence for $s_{+/-}$ pairing

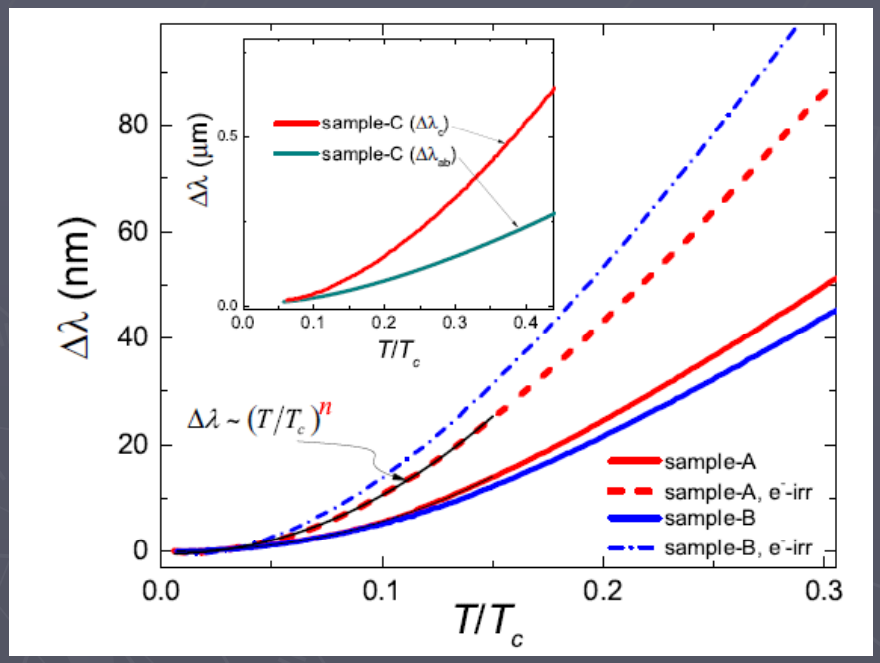


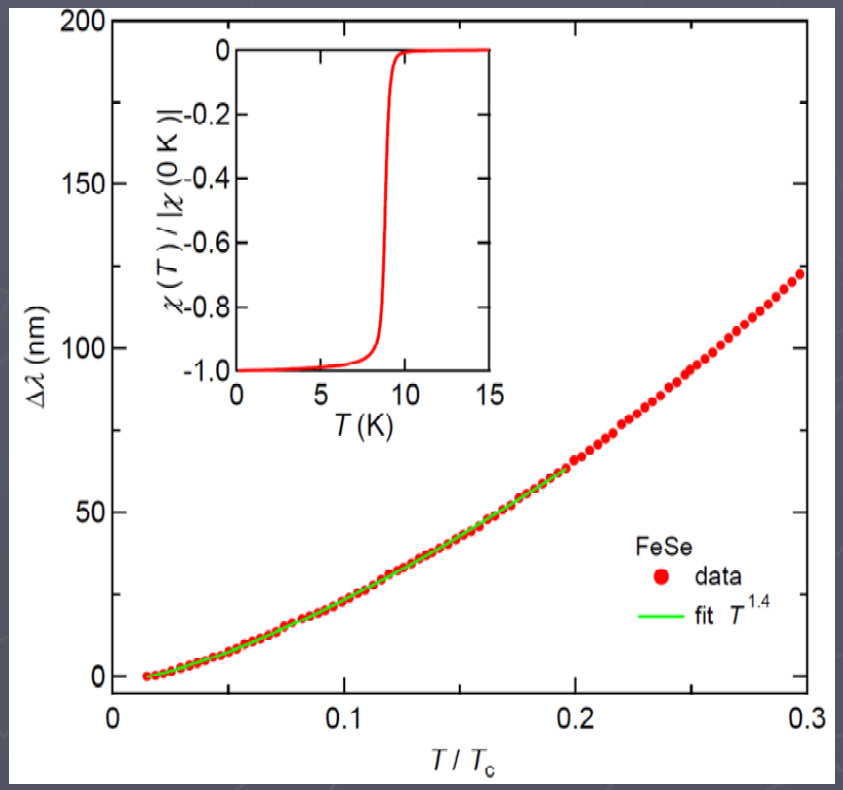


Prozorov expt.

T_c and penetration depth measurements on FeSe, + e^- irradiation

Part 1: observation of a small gap





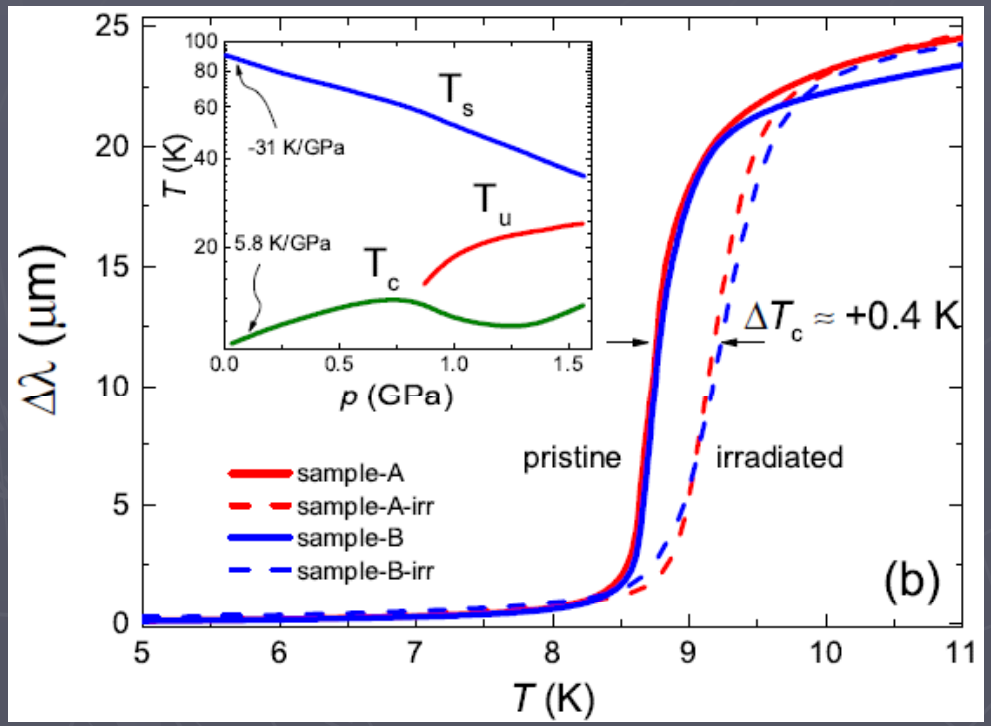
S.Teknowijoyo et al, arXiv:1605.04170 Compare Kasahara et al. 2014

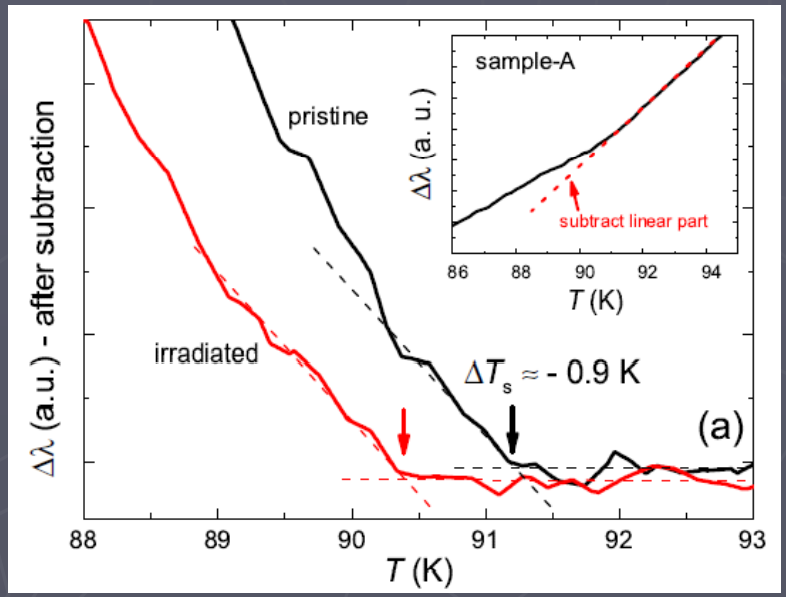
Other recent reports of small gaps: Bourgeois-Hope 2016, Li et al 2016, Jiao et al 2016

Prozorov expt.

Part 2: enhancement of T_c by disorder

S.Teknowijoyo et al, arXiv:1605.04170





e^- disorder increases T_c

e^- disorder decreases T_s

Explanations? $T_s\downarrow$, $T_c\uparrow$

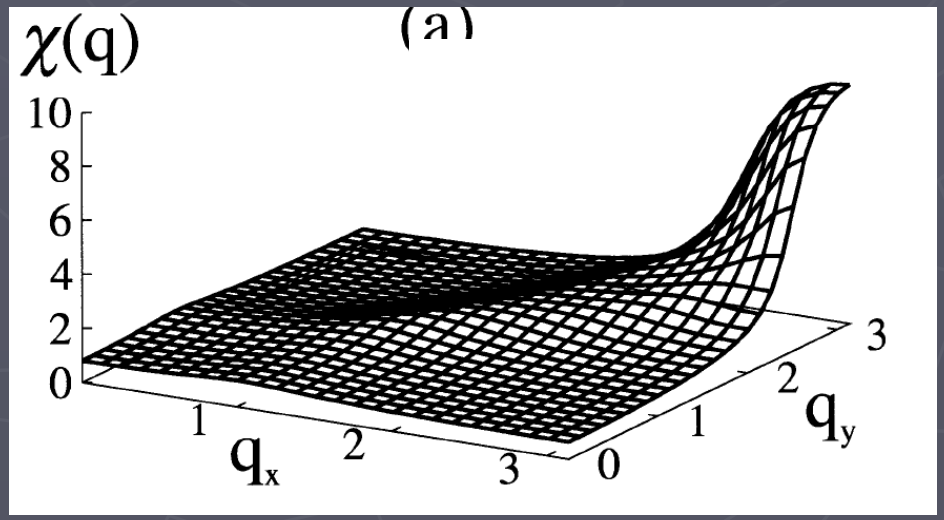
- Pairbreaking effect must be minimal to allow alternate, pair enhancing mechanism to win: s_{++} state? ✗ Mostly small-q scattering? ✓
- Chemical pressure? ✗ Irradiation *expands* lattice, + effect 10x too small
- Impurities may favor one type of spin order, break Glasbrenner et al – style degeneracy ?
- Impurities can enhance pair interaction locally ?
- Impurities can favor SC *competing* with nematic order ?

Local pair strengthening near impurity I

What will happen in a *correlated* gas
when a *nonmagnetic* impurity is inserted?

Simplest approach: describe
background correlations with RPA

$$\chi = \frac{\chi_0(T)}{1 - U\chi_0(T)}$$



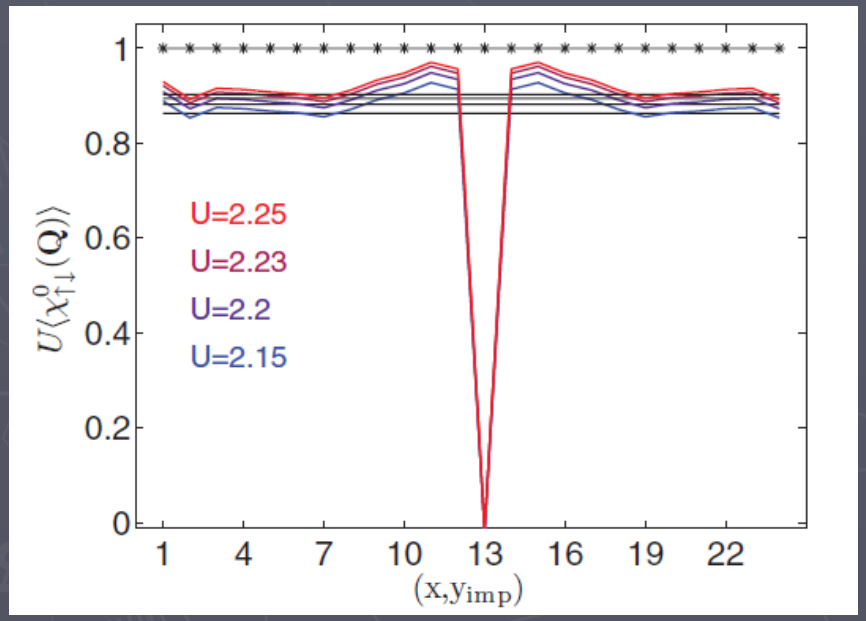
Idea (Nunner et al 2005): impurities can enhance *pairing interaction* locally by nearly freezing π,π spin fluctuations

RPA for general system:

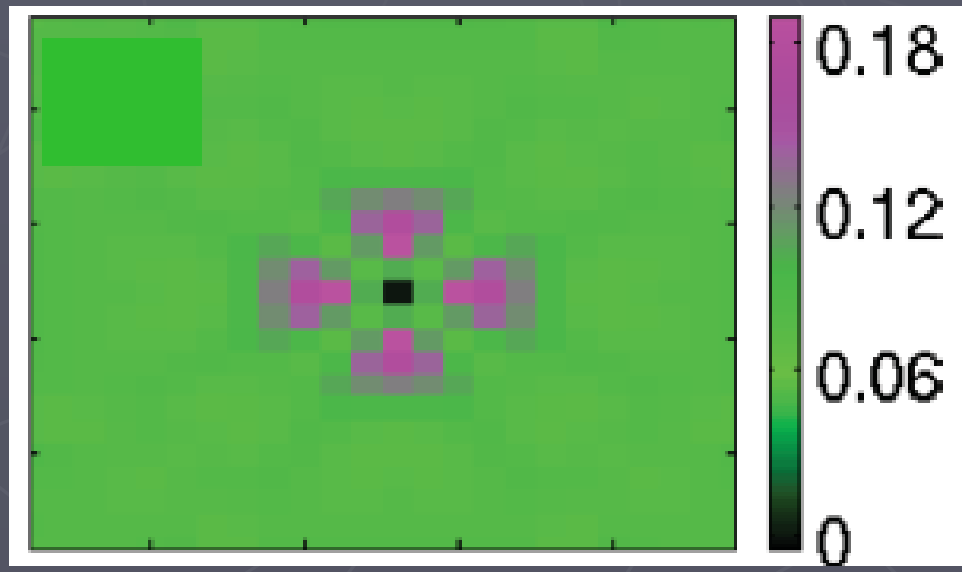
$$\chi(\mathbf{r},\mathbf{r}') = \chi_0(\mathbf{r},\mathbf{r}') + U\sum_{\mathbf{r}''}\chi_0(\mathbf{r},\mathbf{r}'')\chi(\mathbf{r}'',\mathbf{r}')$$

Impurity: Fourier transform: $\chi(\mathbf{q},\mathbf{r}_i)$

Proximity to Stoner criterion



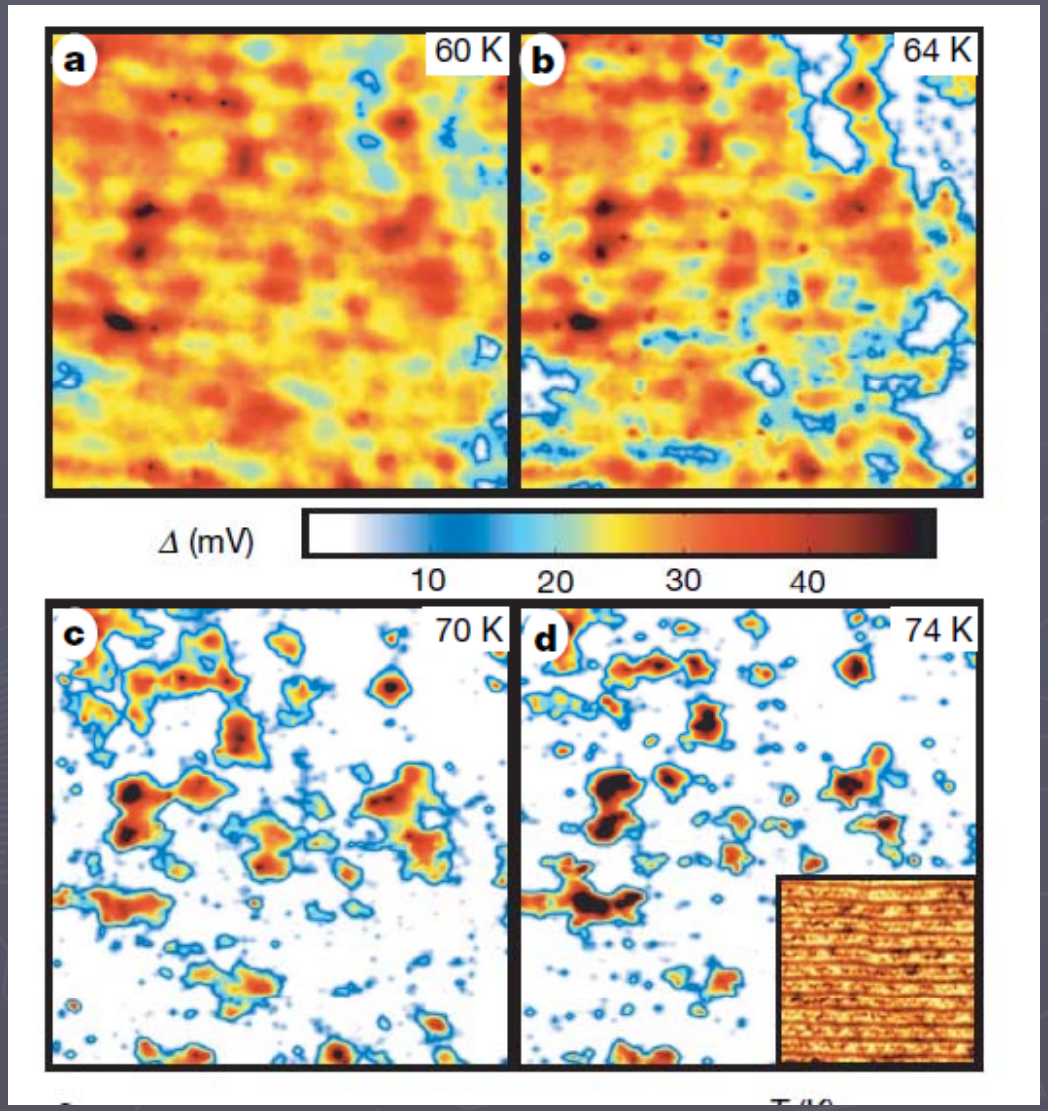
d-wave gap



Rømer et al 86, 054507(2012)

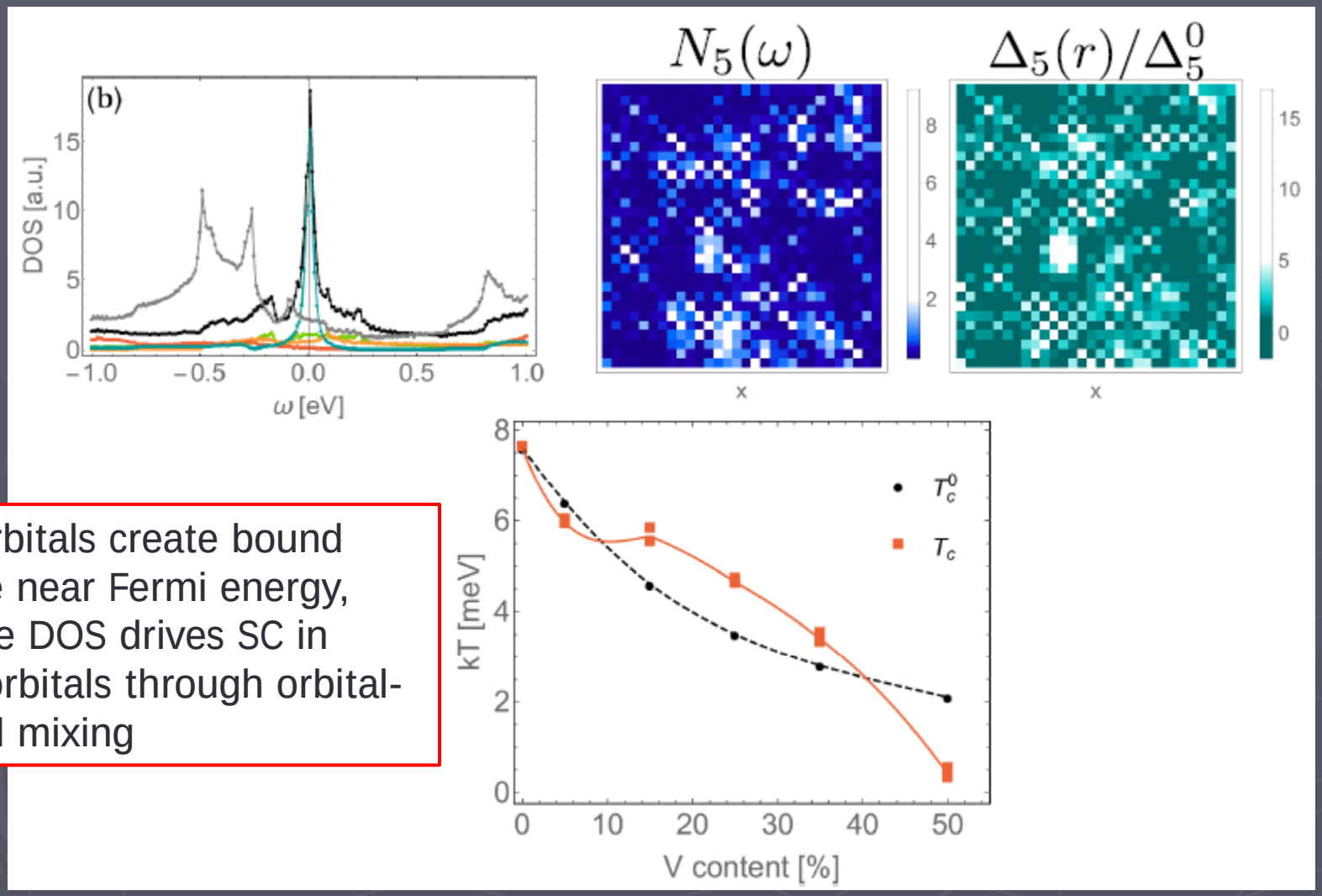
Strong coupling version of same phenomenon: Maska et al PRL 2007, Foyevstsova et al PRB 2010

Consequences – prediction for experiment: percolating set of islands just below T_c



Overdoped BSCCO
T_c=65K
Gomes et al 2008

Local pair strengthening near impurity II



E_g orbitals create bound state near Fermi energy, Large DOS drives SC in T_{2g} orbitals through orbital-band mixing

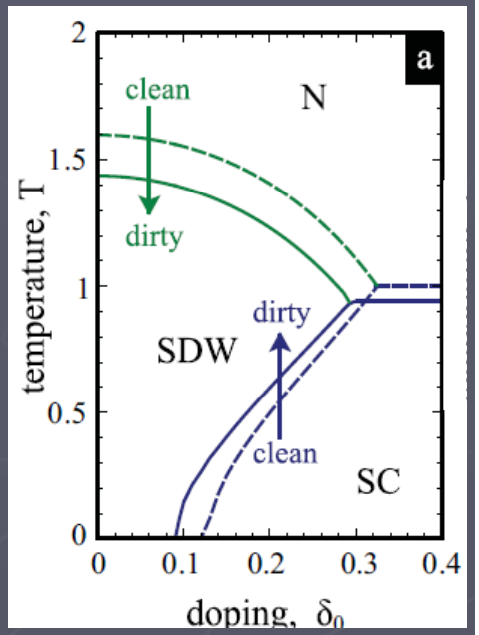
Slide kindly provided by Maria Gastiasoro

Competition of nematic order & SC + disorder

Analogy with Fernandes et al, Phys. Rev. B 85, 140512: competition of magnetic and superconducting order

Idea: both intra- and interband scattering suppress SDW; only interband scattering suppresses isotropic $s_{+/-}$

Problem: no LR magnetic order in FeSe, only nematic (q=0) order. Also: since SC is highly anisotropic, both intra, interband should suppress T_c



Toy model for interplay of SC, nematicity and disorder (Mishra and PJH 2016)

$$H = \sum_k \varepsilon_k n_k + \frac{U}{2}\sum_{kk'} d_k d_{k'} n_k n_{k'} \rightarrow \sum_k \varepsilon_k n_k + \frac{U}{2}\sum_k \theta_k n_k$$

$$\theta_k = d_k \sum_{k'} \langle d_{k'} n_{k'} \rangle; \; d_k = \cos 2\phi$$

Yamase et al PRB 2005
Mean field theory of d-wave Pomeranchuk instability

Competition of nematic order & SC + disorder

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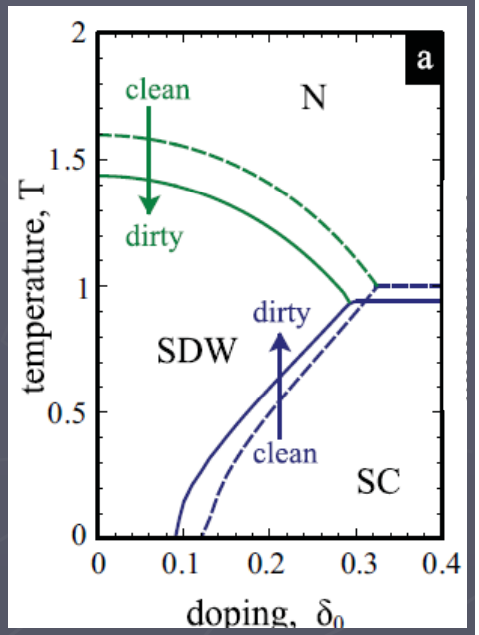

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Yamase et al PRB 2005
Mean field theory of d-wave Pomeranchuk instability

Competition of nematic order & SC + disorder

Bare nematic transition

$$T_{nem} = \frac{\mu}{2\tanh^{-1}\left(4\lambda_{nem}^{-1}\right)}$$

$$\lambda_{nem} = m|U|/2\pi$$

Include disorder:

$$\Sigma_{nem} = n_{imp}|V_{imp}|^2 \sum_{k'} \frac{1}{i\omega - x - \Theta_{k'}}$$

Anisotropic s-wave SC with nematic order

$$\Delta = \Delta_0 \frac{(1 + r\cos 2\phi)}{\sqrt{1 + r^2/2}}$$

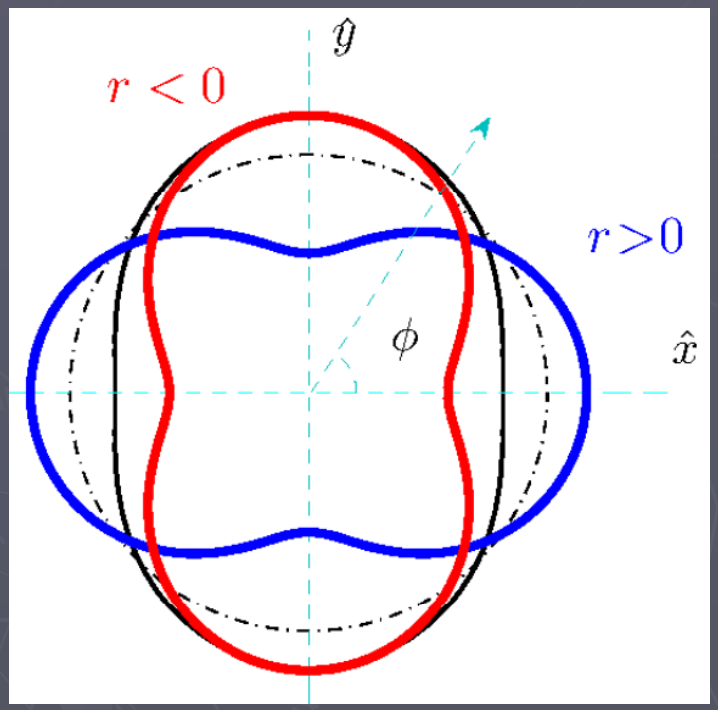
$$G = -\frac{i\omega\tau_0 + (\xi_k + \Theta_k)\tau_3 + \Delta\tau_1}{\omega^2 + (\xi_k + \Theta_k)^2 + \Delta^2}$$

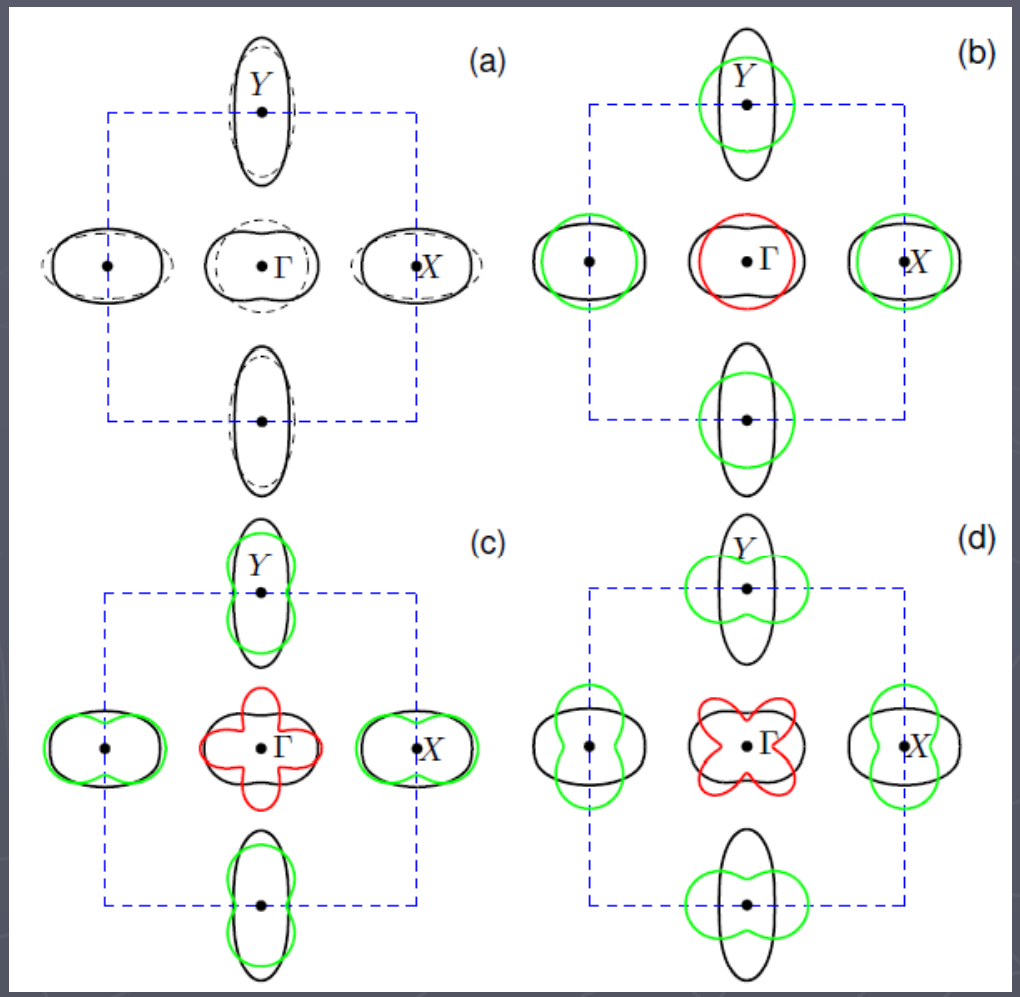
Gap equation with disorder

$$\Delta_0 = 2T \sum_{\omega>0,k'} V_0 \frac{(1 + r\cos 2\phi')}{\sqrt{1 + r^2/2}} \frac{\tilde{\Delta}_{k'}}{\tilde{\omega}^2 + (\xi_k + \Theta_k)^2 + \tilde{\Delta}^2}$$

$$\Sigma = n_{imp}|V_{imp}|^2 \sum_{k'} \frac{i\tilde{\omega}\tau_0 + (\xi_k + \Theta_k)\tau_3 + \tilde{\Delta}\tau_1}{\tilde{\omega}^2 + (\xi_k + \Theta_k)^2 + \tilde{\Delta}^2}$$

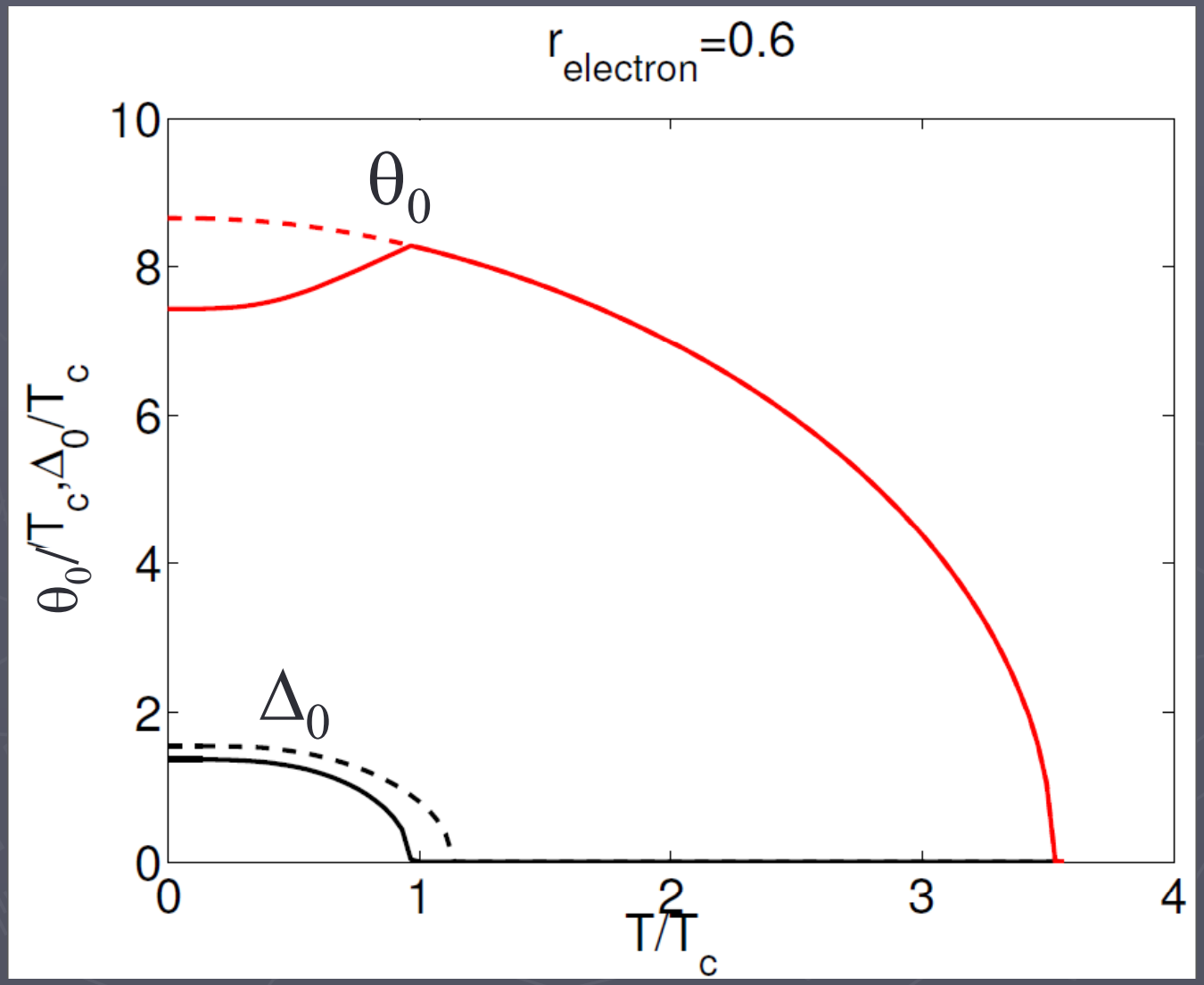
Competition of nematic order & SC



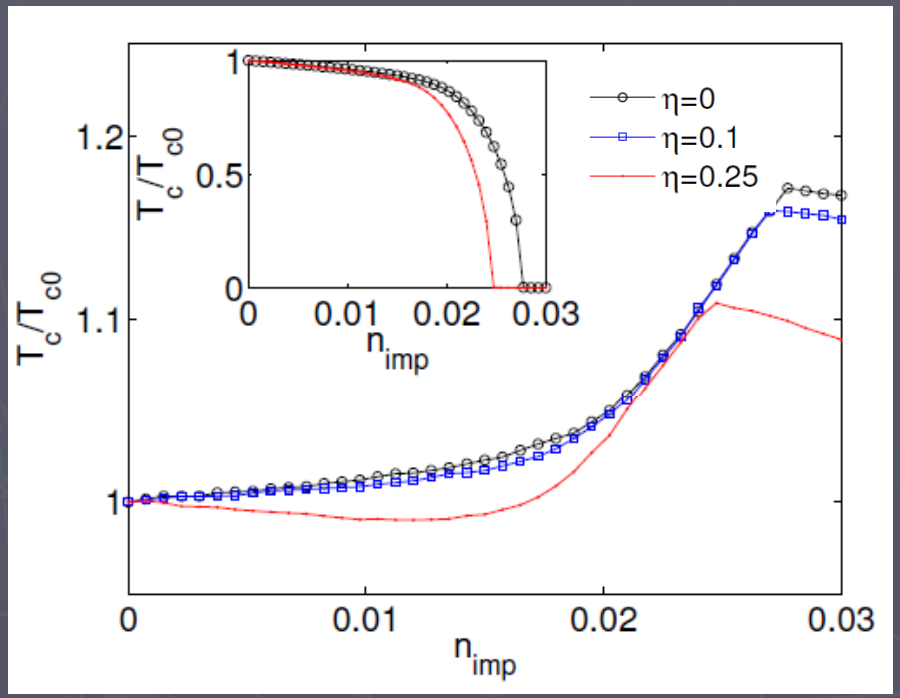


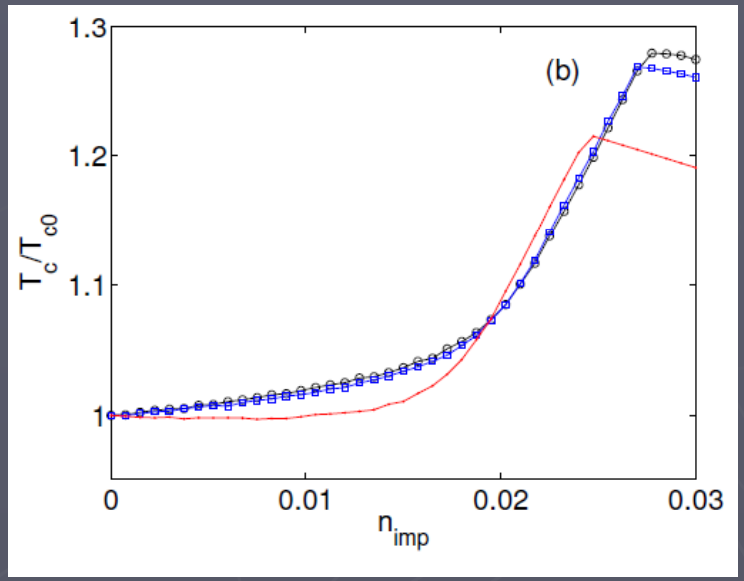
$$\Delta_n(k) = \Delta_0(1+rY_n(k))$$

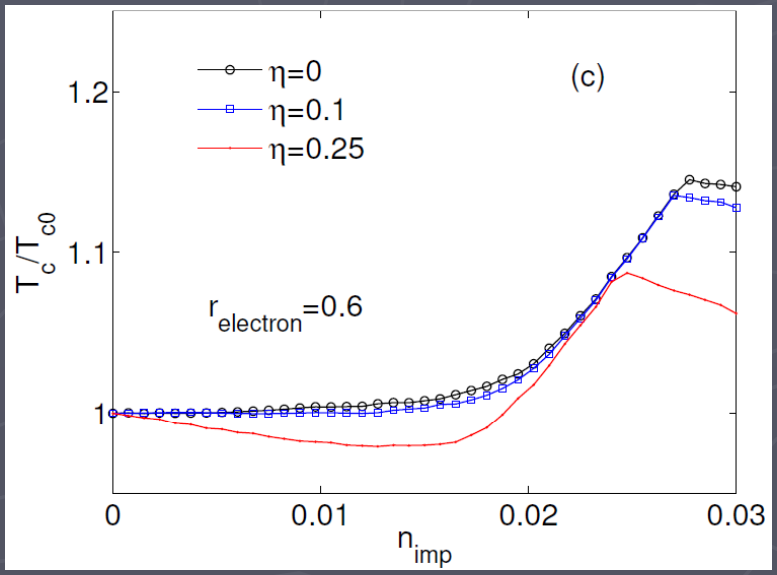
Competition of nematic order & SC



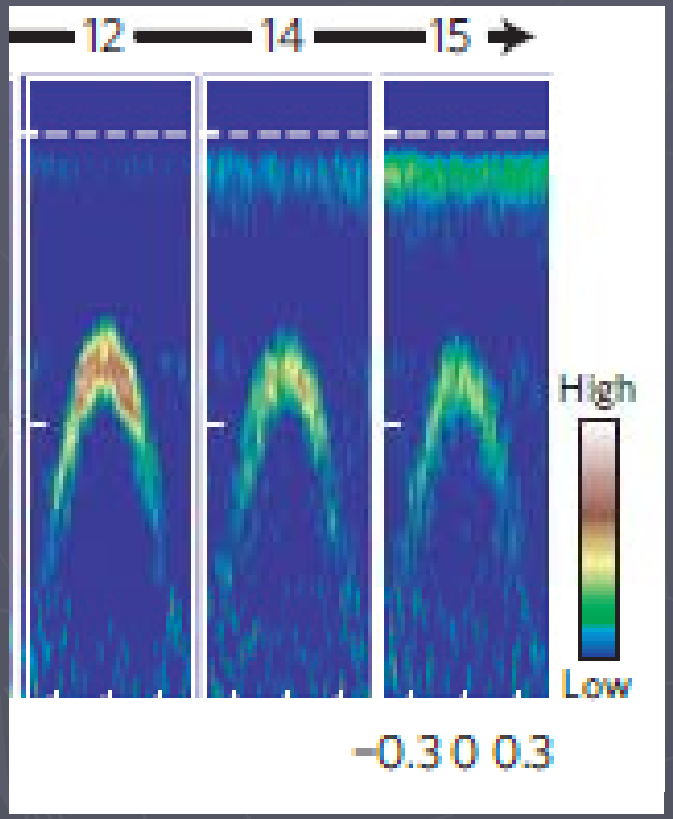
Competition of nematic order & SC + disorder

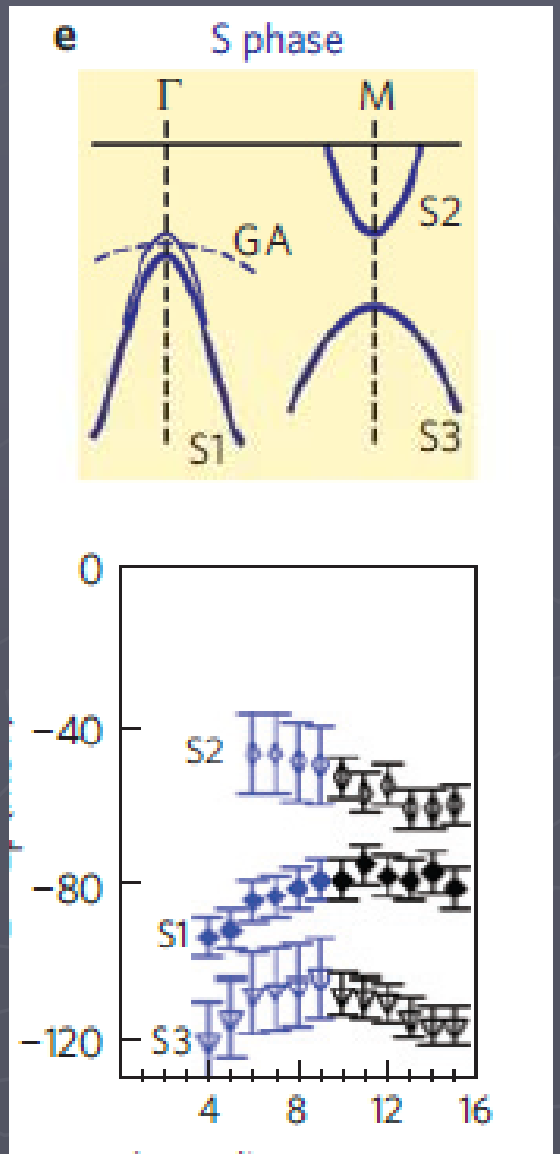






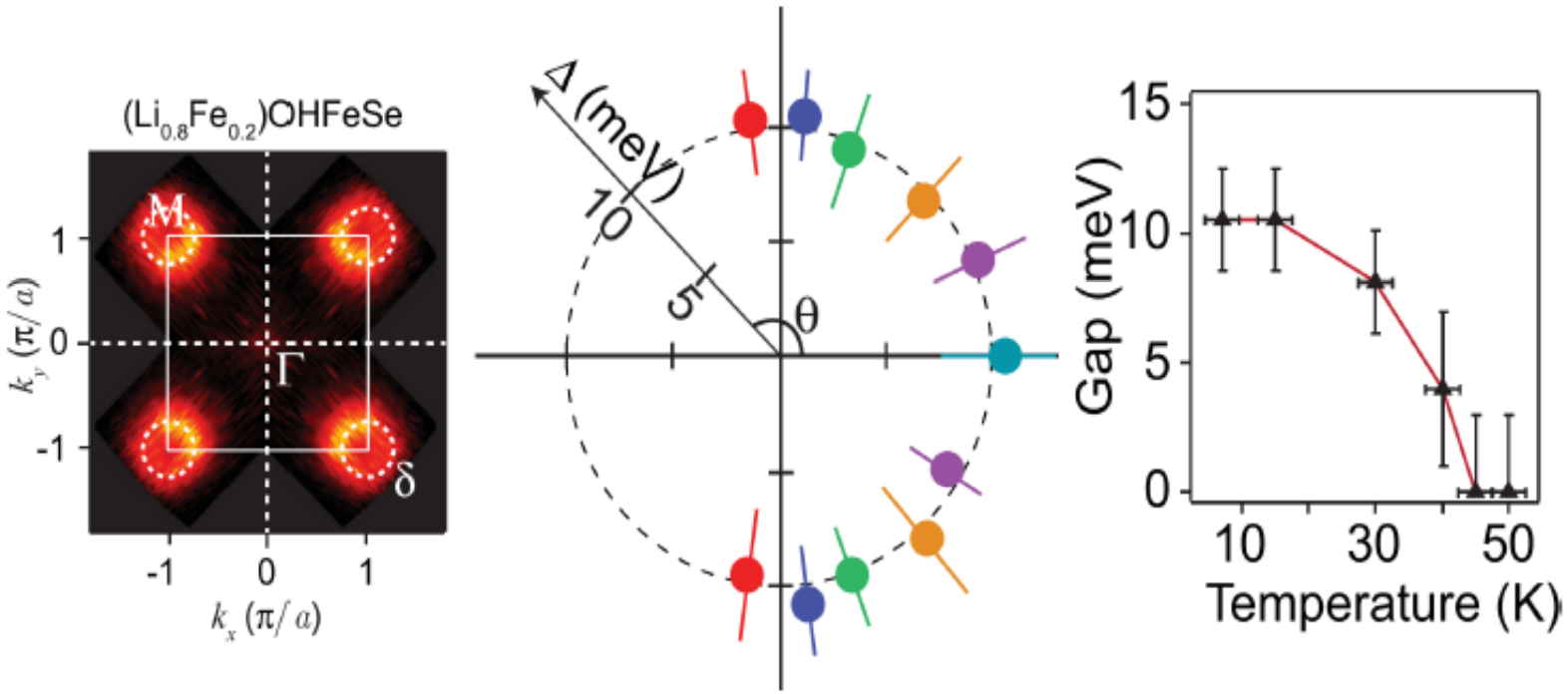
Incipient bands in Fe/STO monolayers





FeSe based system without additional hole-pocket at FL

- FeSe intercalates:

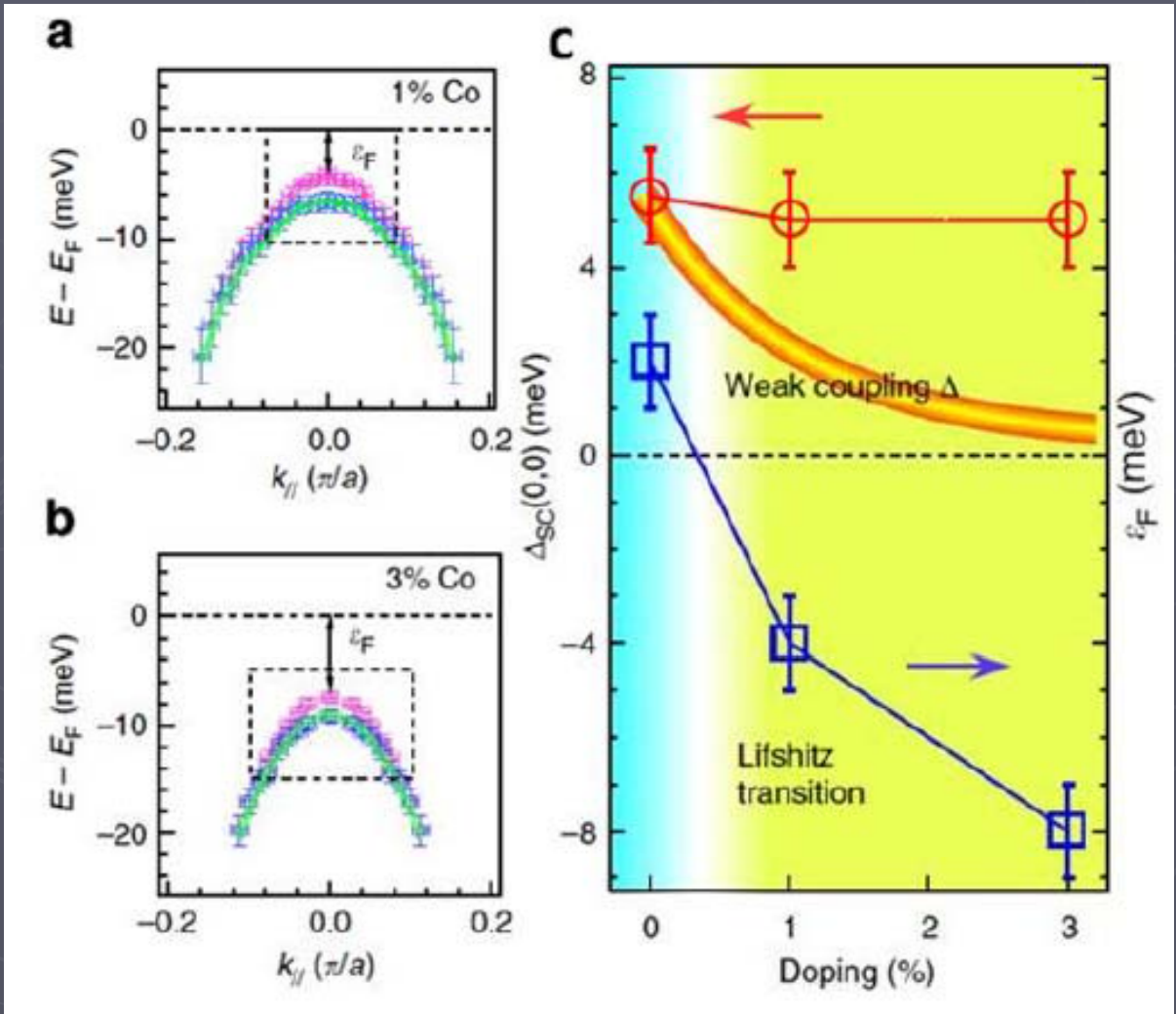


X. H. Niu *et al.* PRB **92**, 060504(R) (2015)

- T_c's of 35 – 45K

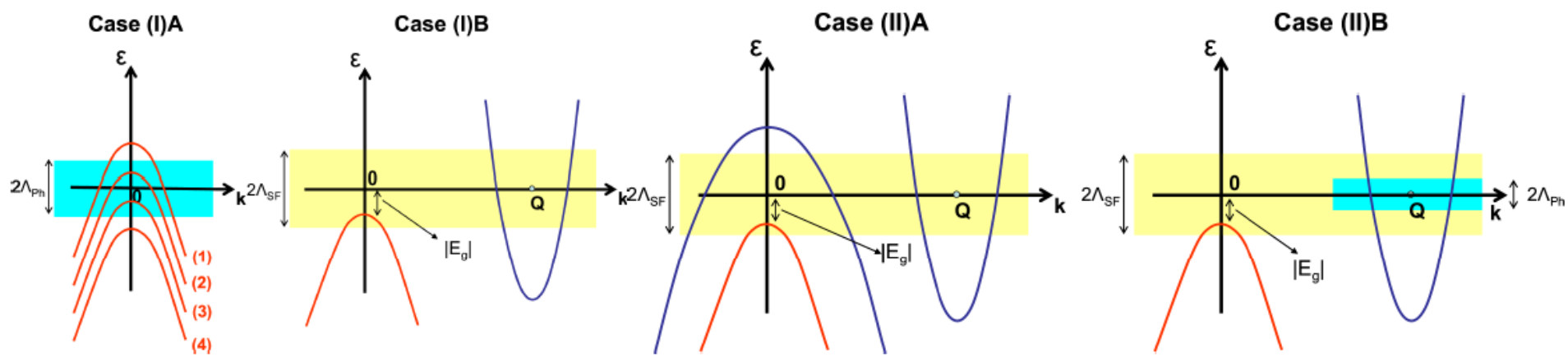
Can incipient bands contribute to SC? LiFeAs

Miao et al. Nat. Comm (2014).



Role of incipient bands in FeSC

Chen, Maiti, Linscheid, PH PRB 92, 224514 (2015)



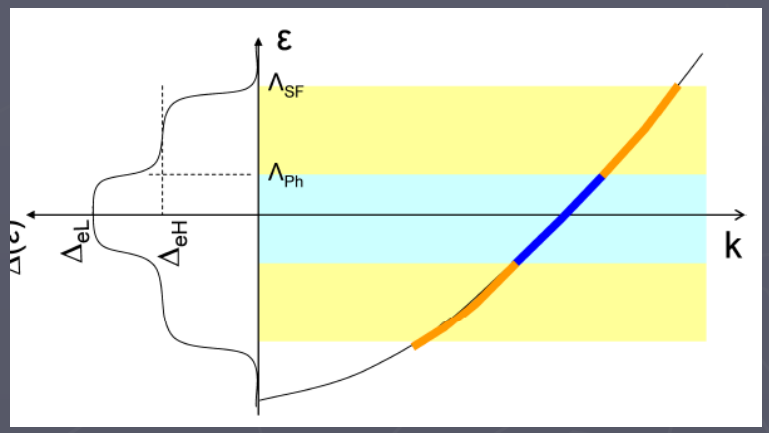
- Case I: SC caused by incipient bands
- Case II SC caused by FS bands, induced in incipient bands

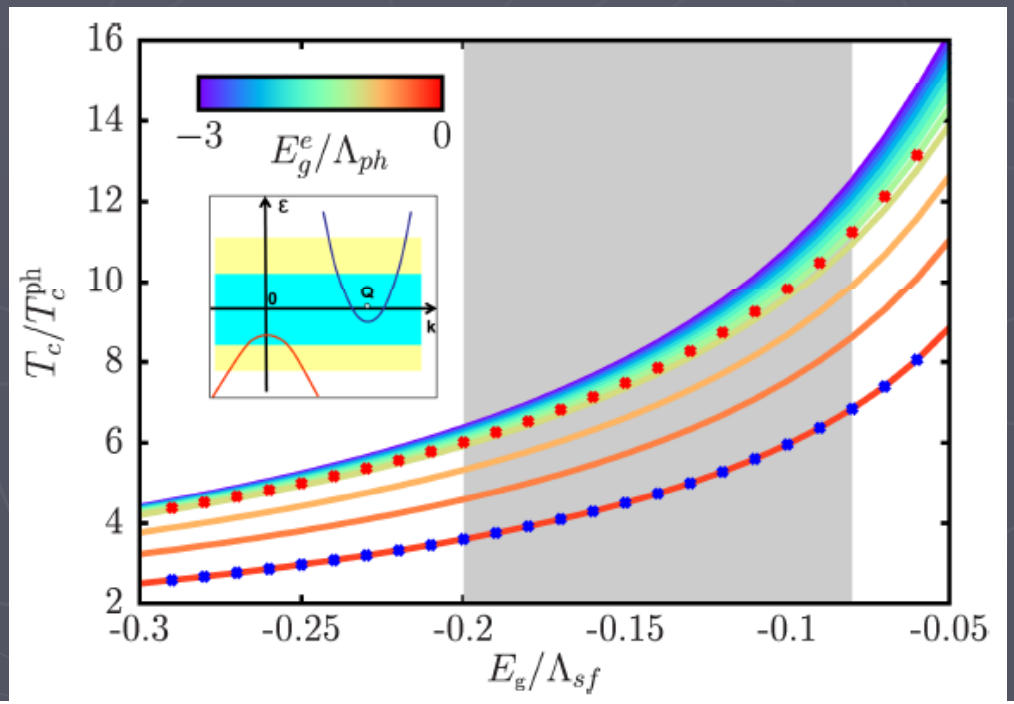
Conclusion: weak coupling multiband BCS theory with constant interactions can account for large gaps on incipient bands *IF* SC is supported by pairing interactions at the Fermi level.

Multiband BCS for Case II(B): FeSe/STO monolayers

$$\Delta_{eL} = -V_{ph}\Delta_{eL}L_{eL} - V_{sf}\Delta_h L_h,$$
$$\Delta_{eH} = -V_{sf}\Delta_h L_h,$$
$$\Delta_h = -2V_{sf}(\Delta_{eL}L_{eL} + \Delta_{eH}L_{eH})$$

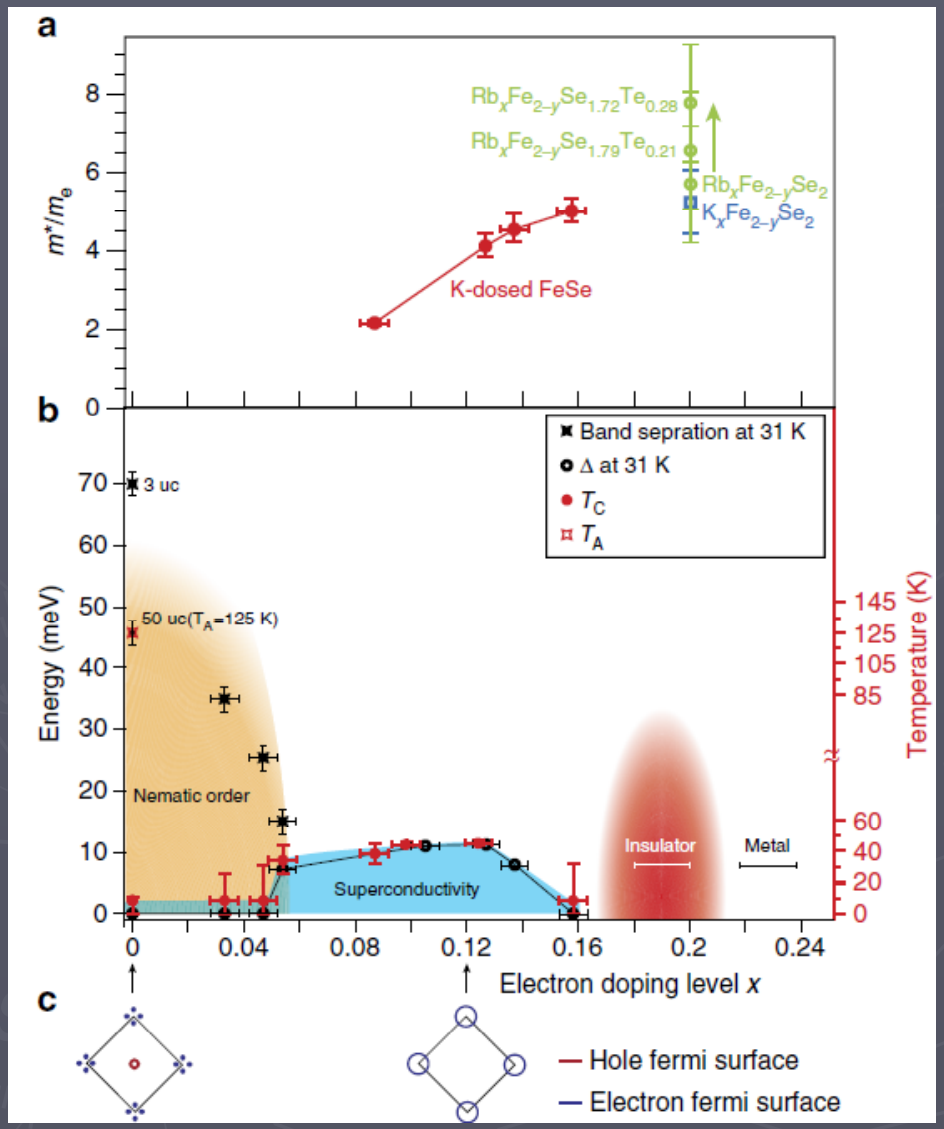
$$L_{eL} = 2\int_0^{\Lambda_{ph}} d\varepsilon N_e \frac{\tanh\frac{E_{eL}}{2T}}{2E_{eL}},$$
$$L_{eH} = 2\int_{\Lambda_{ph}}^{\Lambda_{sf}} d\varepsilon N_e \frac{\tanh\frac{E_{eH}}{2T}}{2E_{eH}},$$
$$L_h = \int_{-\Lambda_{sf}}^{E_g} d\varepsilon \frac{m}{2\pi}\frac{\tanh\frac{E_h}{2T}}{2E_h}.$$



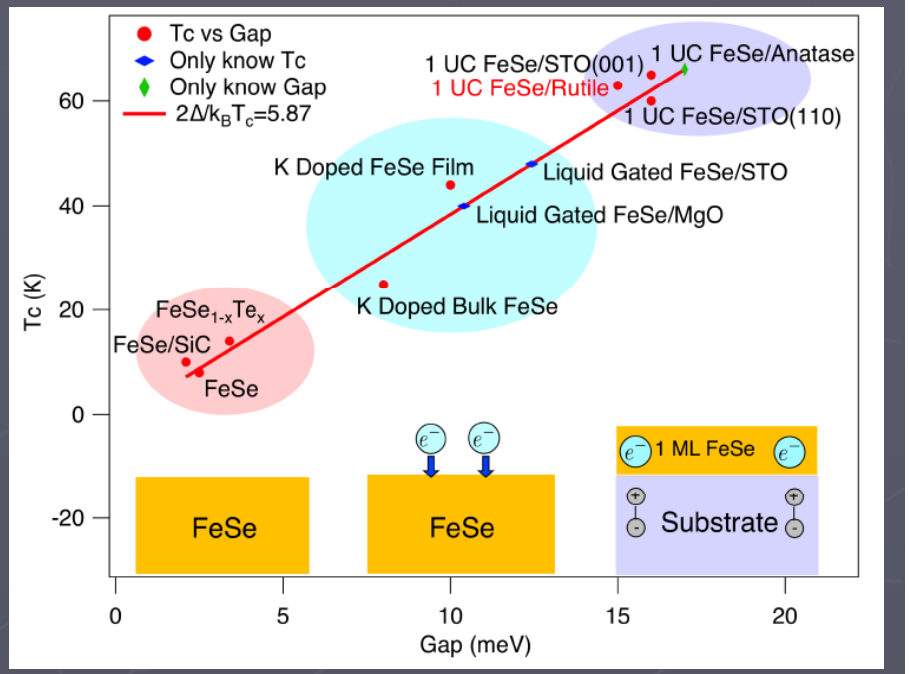


SF interaction with incipient band
Can bootstrap weak phonon interaction!

But: high T_c only upon e-doping: incipient hole band moves *further* away



Wen et al Nat. Comm. 2016



Rebec et al aXv:1606.09358

Also: Song et al PRL 2016
Miyata et al Nat. Comm 2016

Dynamical spin fluctuation interaction of FS bands with incipient band

A. Linscheid et al arXiv:1603.03739

- With local, constant interaction U

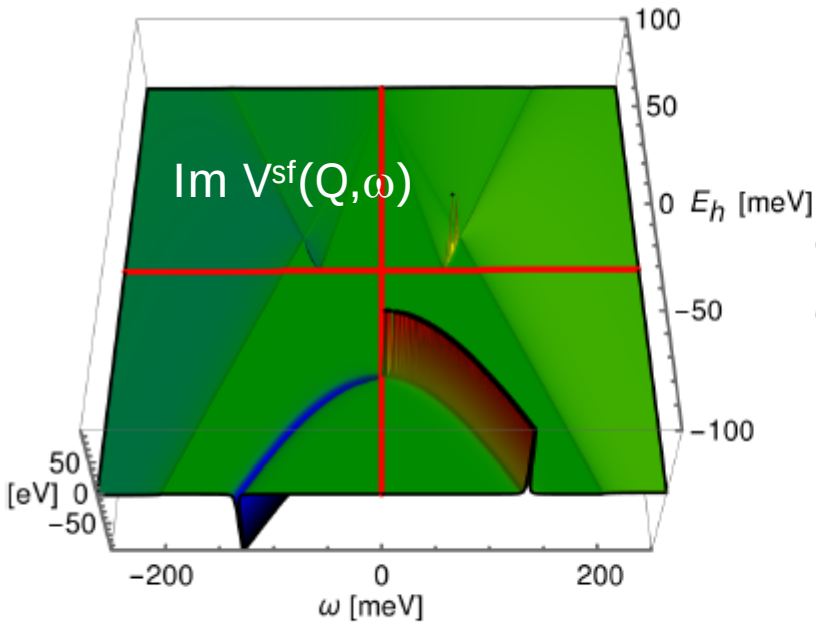
$$V_{\mathrm{sf}}(\boldsymbol{q}, \mathrm{i}\nu_n) = \frac{U^2[\chi_0^{\mathrm{eh}}(\boldsymbol{q}, \mathrm{i}\nu_n) + \chi_0^{\mathrm{he}}(\boldsymbol{q}, \mathrm{i}\nu_n)]}{1 - U[\chi_0^{\mathrm{eh}}(\boldsymbol{q}, \mathrm{i}\nu_n) + \chi_0^{\mathrm{he}}(\boldsymbol{q}, \mathrm{i}\nu_n)]}$$

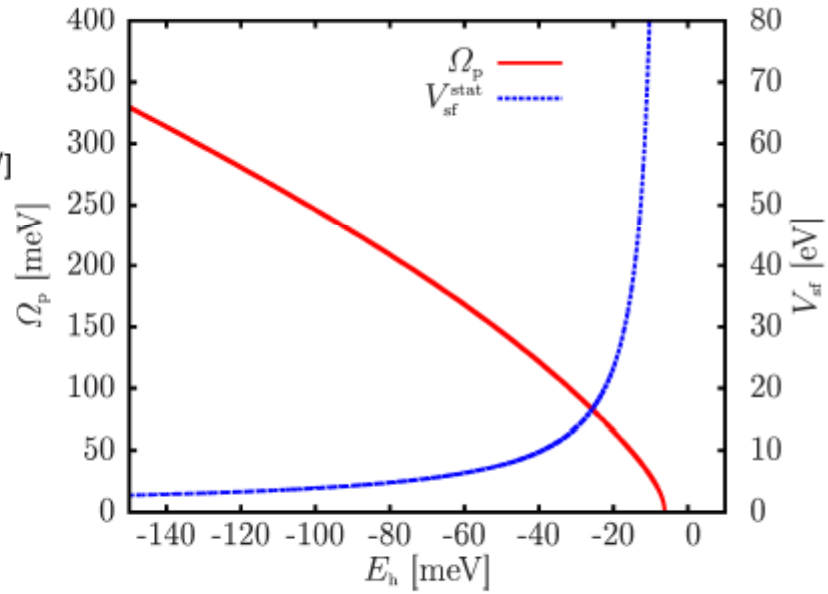
where

$$\begin{aligned} \chi_0^{\mathrm{he}}(\boldsymbol{q}, \mathrm{i}\nu_n) &= \int \mathrm{d}\boldsymbol{k} \frac{f(\varepsilon_{\boldsymbol{k}}^{\mathrm{h}}) - f(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}}^{\mathrm{e}})}{\mathrm{i}\nu_n - (\varepsilon_{\boldsymbol{k}+\boldsymbol{q}}^{\mathrm{e}} - \varepsilon_{\boldsymbol{k}}^{\mathrm{h}})} \\ &\equiv \chi_0^{\mathrm{eh}}(\boldsymbol{q}, -\mathrm{i}\nu_n) \end{aligned}$$

N. F. Berk and J. R. Schrieffer, PRL **17**, 433 (1966)
N. E. Bickers et al. PRL **62**, 961 (1989)
S. Graser et al. New J. Phys. **11**, 025016 (2009)
F. Essenberger, A. Sanna, AL et al. PRB **90**, 214504 (2014)

E_h dependence of the pairing interaction





- Couplings at $E_h \sim E_h^* \ll 0$

$$\Lambda_{\rm sf} \equiv \Omega_{\rm p} \quad \sim \quad \sqrt{|E_h - E_h^*|}$$
$$\lambda_{\rm sf} \equiv V_{\rm sf}(\boldsymbol{Q}, 0) \quad \sim \quad 1/|E_h - E_h^*|$$

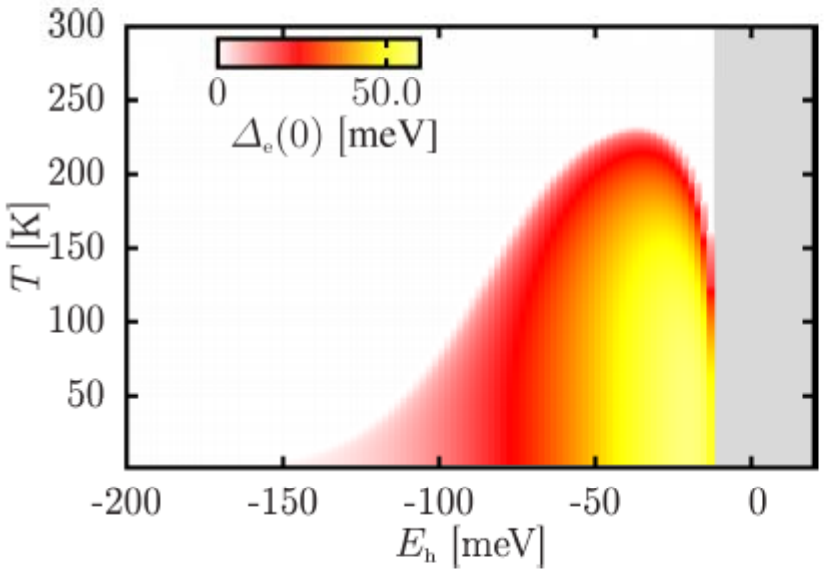
- Allen-Dynes estimate for strong coupling SC:

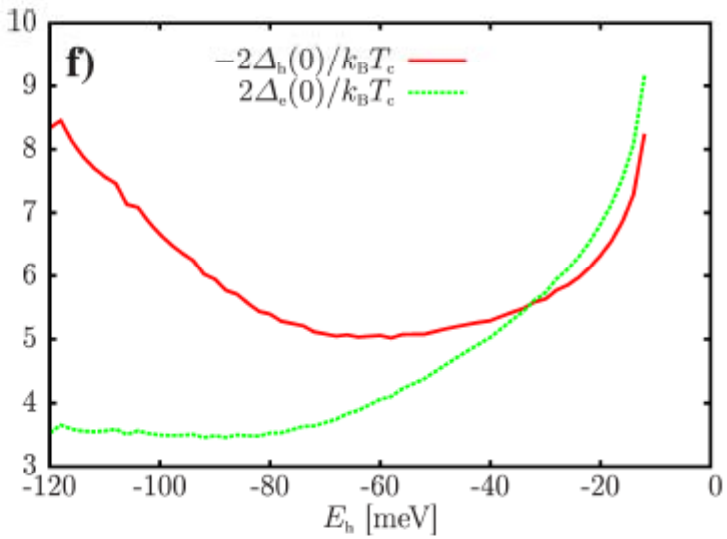
$$T_c(E_h \to E_h^*) \quad \sim \quad \Lambda_{\rm sf}\sqrt{\lambda_{\rm sf}} \equiv const$$

AL, S. Maiti, Y. Wang, S. Johnston, P. J. Hirschfeld, arXiv:1603.03739

Solve incipient Eliashberg equations

Lifschitz transition, magnetic transition nearly coincide!





- Large T_c due to incipient $s_\pm$ pairing
- Non-monotonic $T_c(E_h)$: Optimal trade-off between Λ_{sf} and λ_{sf}

Conclusions

- FeSe is different, complicated (cool)
- “Band engineering” phenomenology
- Prozorov expt: irradiation: $T_s\downarrow$, $T_c\uparrow$
- Discussed some ideas:
  - Impurities break ground state degeneracy
  - Impurities enhance pair interaction locally
    - Spin fluctuation freezing
    - E_g orbital bound state
  - Impurities influence nematic/SC competition
- Incipient bands may be important for monolayers