1. Importance of orbital degrees of freedom

2. Evidence for triplet superconductivity in LiFeAs

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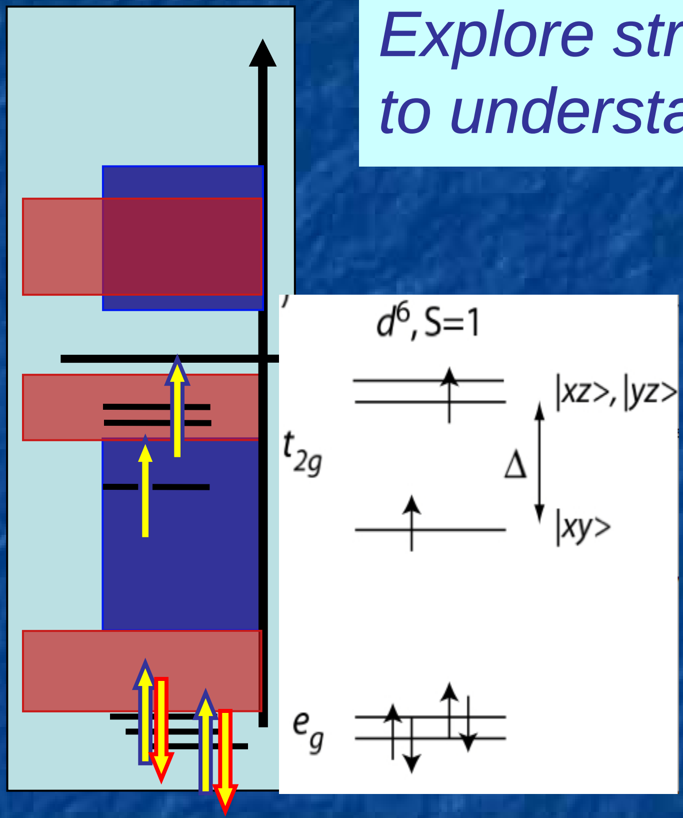
***Seung-Ho Baek*, *Hajo Grafe*, Franziska Hammerath, *Maria Daghofer*, Carsten Timm, *Philip Brydon*, Bernd Buchner**

KITP 12/1/2011

Orbital degrees of freedom

Explore strong coupling spin-orbital fixed points to understand spin-orbital physics in Fe-pnictides



S=1

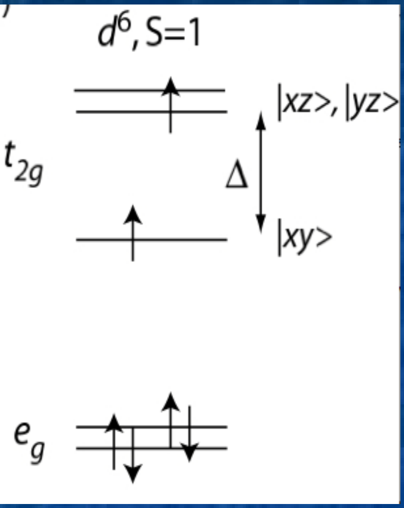
$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_{\mathrm{cf}} + \mathcal{H}_{\mathrm{int}}$$

$$\mathcal{H}_t = -\sum_{(i,j)} \sum_{\alpha\beta,\sigma} t_{\alpha\beta}^{(i,j)} \; d_{i\alpha\sigma}^{\dagger} d_{j\beta\sigma}$$

$$\mathcal{H}_{\mathrm{cf}} = \sum_{i\alpha} \epsilon_{\alpha} \hat{n}_{i\alpha}$$

Kruger, Kumar, Zaanen, JvdB, *PRB 79, 054504 (2009)*
Sawatzky, Elfimov, JvdB, Zaanen *EPL 86, 17006 (2009)*
Chen, Moritz, JvdB, Devereaux, Singh *PRB 80, 180418 (2009)*
Wang, JvdB, et al. *PRB 80, 014508 (2009)*
Giovannetti, Kumar, JvdB, *Phys. B. 403, 3653 (2008)*

Effective Kugel-Khomskii model for t_{2g} doublet



$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_{\rm cf} + \mathcal{H}_{\rm int}$$

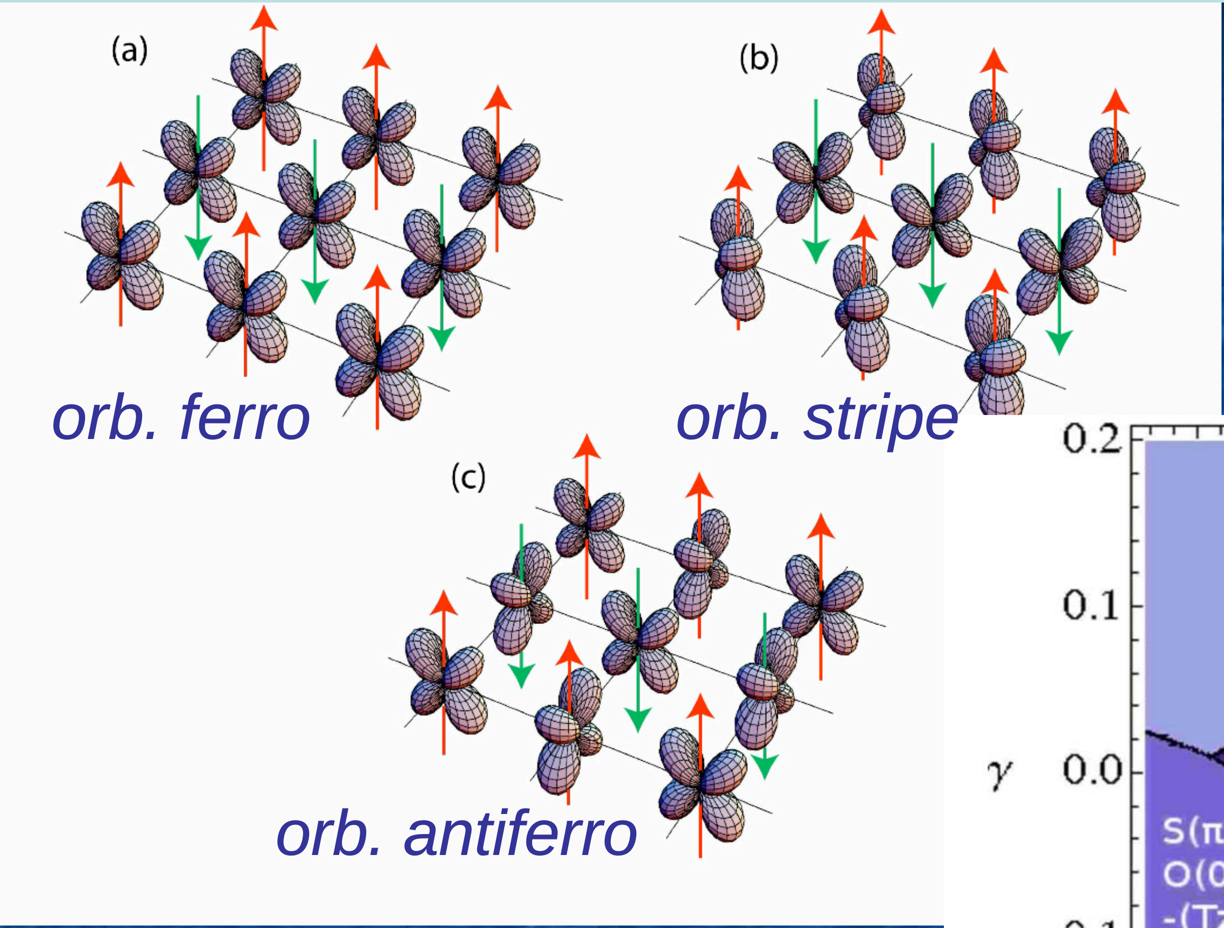
$$\mathcal{H}_t = -\sum_{(i,j)} \sum_{\alpha\beta,\sigma} t_{\alpha\beta}^{(i,j)} \, d_{i\alpha\sigma}^{\dagger} d_{j\beta\sigma} \qquad \mathcal{H}_{\rm cf} = \sum_{i\alpha} \epsilon_\alpha \hat{n}_{i\alpha}$$

$$\mathcal{H}_{\rm int} = U \sum_{i\alpha} \hat{n}_{i\alpha\uparrow}\hat{n}_{i\alpha\downarrow} + \frac{1}{2}\left(U - \frac{5}{2}J_H\right) \sum_{i\alpha\beta}^{\alpha\neq\beta} \hat{n}_{i\alpha}\hat{n}_{i\beta} + J_H \sum_{i\alpha\beta}^{\alpha\neq\beta} d_{i\alpha\uparrow}^{\dagger} d_{i\alpha\downarrow}^{\dagger} d_{i\beta\downarrow} d_{i\beta\uparrow} - J_H \sum_{i\alpha\beta}^{\alpha\neq\beta} \hat{\mathbf{S}}_{i\alpha}\hat{\mathbf{S}}_{i\beta}$$

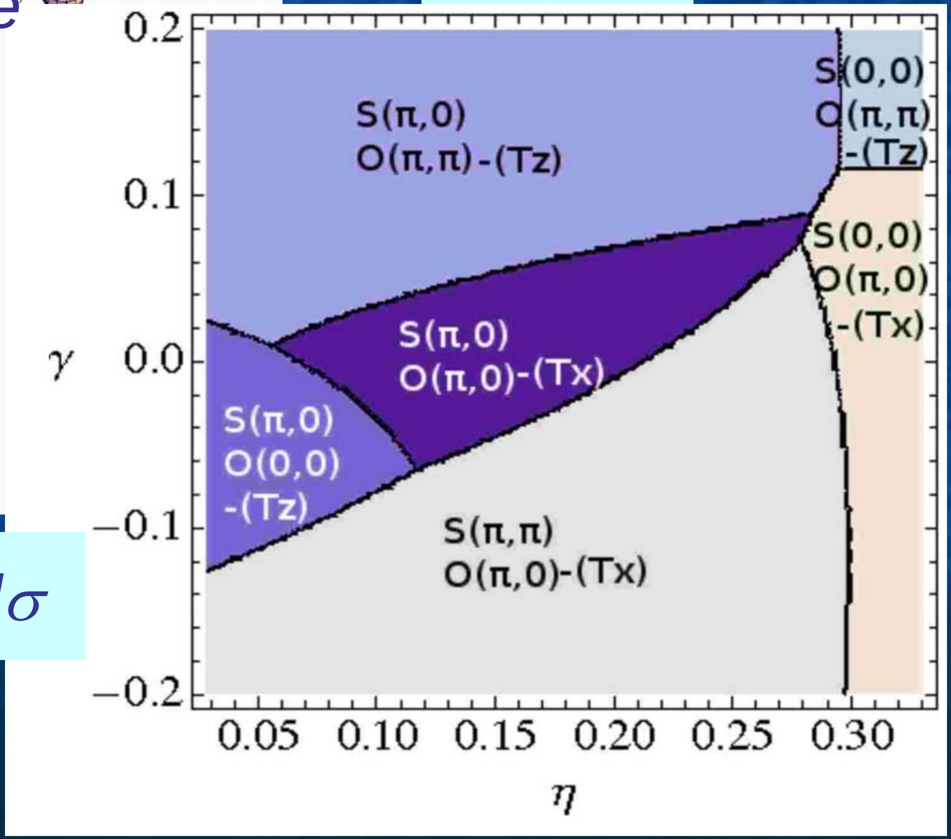
$$\mathcal{H}_{\rm KK}^{(i,j)} = -\sum_{\tau_i,\tau_j} \sum_{s_i,s_j} J_{\tau_i,\tau_j,s_i,s_j}^{(i,j)} A_{\tau_i,\tau_j}^{(i,j)}(\hat{\mathbf{T}}_i, \hat{\mathbf{T}}_j) \times B_{s_i,s_j}(\hat{\mathbf{S}}_i, \hat{\mathbf{S}}_j)$$

Kruger, Kumar, Zaanen, JvdB, *PRB 79, 054504 (2009)*

Spin-Orbital Ordered Phases

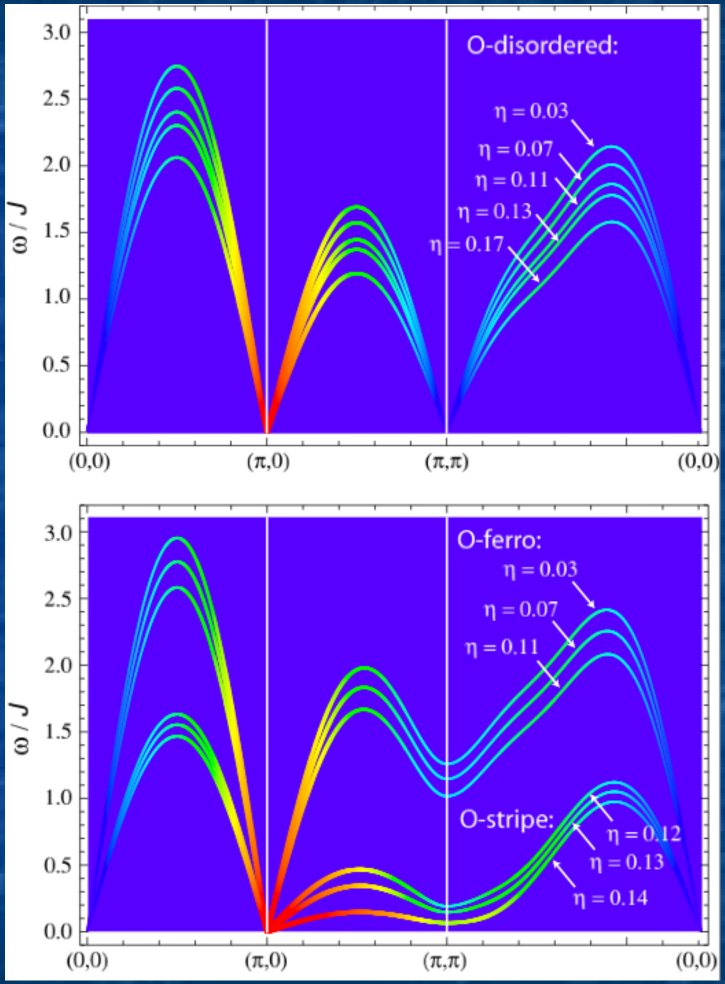


$\eta = J_H / U$



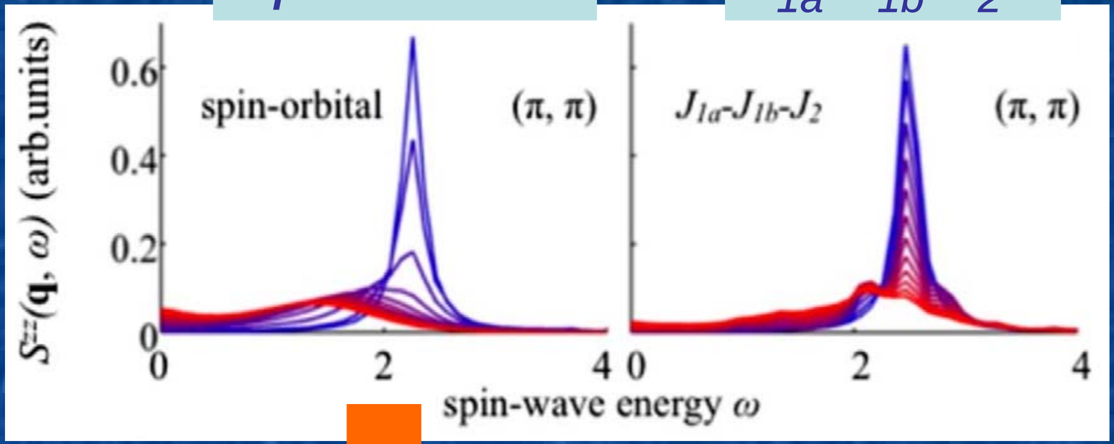
$\gamma = pd\pi / pd\sigma$

Spin Excitations & T-Dependence



Spin-Orbital

J_{1a}-J_{1b}-J_2



Collapse of coherent
(π,π) magnon
due to orbital fluctuations

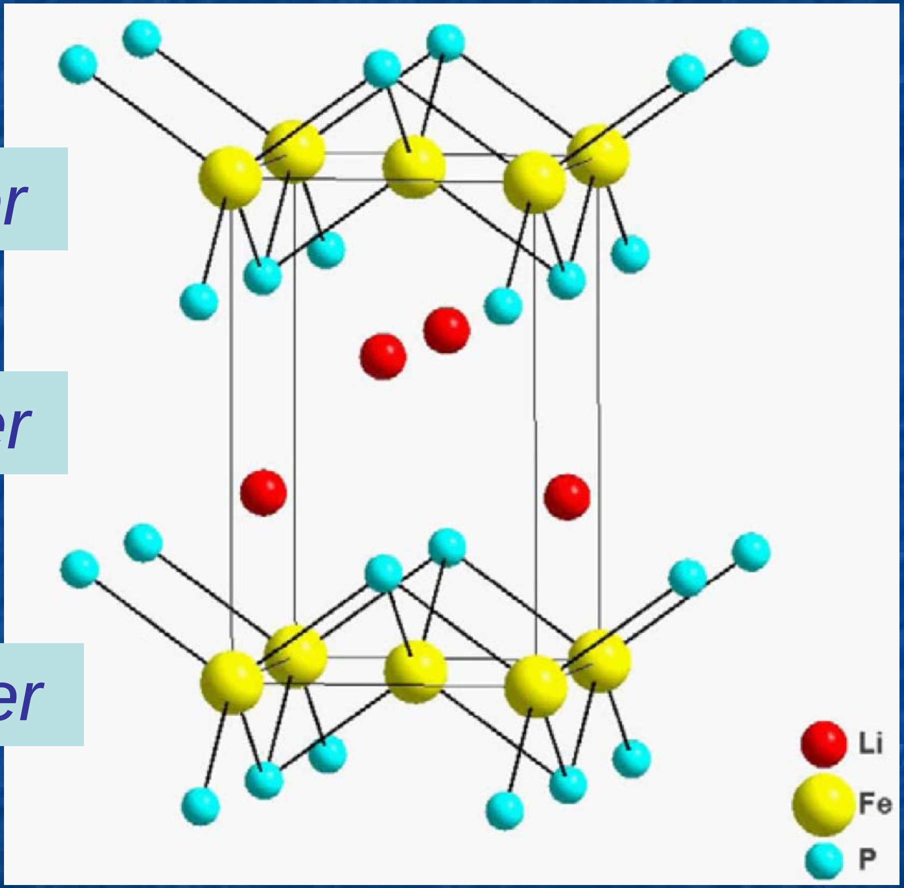
Kruger, Kumar, Zaanen, JvdB, *PRB 79, 054504 (2009)*
Chen, Moritz, JvdB, Devereaux, Singh *PRB 80, 180418 (2009).*

Li-Fe-As structure 1-1-1

FeAs layer

Li - Li layer

FeAs layer



Absence of surface states:

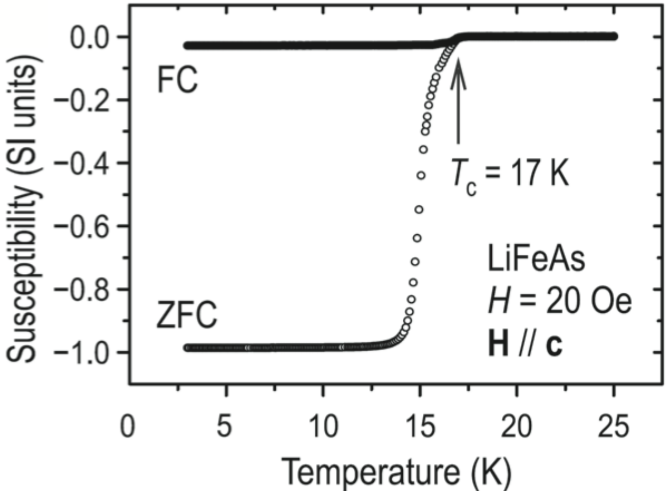
Lankau, Koepernik, Borisenko, Zabolotnyy, Buchner, JvdB, Eschrig, PRB 82, 184518 (2010)

opposed to 122's:

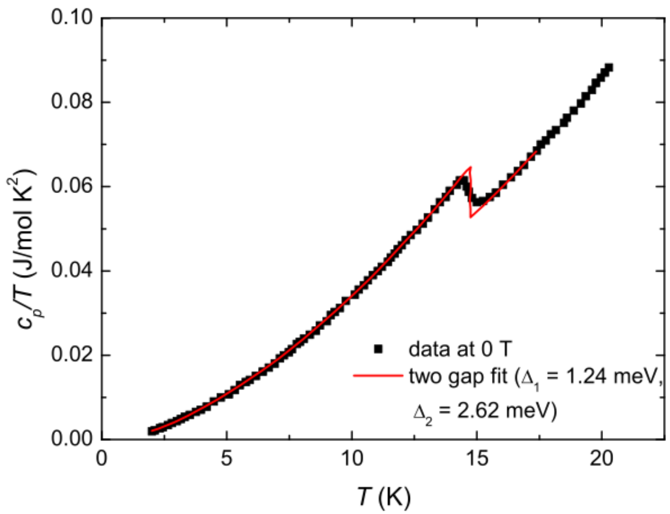
Heumen, Vuorinen, Koepernik, Massee, Huang, Shi, Klei, Goedkoop, Lindroos, JvdB, Golden, PRL, in press

stochiometric superconductor T_c ~18K

LiFeAs crystal quality



--Sharp Tc
--100% superconducting volume fraction



Supplementary Figure 2 Specific heat versus temperature for zero magnetic field. The figure has been reproduced from U. Stockert *et al*. (*S4*).

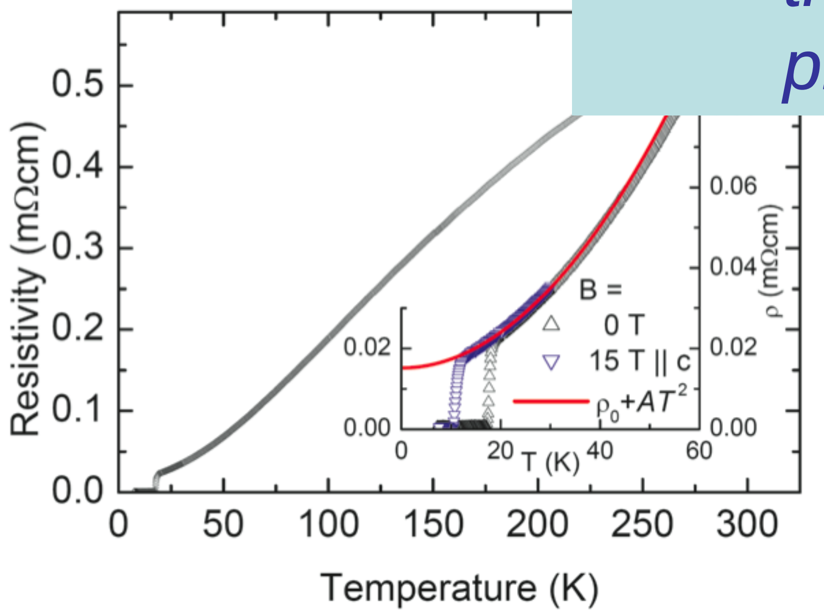
--Very sharp Tc in specific heat

Baek, Grafe, Hammerath, Fuchs, Harnagea, Wurmehl, JvdB & Buchner

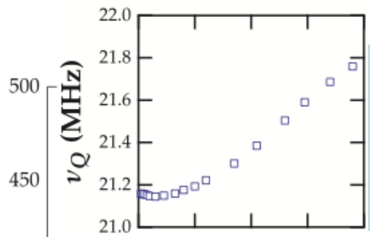
LiFeAs crystal quality

-- R

-- NQR line width ~80 kHz, better than any other pnictide



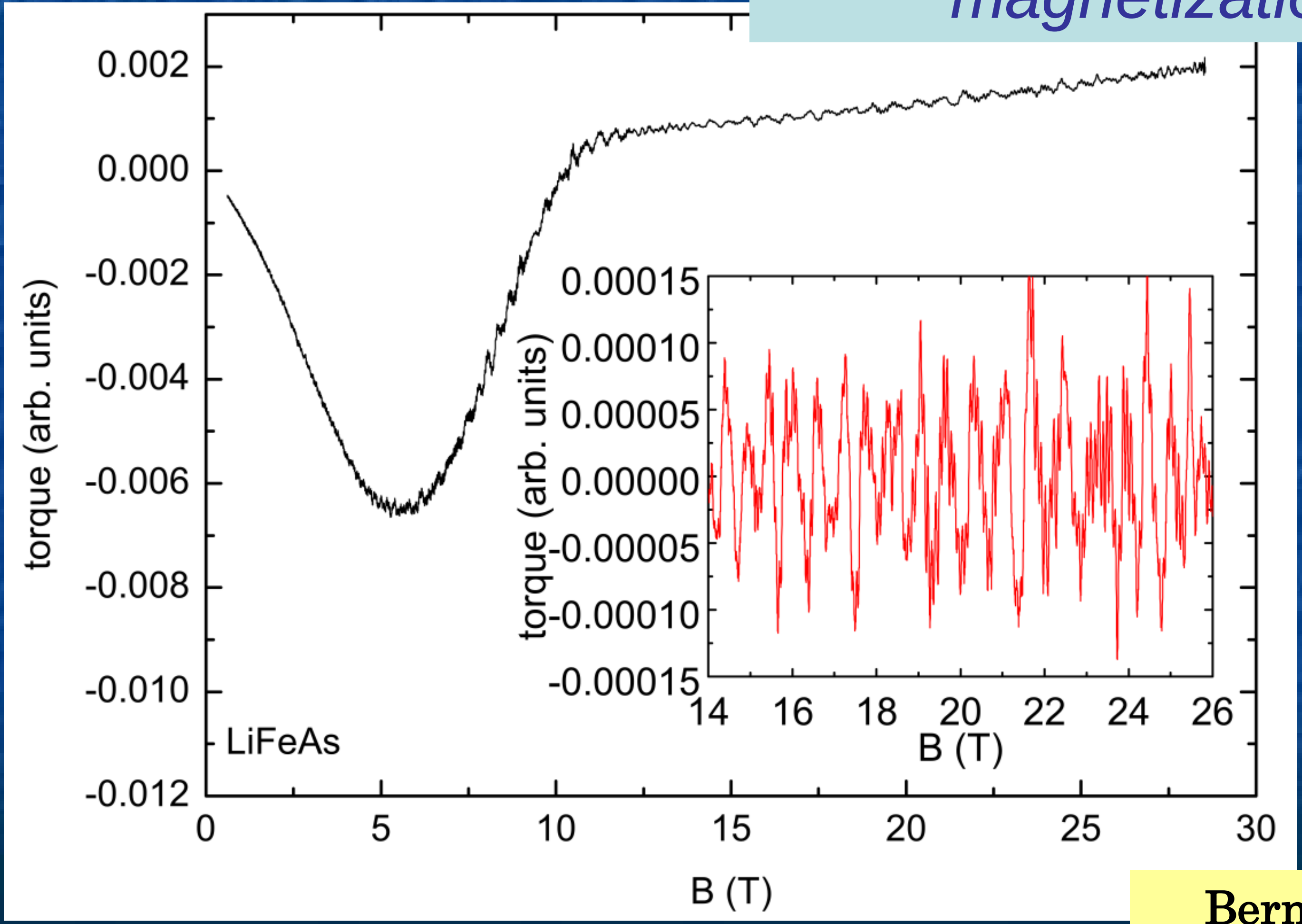
Supplementary Figure 3 Resistivity versus temperature for LiFeAs. Inset: magnetic field dependence and residual resistivity. Figure courtesy of O. Heyer (*S5*).



Supplementary Figure 4 NQR spectra as a function of temperature at zero magnetic field. The quadrupole resonance frequency, ν_Q, decreases with decreasing temperature and saturates at low temperatures. Below T_c, it slightly upturns.

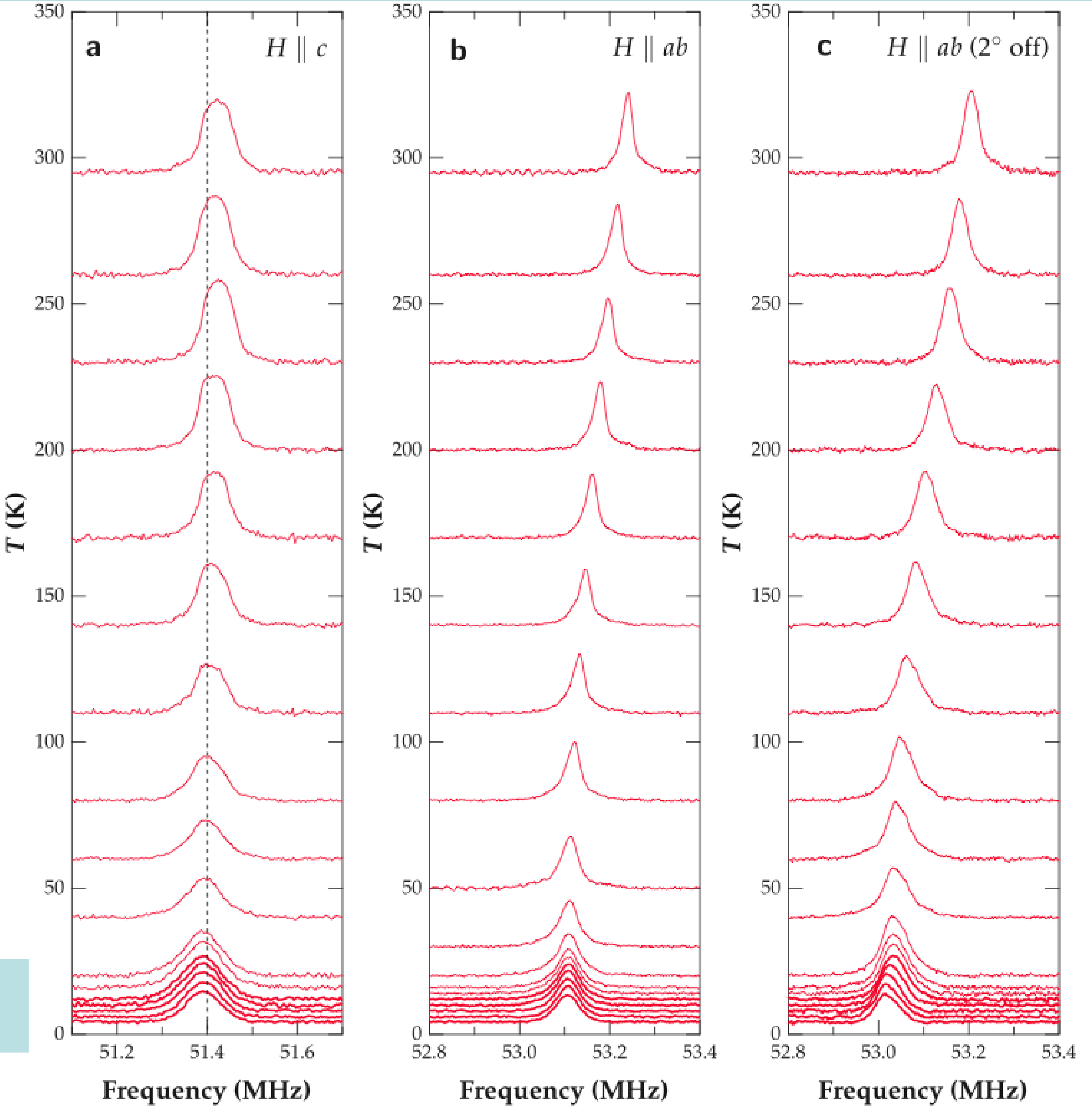
LiFeAs crystal quality

-- Quantum oscillations in magnetization (dHvA)



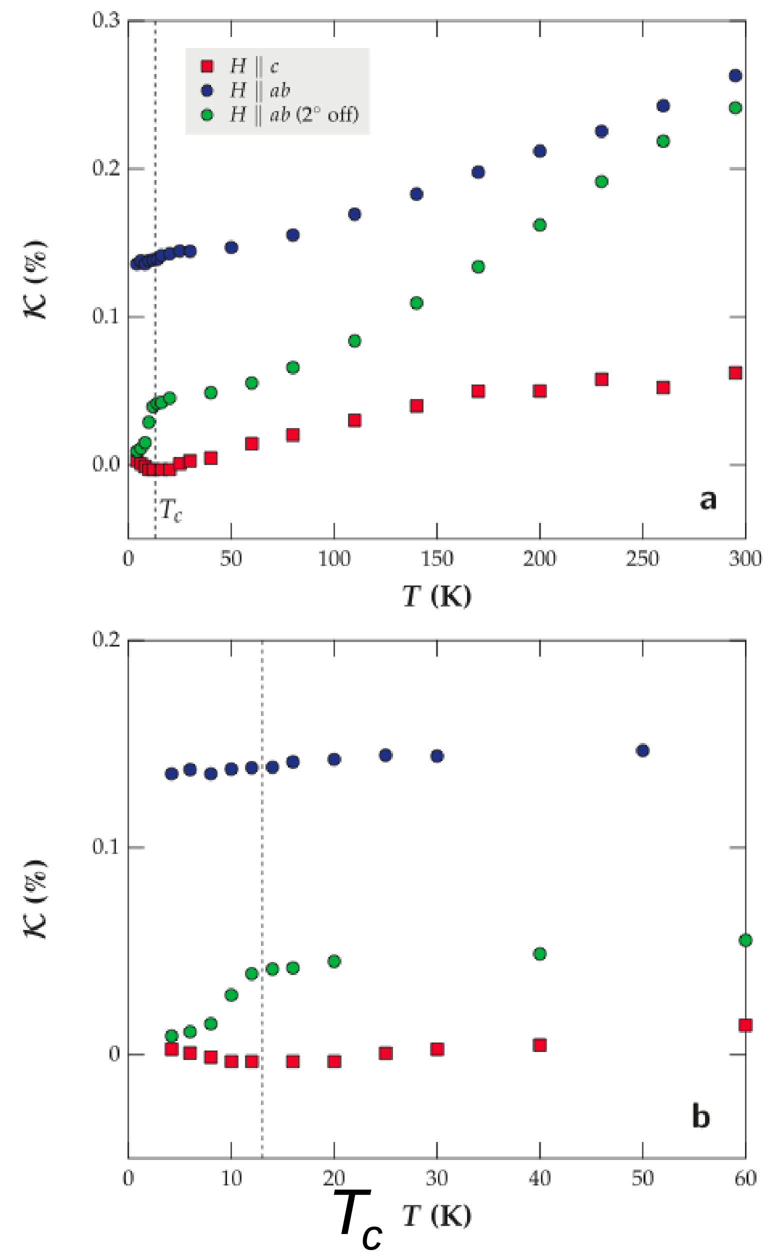
Bernd Buchner *et al.*

^{75}As NMR Knight shift



$T<T_c$

^{75}As NMR

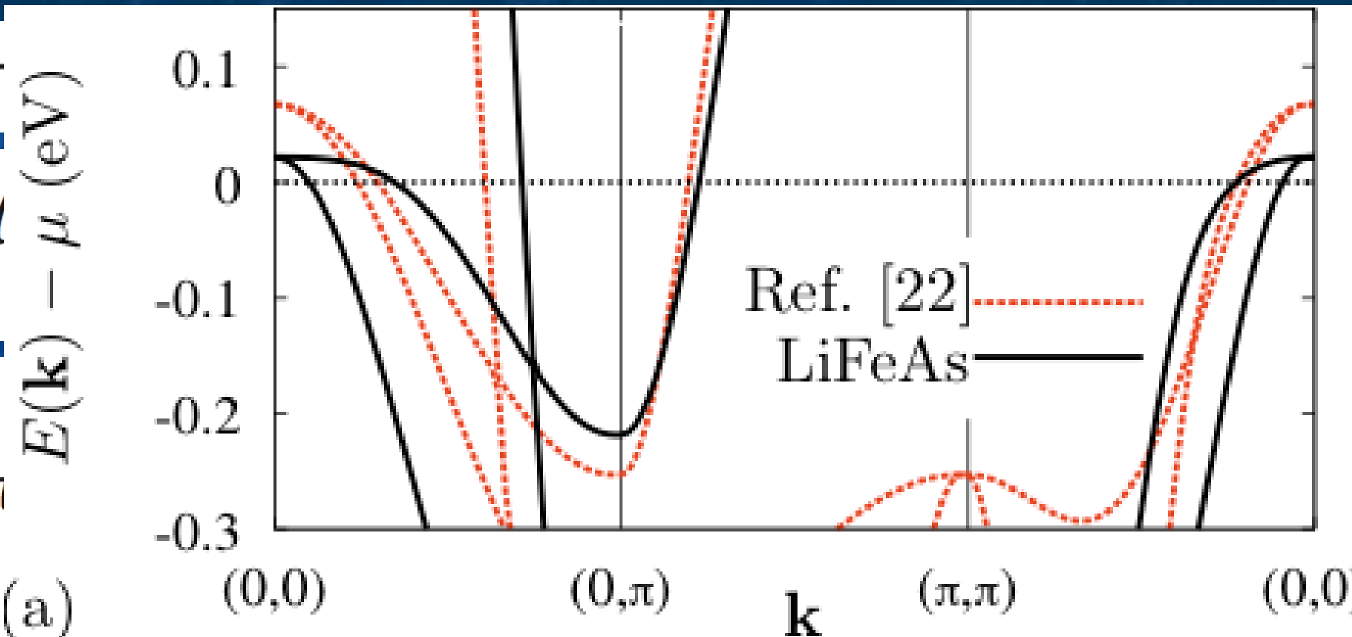


This constant K_{ab} **only** compatible with triplet superconductivity

The strong angle dependence is particular and interesting

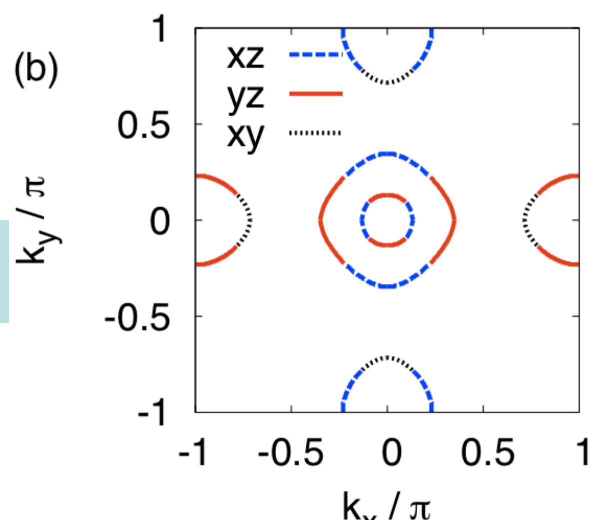
Baek, Grafe, Hammerath, Fuchs, Harnagea, Wurmehl, JvdB & Buchner

Capturing the electronic structure of LiFeAs



$\alpha \neq \beta$

$+ J_H \sum$ ... $\hat{S}_{i\beta}$



Poor nesting

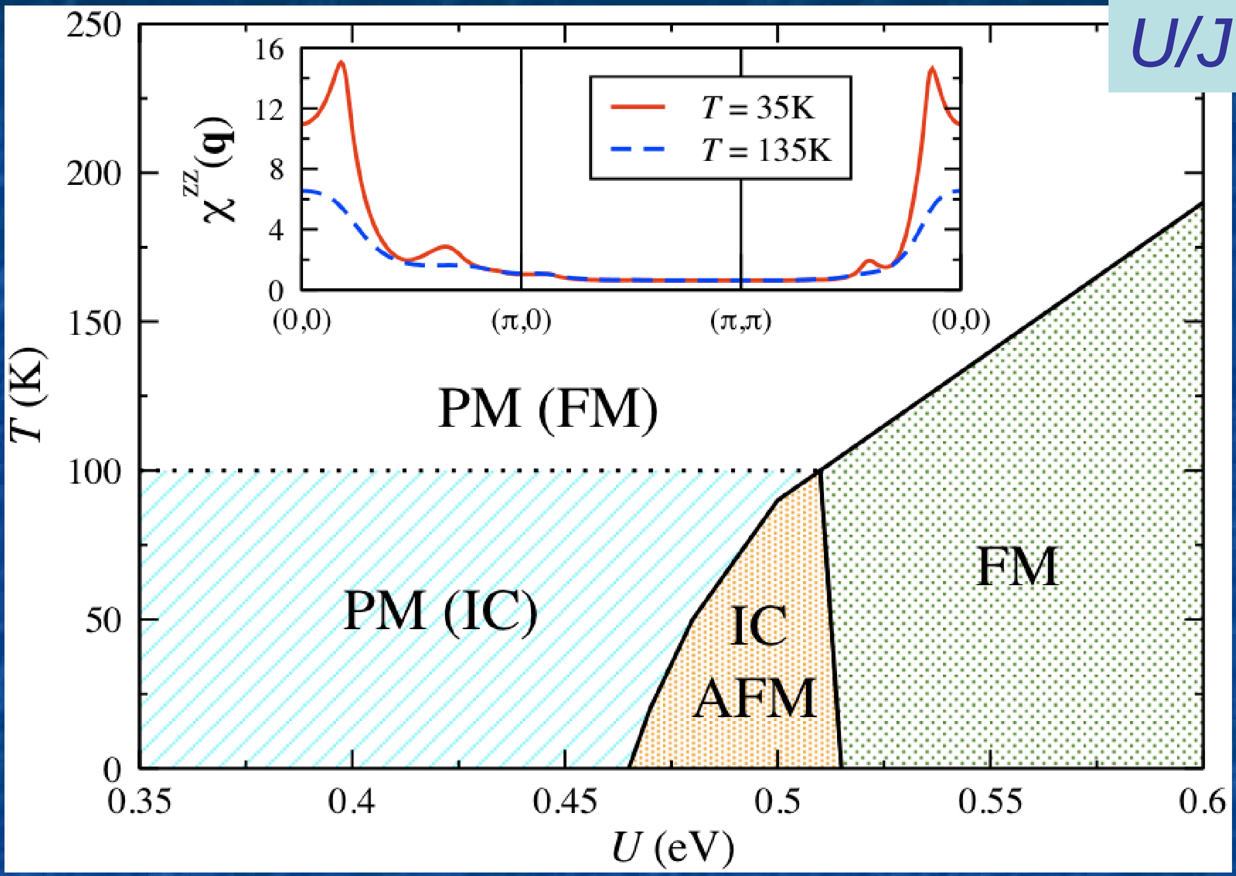
Matches ARPES

Borisenko *et al.*, PRL 2101

Brydon, Daghofer, Timm & JvdB
arXiv:1009:3104
PRB, in press

Magnetic phases

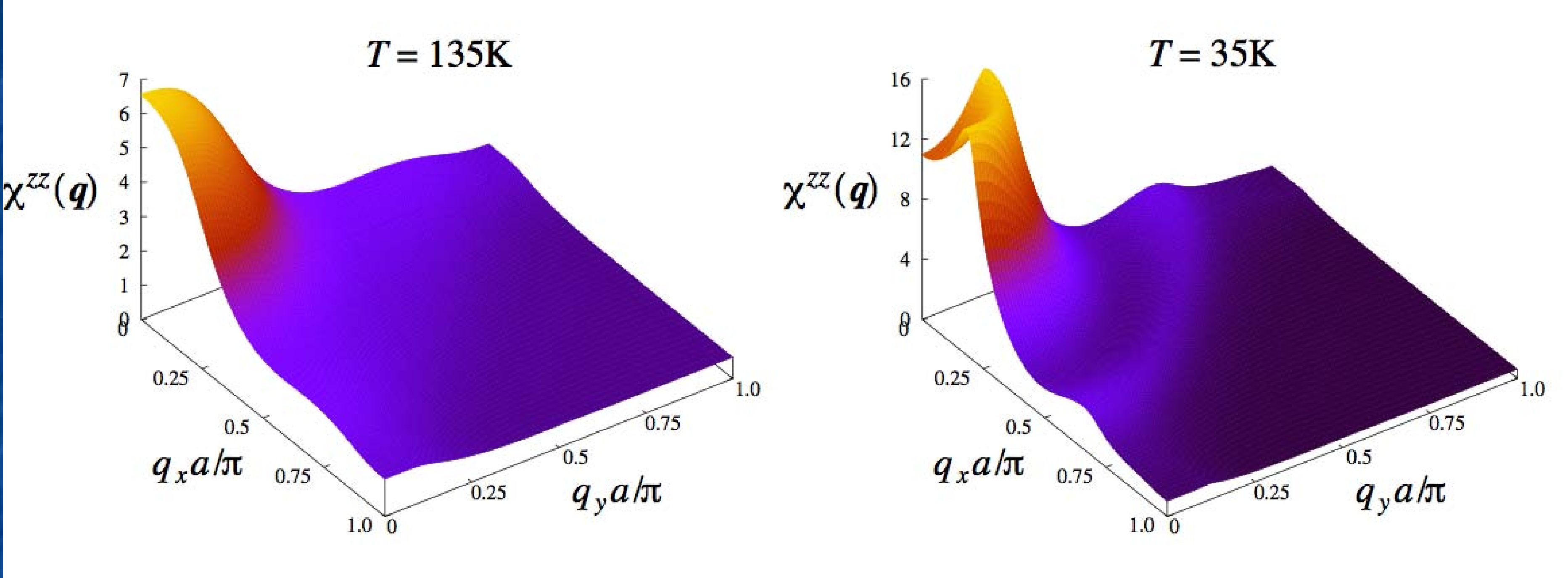
U/J=4



--Mean field

--Analysis of magnetic instabilities in RPA

Magnetic susceptibility



radius of crater is twice radius inner hole pocket

Brydon *et al.*

SC instabilities

Pairing vertex within fluctuation exchange approximation

Scalapino, Loh, Hirsch, PRB 34,8190 (1986)

Graser, Maier, Hirschfeld, Scalapino, NJP 11, 025016 (2009)

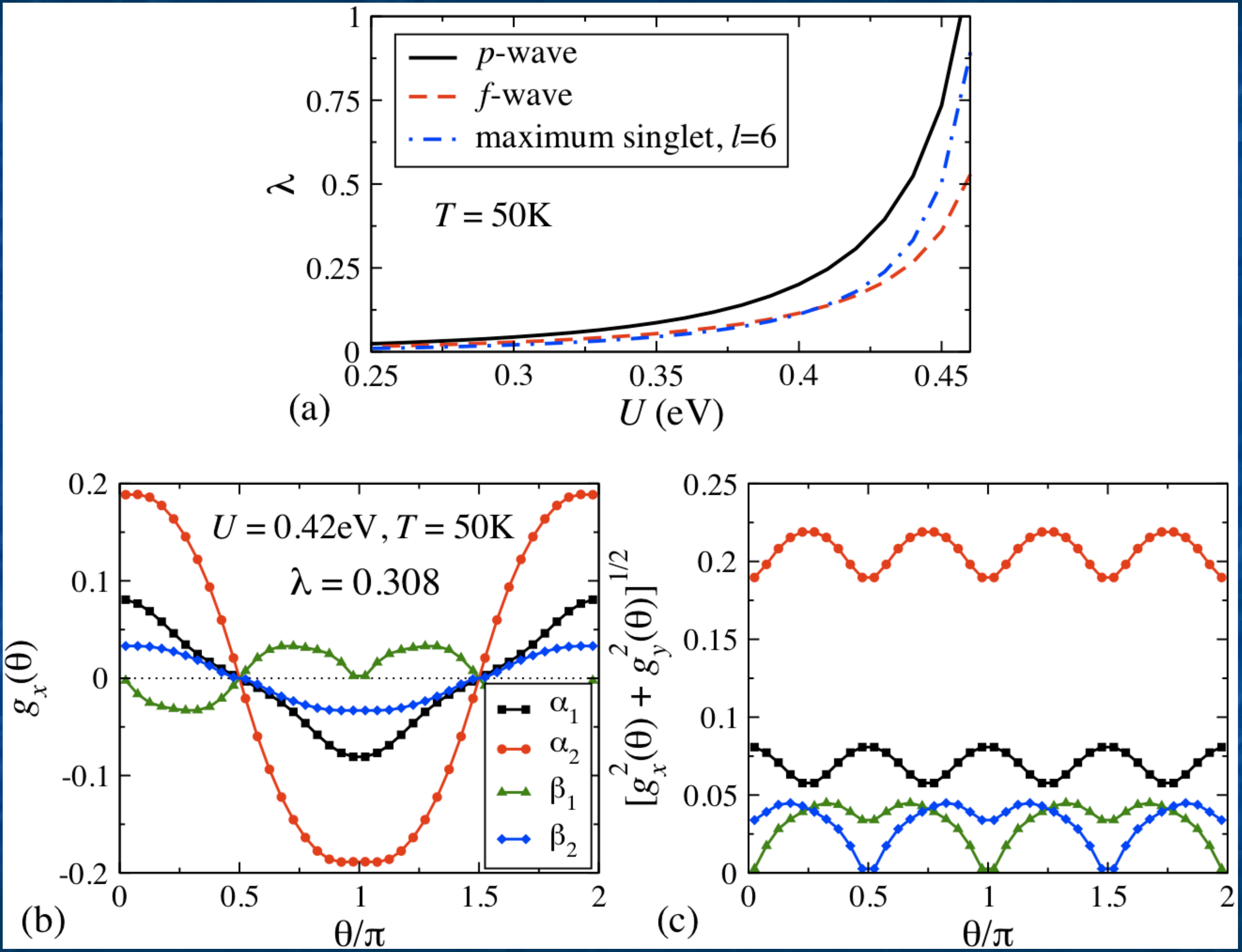
$$\hat{\Gamma}^s(\mathbf{k},\mathbf{k}',\omega) = \left[\frac{3}{2}\hat{U}^S\hat{\chi}^S(\mathbf{k}-\mathbf{k}',\omega)\hat{U}^S + \frac{1}{2}\hat{U}^S - \frac{1}{2}\hat{U}^C\hat{\chi}^C(\mathbf{k}-\mathbf{k}',\omega)\hat{U}^C + \frac{1}{2}\hat{U}^C\right]$$

$$\hat{\Gamma}^t(\mathbf{k},\mathbf{k}',\omega) = \left[-\frac{1}{2}\hat{U}^S\hat{\chi}^S(\mathbf{k}-\mathbf{k}',\omega)\hat{U}^S + \frac{1}{2}\hat{U}^S - \frac{1}{2}\hat{U}^C\hat{\chi}^C(\mathbf{k}-\mathbf{k}',\omega)\hat{U}^C + \frac{1}{2}\hat{U}^C\right]$$

Determine leading pairing instability from

$$-\sum_j \oint_{C_j} \frac{dk'_{\parallel}}{4\pi^2 v_{F,j}(\mathbf{k}')} \Gamma^{\nu}_{ij}(\mathbf{k},\mathbf{k}') g_\nu(\mathbf{k}') = \lambda g_\nu(\mathbf{k})$$

Leading SC instability and gap



Brydon, Daghofer, Timm & JvdB, arXiv:1009:3104, PRB, in press

Conclusions

Orbital degrees of freedom / nematic correlations relevant in iron pnictides

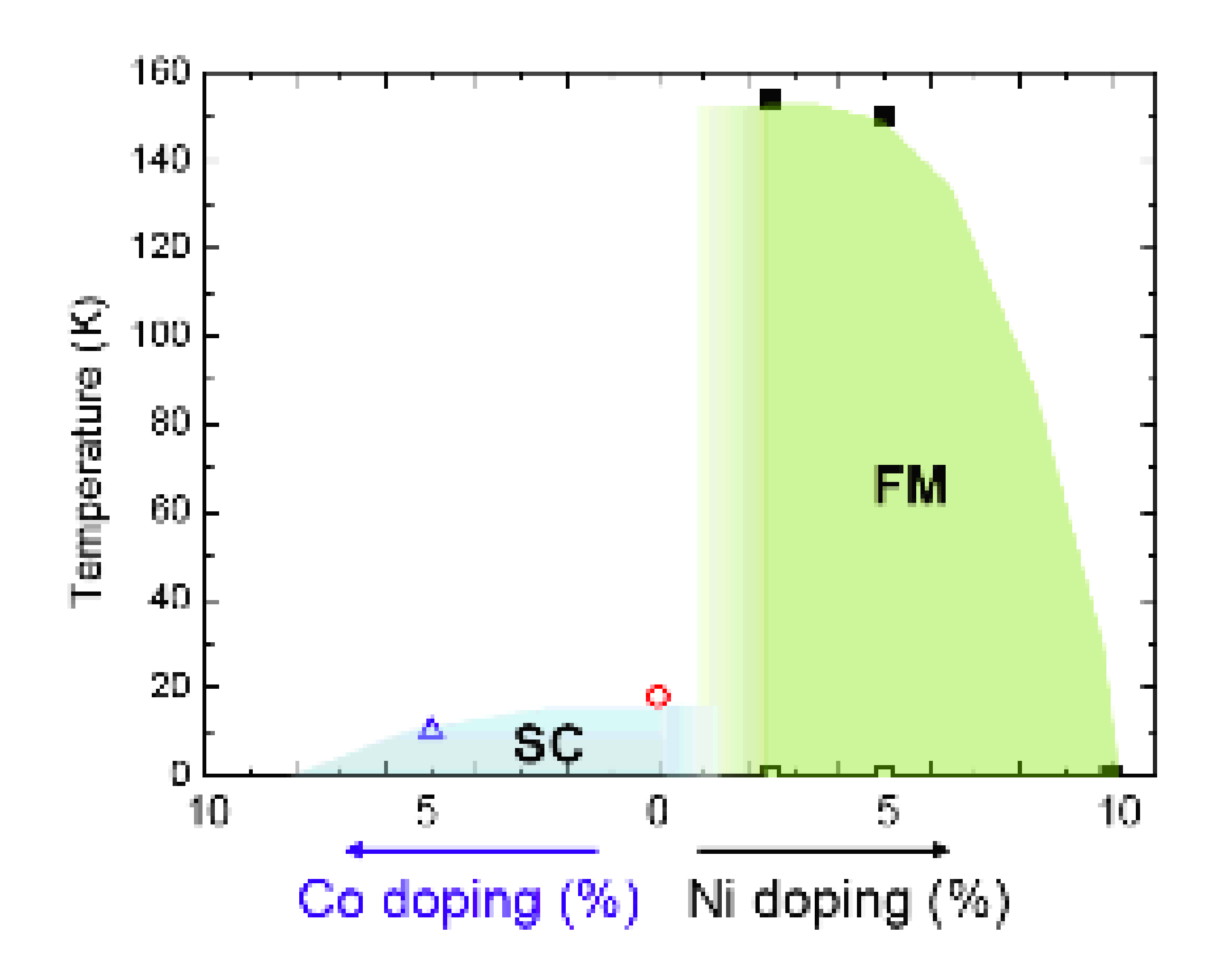
LiFeAs has a triplet superconducting phase

experiment + theory

LiFeAs close to ferromagnetic instability

theory + ...

Magnetic Instability of LiFeAs



Bernd Buchner *et al.*