Hunds interaction, spin-orbit coupling and the mechanism of superconductivity in heavily hole-doped iron pnictides

Oskar Vafek

National High Magnetic Field Laboratory

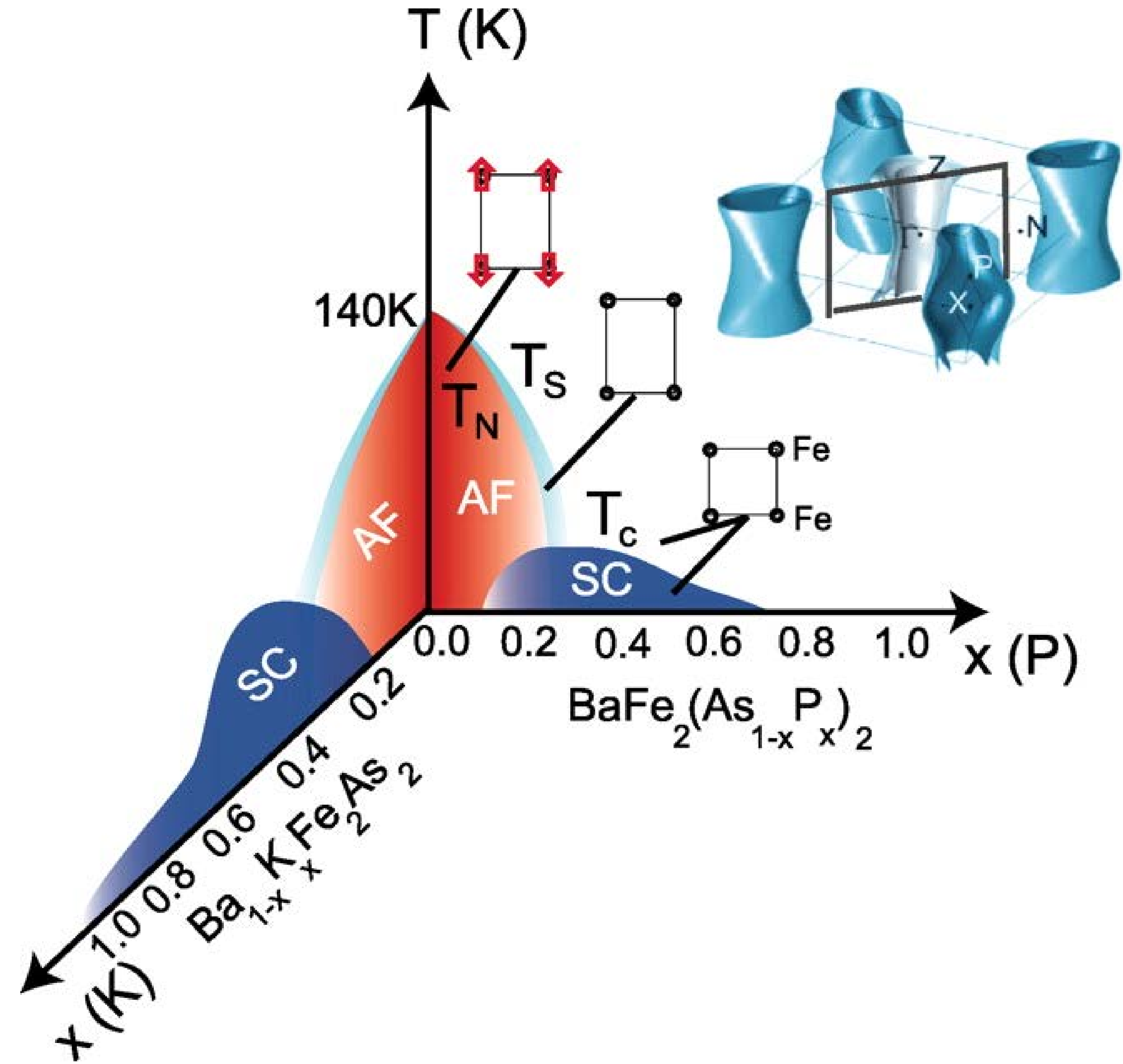
and

Florida State University

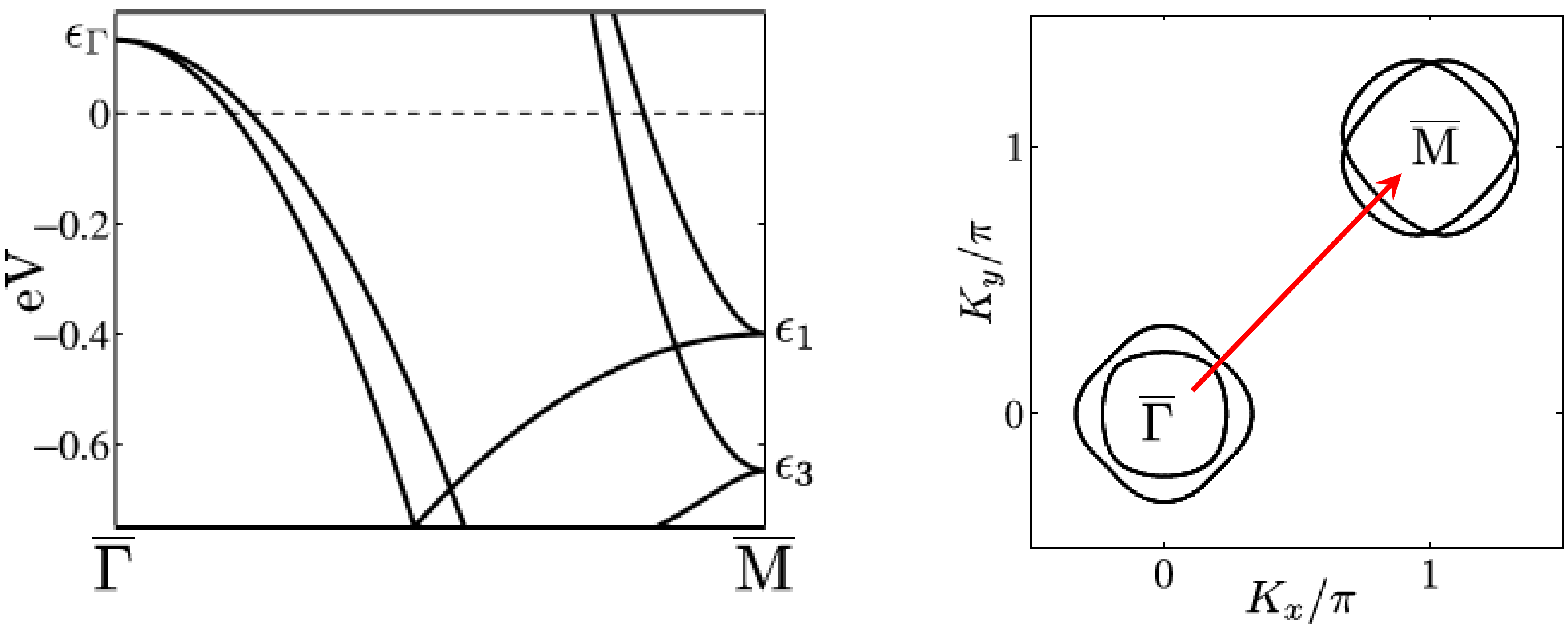
Tallahassee, FL

Collaborator

Andrey Chubukov

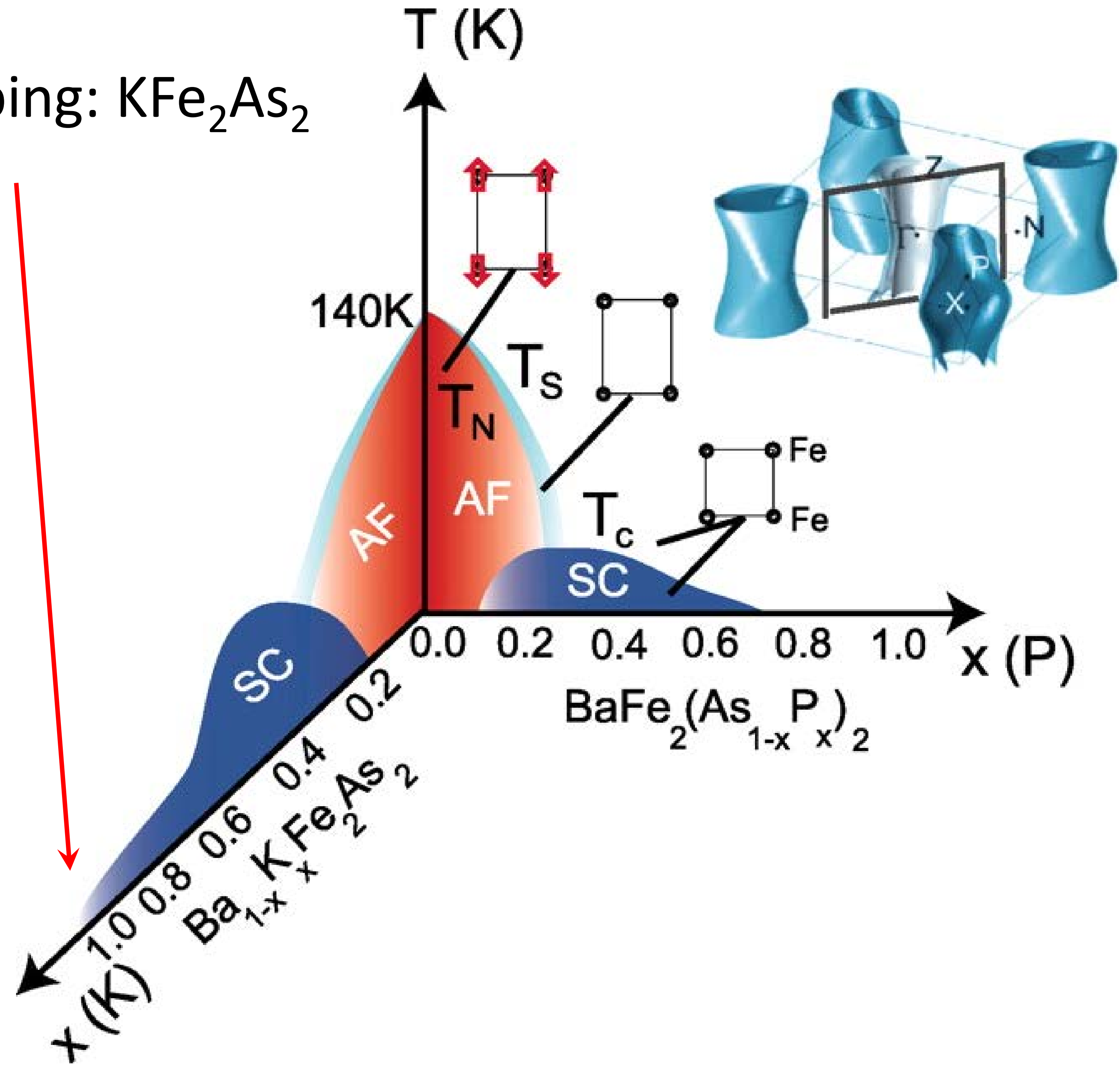


T (K)
140K
T_N
T_S
AF
AF
T_c
SC
SC
Fe
Fe
Z
Γ
N
P
X
0.0 0.2 0.4 0.6 0.8 1.0
x (P)
$BaFe_2(As_{1-x}P_x)_2$
0.2 0.4 0.6 0.8 1.0
x (K)
$Ba_{1-x}K_xFe_2As_2$

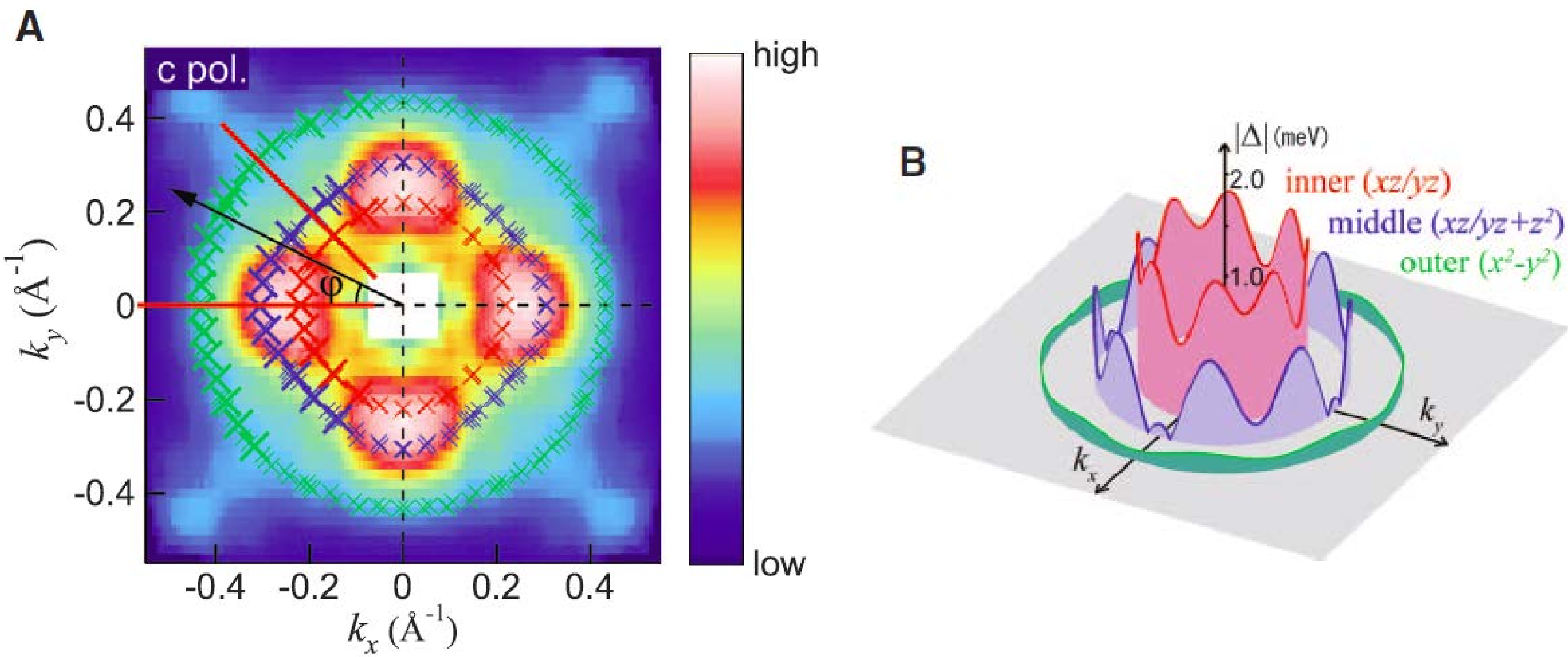


ϵ_Γ
0
−0.2
−0.4
−0.6
eV
ϵ_1
ϵ_3
$\overline{\Gamma}$
$\overline{\mathrm{M}}$
K_y/π
K_x/π
0
1

Strong hole doping: KFe_2As_2
($T_c \approx 3K$)



KFe_2As_2



Okazaki et.al.
Science (2012)

Even if the pairing symmetry is s-wave, or more precisely A_{1g}, such experiments indicate that the Cooper pairs have a richer internal structure that those of conventional sc.

(Caricature of the…) Basic idea (Γ point)

$$\psi_\sigma^\dagger = \left(d_{xz,\sigma}^\dagger, d_{yz,\sigma}^\dagger\right)$$

Cooper pair: $\psi_\alpha^\dagger M \psi_\beta^*$

		Kanamori Hamiltonian
s++ wave (A_{1g})	$\Delta_0 \psi_\alpha^\dagger 1 i\sigma_2^{\alpha\beta} \psi_\beta^*$	$(U+J')/2$
d_{xy} wave (B_{2g})	$\Delta_1 \psi_\alpha^\dagger \tau_1 i\sigma_2^{\alpha\beta} \psi_\beta^*$	$(U'+J)/2$
$d_{x^2-y^2}$ wave (B_{1g})	$\Delta_3 \psi_\alpha^\dagger \tau_3 i\sigma_2^{\alpha\beta} \psi_\beta^*$	$(U-J')/2$
triplet (A_{2g})	$\vec{\Delta}_2 \cdot \psi_\alpha^\dagger \tau_2 (i\sigma_2\vec{\sigma})^{\alpha\beta} \psi_\beta^*$	$(U'-J)/2$

OV and A. Chubukov, PRL **118**, 087003 (2017)

(Caricature of the...) Basic idea (Γ point)

$$\psi_\sigma^\dagger = \left(d_{xz,\sigma}^\dagger, d_{yz,\sigma}^\dagger\right)$$

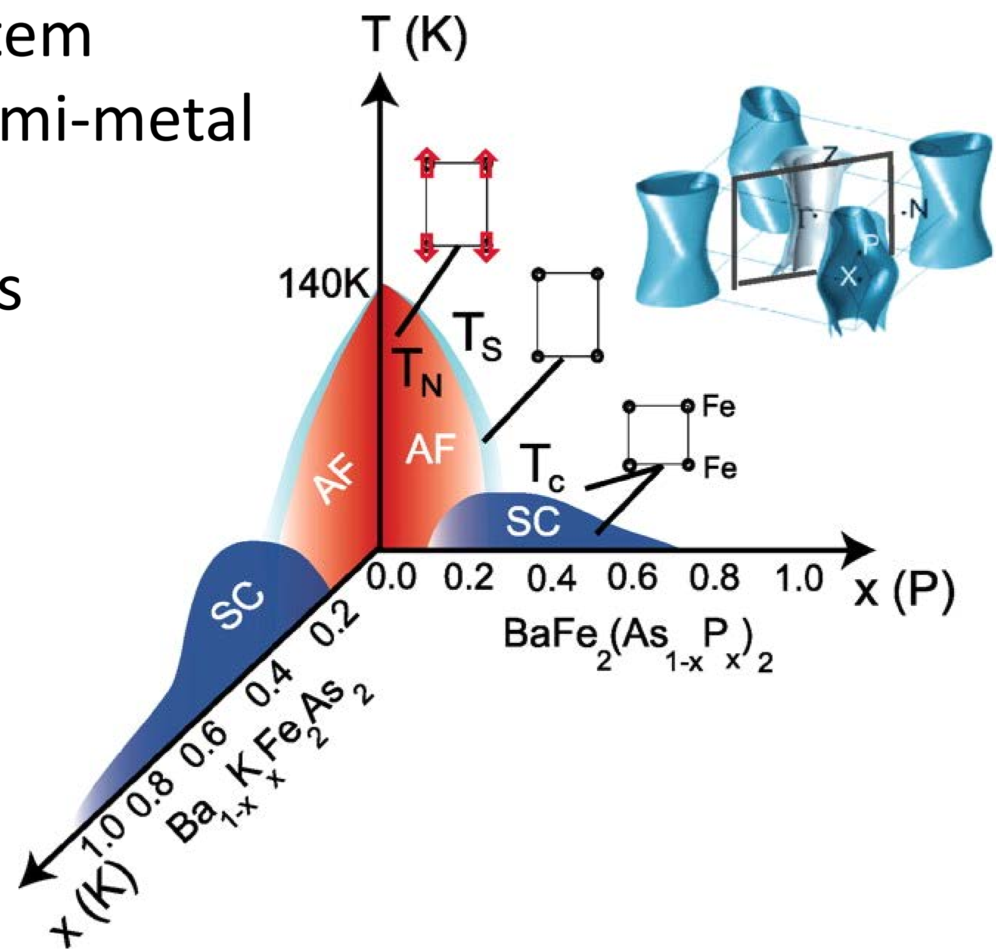
Cooper pair: $\psi_\alpha^\dagger M \psi_\beta^*$

s++ wave (A_{1g})	$\Delta_0 \psi_\alpha^\dagger 1 i\sigma_2^{\alpha\beta} \psi_\beta^*$
d_{xy} wave (B_{1g})	$\Delta_1 \psi_\alpha^\dagger \tau_1 i\sigma_2^{\alpha\beta} \psi_\beta^*$
$d_{x^2-y^2}$ wave (B_{2g})	$\Delta_3 \psi_\alpha^\dagger \tau_3 i\sigma_2^{\alpha\beta} \psi_\beta^*$
triplet (A_{2g})	$\vec{\Delta}_2 \cdot \psi_\alpha^\dagger \tau_2 (i\sigma_2 \vec{\sigma})^{\alpha\beta} \psi_\beta^*$ → (Spin orbit coupling) → s+- wave (A_{1g}) + Eg

OV and A. Chubukov, PRL **118**, 087003 (2017)

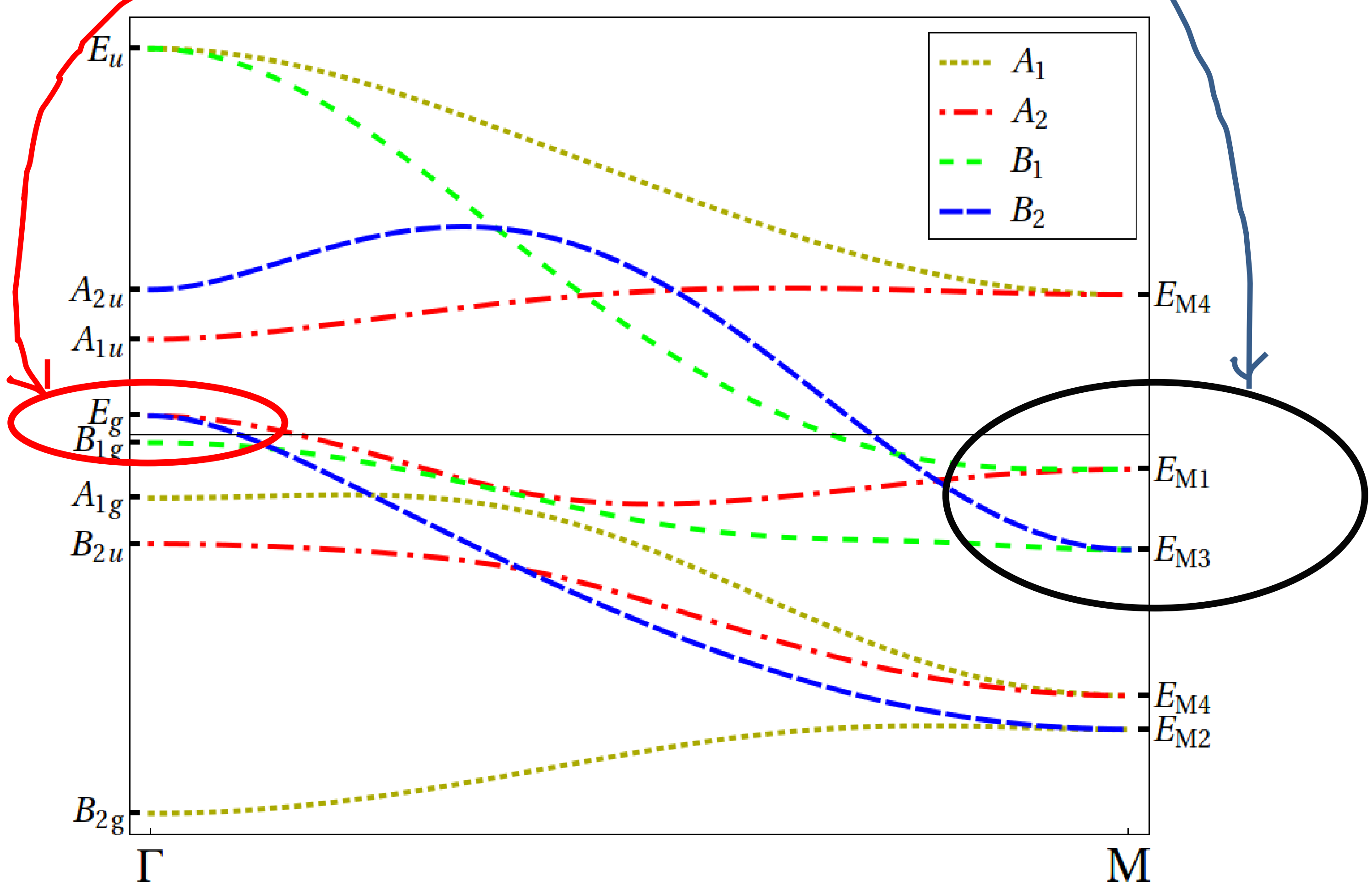
Low carrier density, quasi 2D system
parent state is a compensated semi-metal

=> Luttinger’s theory of invariants



Full tight banding band structure and the low energy `spinor’

$$\psi_\sigma(\mathbf{k}) = \begin{pmatrix} \psi_{X,\sigma}(\mathbf{k}) \\ \psi_{Y,\sigma}(\mathbf{k}) \\ \psi_{\Gamma,\sigma}(\mathbf{k}) \end{pmatrix}$$



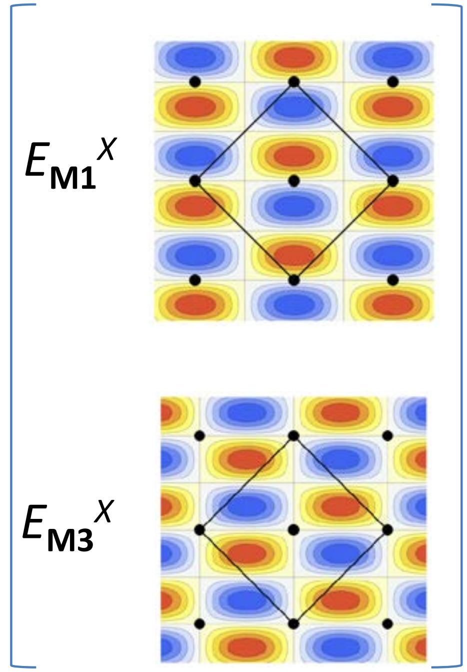
Cvetkovic and OV, PRB **88**, 134510 (2013)

Low-energy effective theory

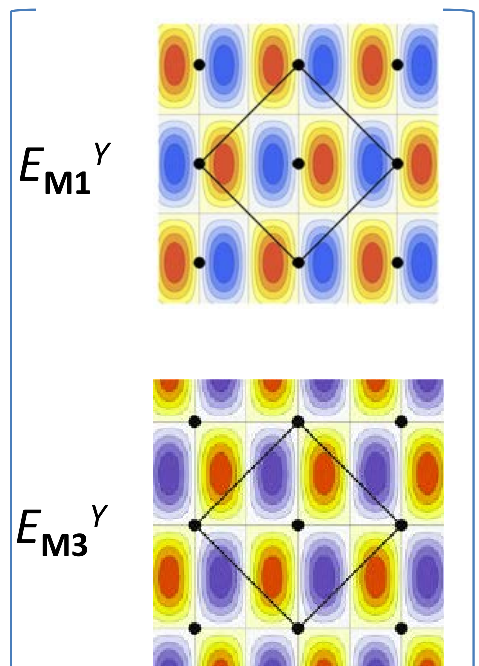
Low-energy spinor
(Γ: E_g states; **M**: E_{M1} and E_{M3} states):

$$\psi_\sigma(\mathbf{k}) = \begin{pmatrix} \psi_{X,\sigma}(\mathbf{k}) \\ \psi_{Y,\sigma}(\mathbf{k}) \\ \psi_{\Gamma,\sigma}(\mathbf{k}) \end{pmatrix}$$

$$\begin{bmatrix} Yz_A+Yz_B \\ -Xz_A-Xz_B \end{bmatrix}$$



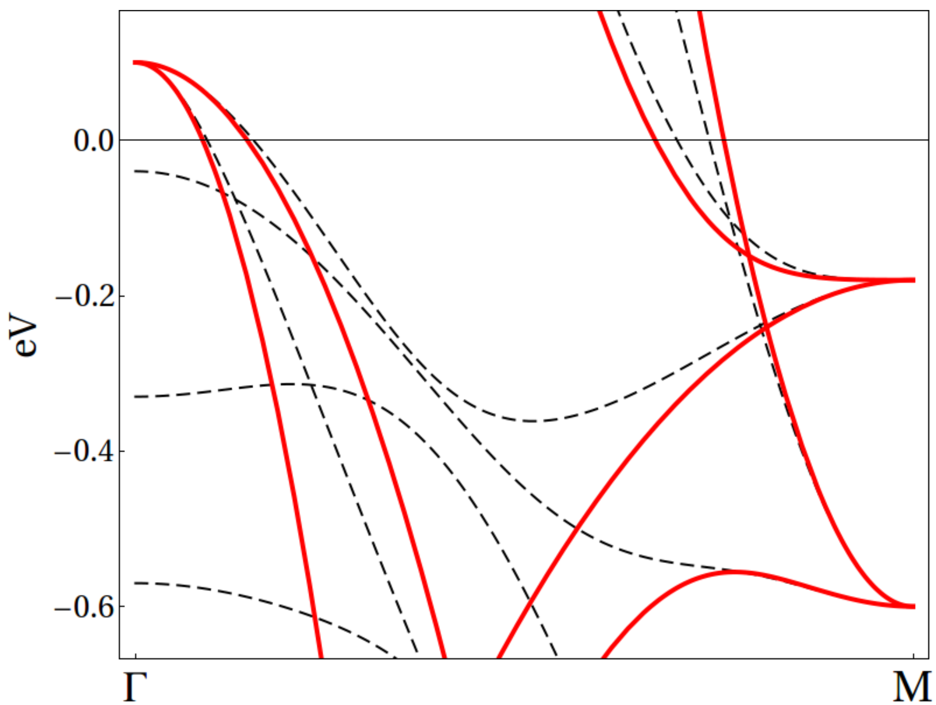
ODD under n-glide

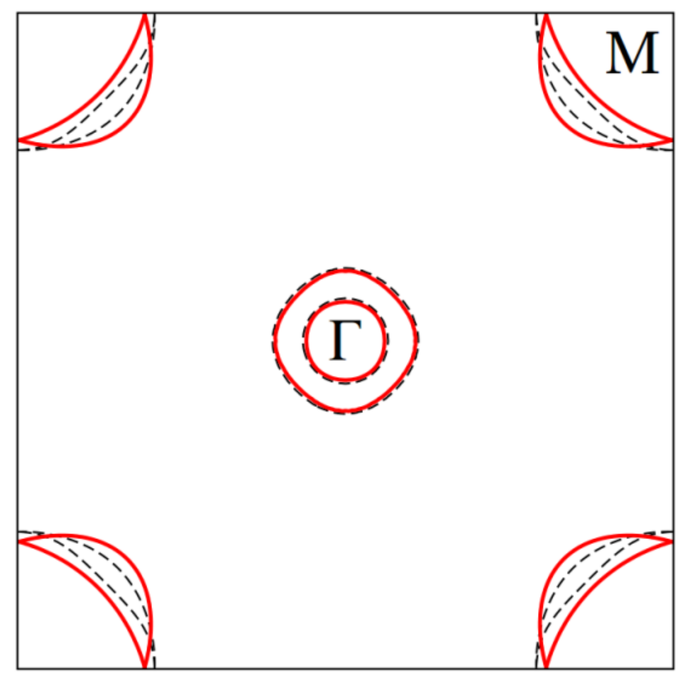


EVEN under n-glide

=> Do not mix (at k_z=0)

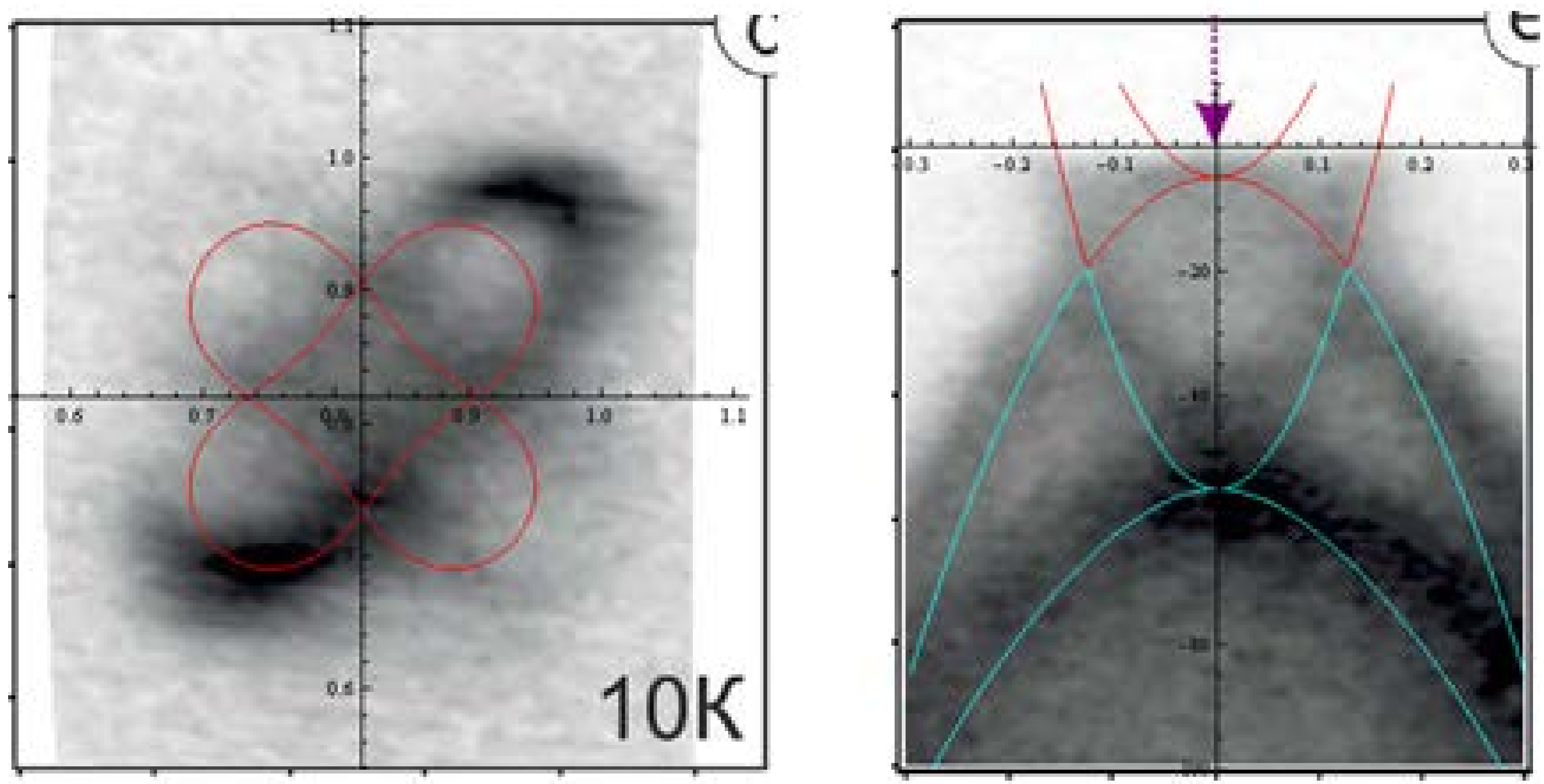
Comparison of the low-energy effective theory and the tight binding models





K. Kuroki, *et al.*, PRL **101**, 087004 (2008)

Fit to the bulk FeSe ARPES (assumed tetragonal)



Fedorov et. al Scientific **Reports** 6:36834 (2016)

Effective Hamiltonian

$$\mathcal{H} = H_0 + H_{int}$$

$$H_0 = \sum_{\mathbf{k}} \sum_{\alpha,\beta=\uparrow,\downarrow} \psi^\dagger_{\mathbf{k},\alpha} \left(h_{\mathbf{k}} \delta_{\alpha\beta} + h^{SO} s^z_{\alpha\beta} \right) \psi_{\mathbf{k},\beta}$$

$$h_{\mathbf{k}} = \begin{pmatrix} \mu - \frac{\mathbf{k}^2}{2m} + b k_x k_y & c\left(k_x^2 - k_y^2\right) \\ c\left(k_x^2 - k_y^2\right) & \mu - \frac{\mathbf{k}^2}{2m} - b k_x k_y \end{pmatrix}$$

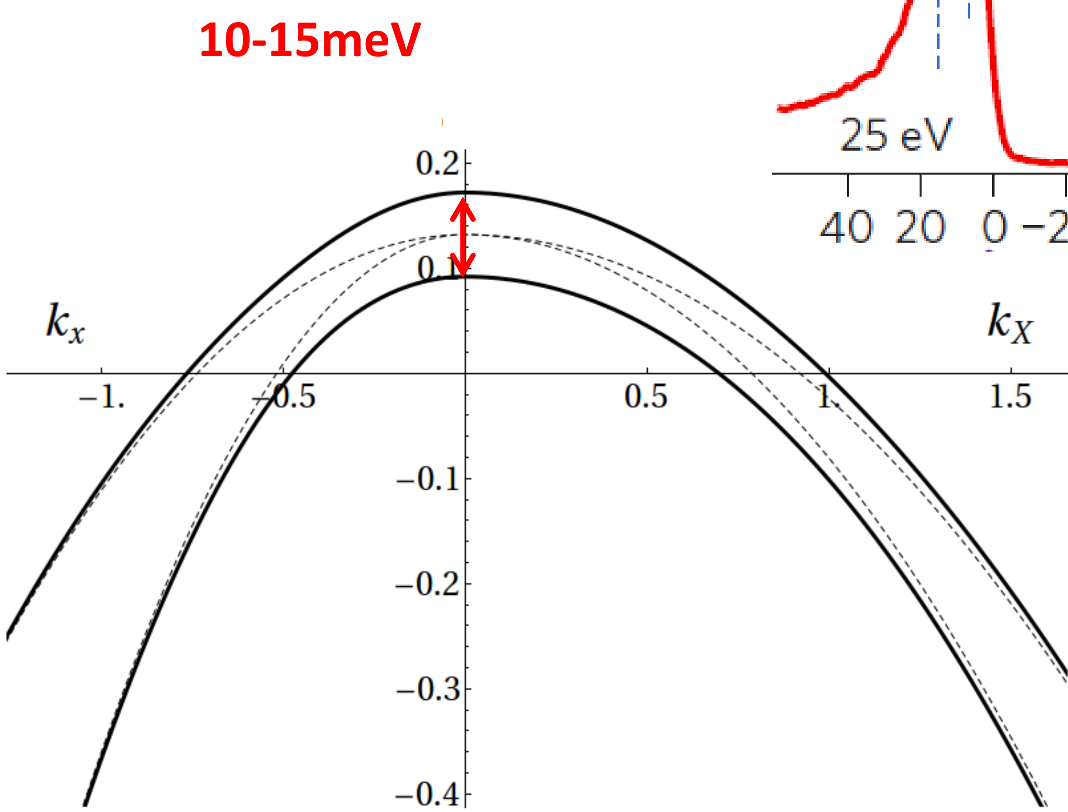
$$h^{SO} = \lambda \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

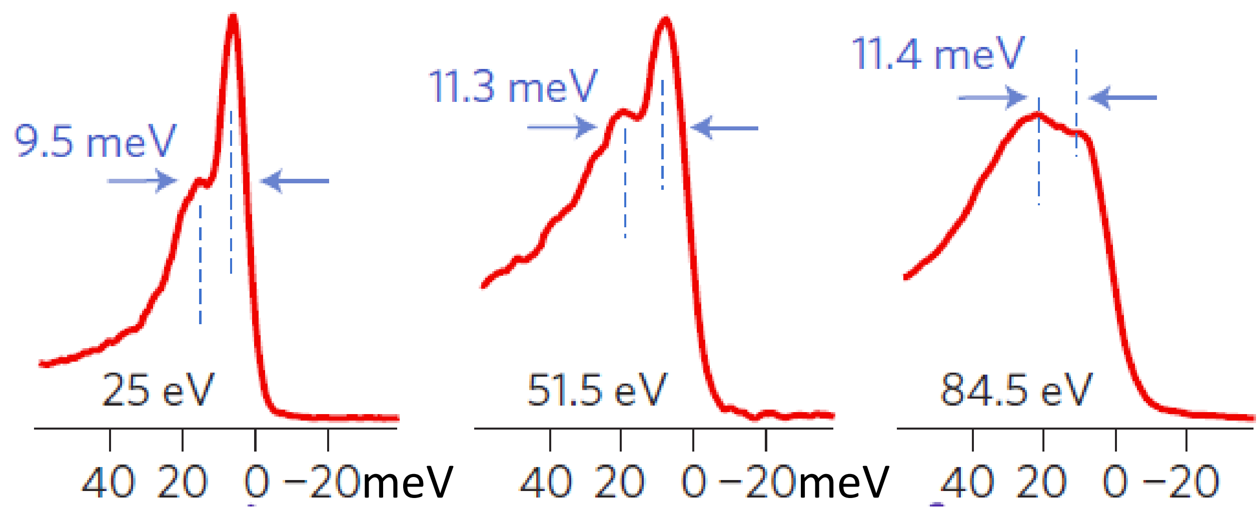
$$H_{int} = \sum_{j=0}^{3} \frac{g_j}{2} \int d^2\mathbf{r} : \psi^\dagger_\sigma(\mathbf{r}) \tau_j \psi_\sigma(\mathbf{r}) \psi^\dagger_{\sigma'}(\mathbf{r}) \tau_j \psi_{\sigma'}(\mathbf{r}) :$$

OV and A. Chubukov, PRL **118**, 087003 (2017)

Spin-orbit interaction in the low-energy effective theory

The effect on the spectrum





Borisenko et.al.
Nature Physics (2016)

Interaction Hamiltonian

$$
\begin{aligned}
H_{int} &= \sum_{j=0}^{3} \frac{g_j}{2} \int d^2\mathbf{r} :\psi^\dagger_\sigma(\mathbf{r})\tau_j\psi_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r})\tau_j\psi_{\sigma'}(\mathbf{r}): \\
g_0 &= \frac{1}{2}(U+U') + \ldots > 0 \\
g_1 &= J + \ldots > 0 \\
g_2 &= 0 + \ldots > 0 \\
g_3 &= \frac{1}{2}(U-U') + \ldots > 0
\end{aligned}
$$

intra-orbital Hubbard repulsion: U

inter-orbital Hubbard repulsion: U'

Hunds coupling: J

Fierz transformation of the interaction Hamiltonian

$$H_{int} = \sum_{j=0}^{3} \frac{\tilde{g}_j}{2} \int d^2\mathbf{r} \left(\psi_\sigma^\dagger(\mathbf{r})\tau_j \psi_{\sigma'}^*(\mathbf{r})\right) \left(\psi_{\sigma'}^T(\mathbf{r})\tau_j \psi_\sigma(\mathbf{r})\right)$$

where

$$\begin{pmatrix} \tilde{g}_0 \\ \tilde{g}_1 \\ \tilde{g}_2 \\ \tilde{g}_3 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 \end{pmatrix} \begin{pmatrix} g_0 \\ g_1 \\ g_2 \\ g_3 \end{pmatrix}$$

avoid large repulsive U:

$$\tilde{g}_1 = \frac{1}{2}(U' + J) + \ldots > 0$$

$$\tilde{g}_2 = \frac{1}{2}(U' - J) + \ldots$$

← could be attractive!

Symmetry of the pairing

$$\left(\psi_{\sigma}^{\dagger}(\mathbf{r})\tau_2\psi_{\sigma'}^{*}(\mathbf{r})\right)\left(\psi_{\sigma'}^{T}(\mathbf{r})\tau_2\psi_{\sigma}(\mathbf{r})\right) =$$
$$\frac{1}{2}\psi_{\alpha}^{\dagger}(\mathbf{r})\tau_2(s^y\vec{s})_{\alpha\beta}\psi_{\beta}^{*}(\mathbf{r})\cdot\psi_{\alpha'}^{T}(\mathbf{r})\tau_2(\vec{s}s^y)_{\alpha'\beta'}\psi_{\beta'}(\mathbf{r}).$$

pairing channel seemingly corresponds to spin triplet A_{2g}

However, the spin-orbit coupling term in H_0 changes the symmetry to A_{1g} (i.e. s-wave)

OV and A. Chubukov, PRL **118**, 087003 (2017)

Order parameters

$$\Delta_0 = \frac{1}{2}\tilde{g}_0\langle\psi_\alpha^T(\mathbf{r})1(-is^y)_{\alpha\beta}\psi_\beta(\mathbf{r})\rangle$$

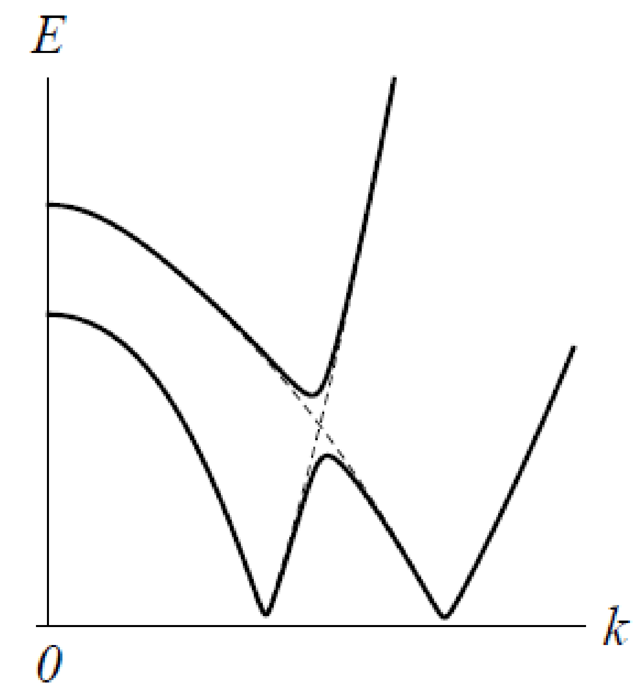
$$\Delta_2 = \frac{1}{2}\tilde{g}_2\langle\psi_\alpha^T(\mathbf{r})\tau_2(is^z s^y)_{\alpha\beta}\psi_\beta(\mathbf{r})\rangle$$

OV and A. Chubukov, PRL **118**, 087003 (2017)

Order parameters and spectrum

$$\mathcal{U}^\dagger H_{BdG}(\mathbf{k})\mathcal{U} = \begin{pmatrix} \xi_+ & 0 & \Delta_0 + \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\Delta_2 & -i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_{\mathbf{k}}^2}} \\ 0 & \xi_- & i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_{\mathbf{k}}^2}} & \Delta_0 - \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\Delta_2 \\ \Delta_0 + \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\Delta_2 & -i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_{\mathbf{k}}^2}} & -\xi_+ & 0 \\ i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_{\mathbf{k}}^2}} & \Delta_0 - \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\Delta_2 & 0 & -\xi_- \end{pmatrix}$$

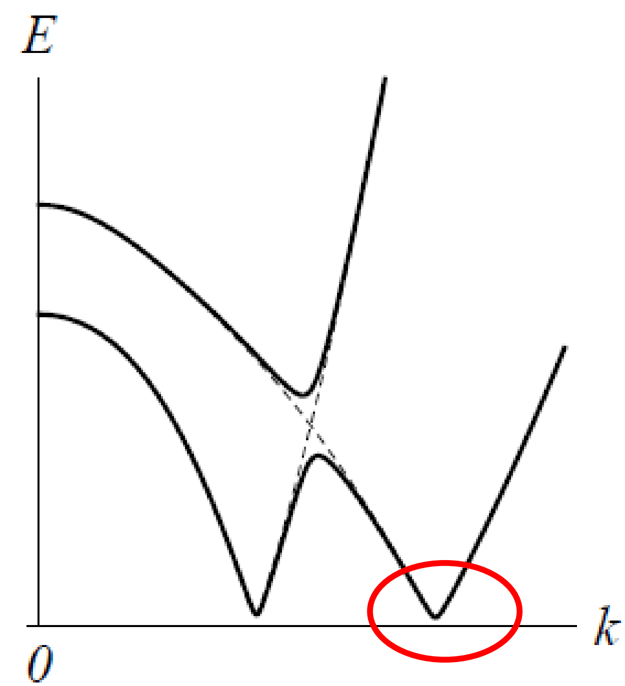
$$h_{\mathbf{k}} + \lambda\tau_2 \quad = \quad A_{\mathbf{k}}\mathbb{1} + \vec{B}_{\mathbf{k}}\cdot\vec{\tau}$$



Order parameters and spectrum

$$\mathcal{U}^\dagger H_{BdG}(\mathbf{k})\mathcal{U} = \begin{pmatrix} \xi_+ & 0 & \Delta_0 + \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & -i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} \\ 0 & \xi_- & i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & \Delta_0 - \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 \\ \Delta_0 + \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & -i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & -\xi_+ & 0 \\ i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & \Delta_0 - \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & 0 & -\xi_- \end{pmatrix}$$

$$h_\mathbf{k} + \lambda\tau_2 = A_\mathbf{k}\mathbb{1} + \vec{B}_\mathbf{k}\cdot\vec{\tau}$$

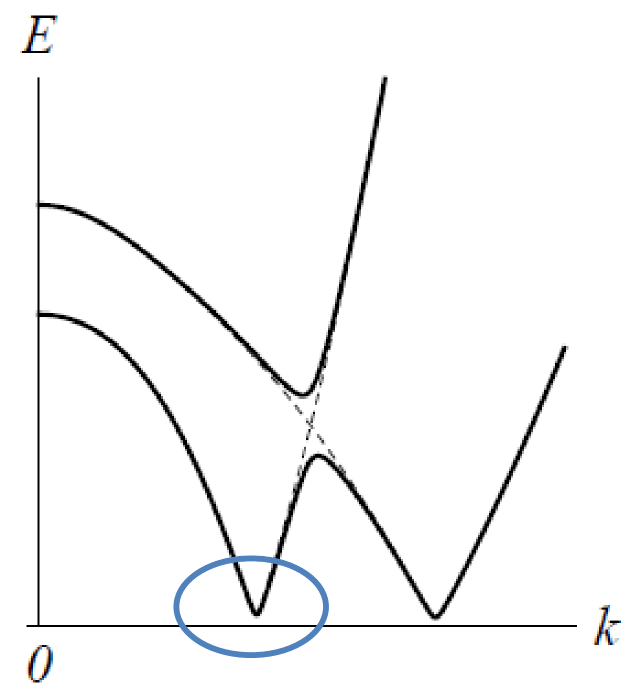


Order parameters and spectrum

$$\mathcal{U}^\dagger H_{BdG}(\mathbf{k})\mathcal{U} =$$

$$\begin{pmatrix} \xi_+ & 0 & \Delta_0 + \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & -i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} \\ 0 & \xi_- & i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & \Delta_0 - \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 \\ \Delta_0 + \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & -i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & -\xi_+ & 0 \\ i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & \Delta_0 - \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & 0 & -\xi_- \end{pmatrix}$$

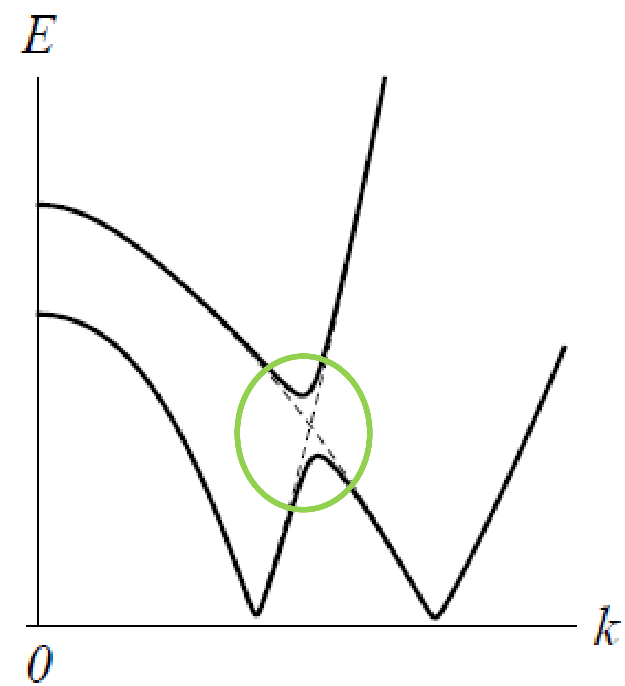
$$h_\mathbf{k} + \lambda\tau_2 = A_\mathbf{k}\mathbb{1} + \vec{B}_\mathbf{k}\cdot\vec{\tau}$$



Order parameters and spectrum

$$\mathcal{U}^\dagger H_{BdG}(\mathbf{k})\mathcal{U} = \begin{pmatrix} \xi_+ & 0 & \Delta_0 + \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & -i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} \\ 0 & \xi_- & i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & \Delta_0 - \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 \\ \Delta_0 + \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & -i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & -\xi_+ & 0 \\ i\Delta_2\sqrt{1-\frac{\lambda^2}{\vec{B}_\mathbf{k}^2}} & \Delta_0 - \frac{\lambda}{|\vec{B}_\mathbf{k}|}\Delta_2 & 0 & -\xi_- \end{pmatrix}$$

$$h_\mathbf{k} + \lambda\tau_2 = A_\mathbf{k}\mathbb{1} + \vec{B}_\mathbf{k}\cdot\vec{\tau}$$



Order parameters and spectrum

$$\frac{\Delta_0(T_c)}{\Delta_2(T_c)} = -\frac{\chi_{02}(T_c)}{\frac{1}{\tilde{g}_0} + \chi_{00}(T_c)} = -\mathcal{C}\,\frac{\lambda}{\mu} \qquad \mathcal{C} > 0$$

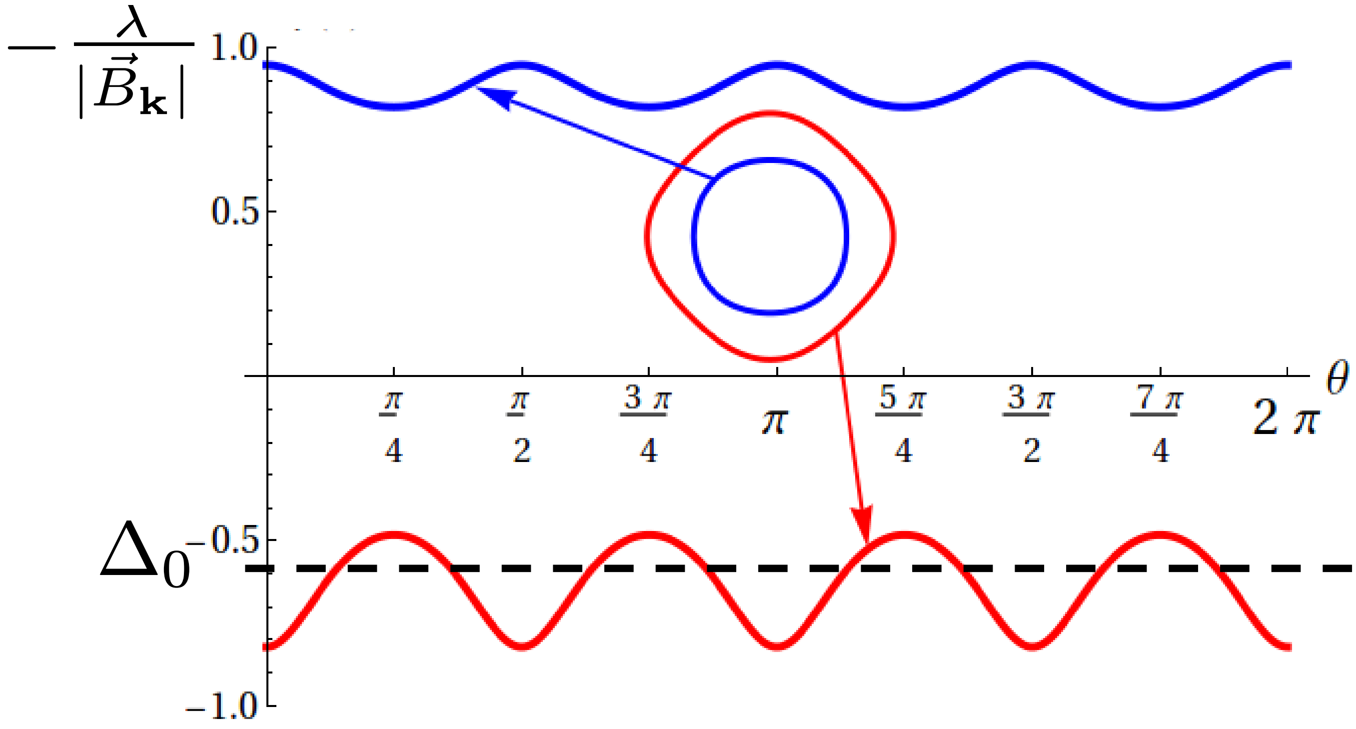
For dominant Δ_2

$$\frac{\Delta_0(T=0)}{\Delta_2(T=0)} = -\mathcal{C}'\,\frac{\lambda}{\mu} \qquad \mathcal{C}' > 0$$

$$\Rightarrow \Delta_0 \pm \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\Delta_2 = \Delta_2 \left(-\mathcal{C}\frac{\lambda}{\mu} \pm \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\right)$$

The anisotropic gap on the outer Fermi surface is (further) reduced by the admixture Δ_0

Order parameters and spectrum

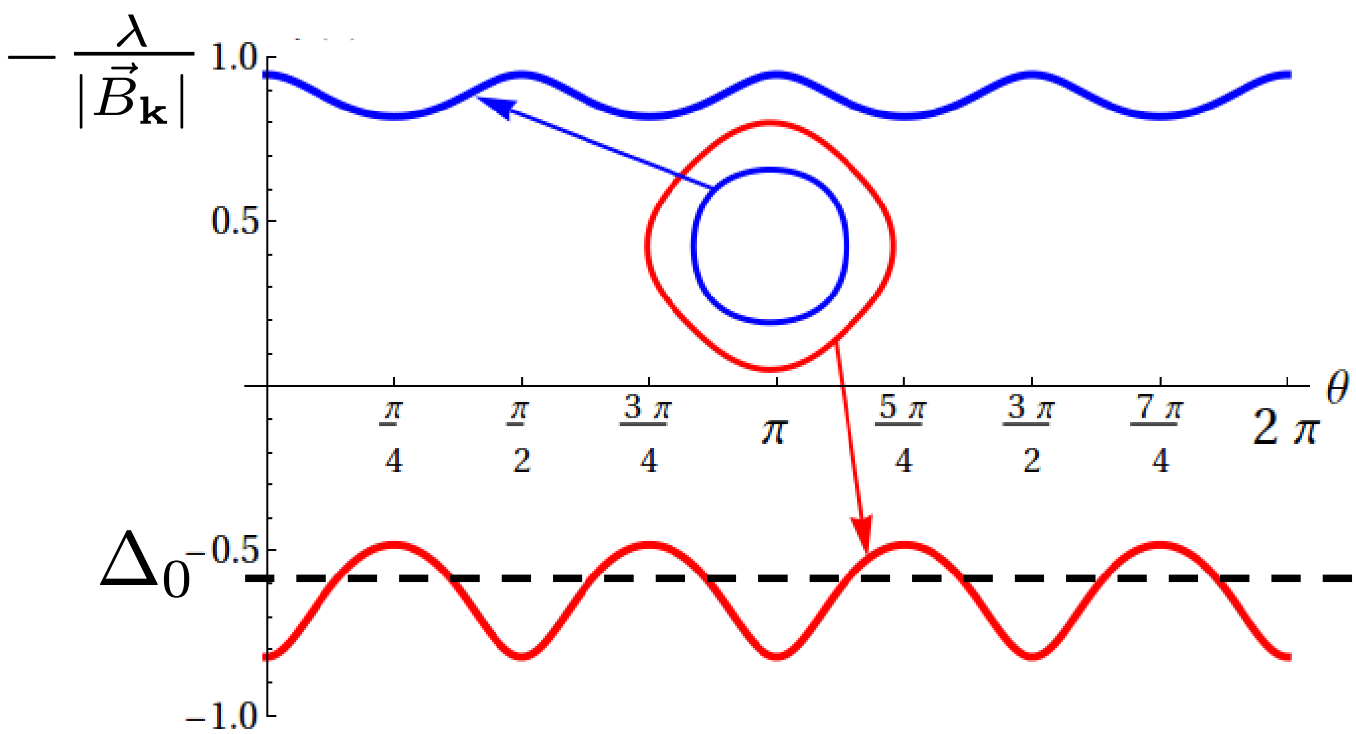


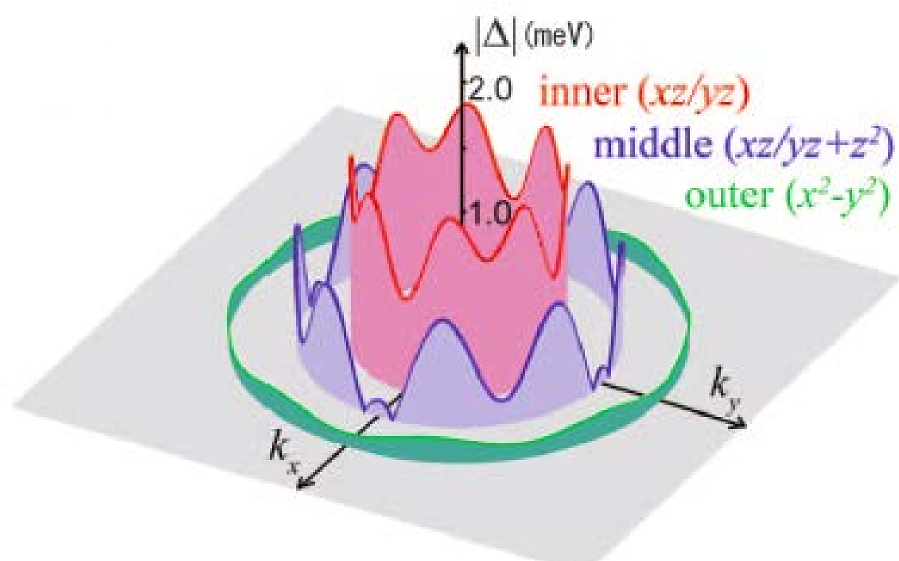
$$\Rightarrow \Delta_0 \pm \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\Delta_2 = \Delta_2\left(-\mathcal{C}\frac{\lambda}{\mu} \pm \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\right) \qquad \mathcal{C} > 0$$

Possibility of accidental nodes but only on the outer Fermi surface

The fourfold anisotropy leads to 8 such nodes

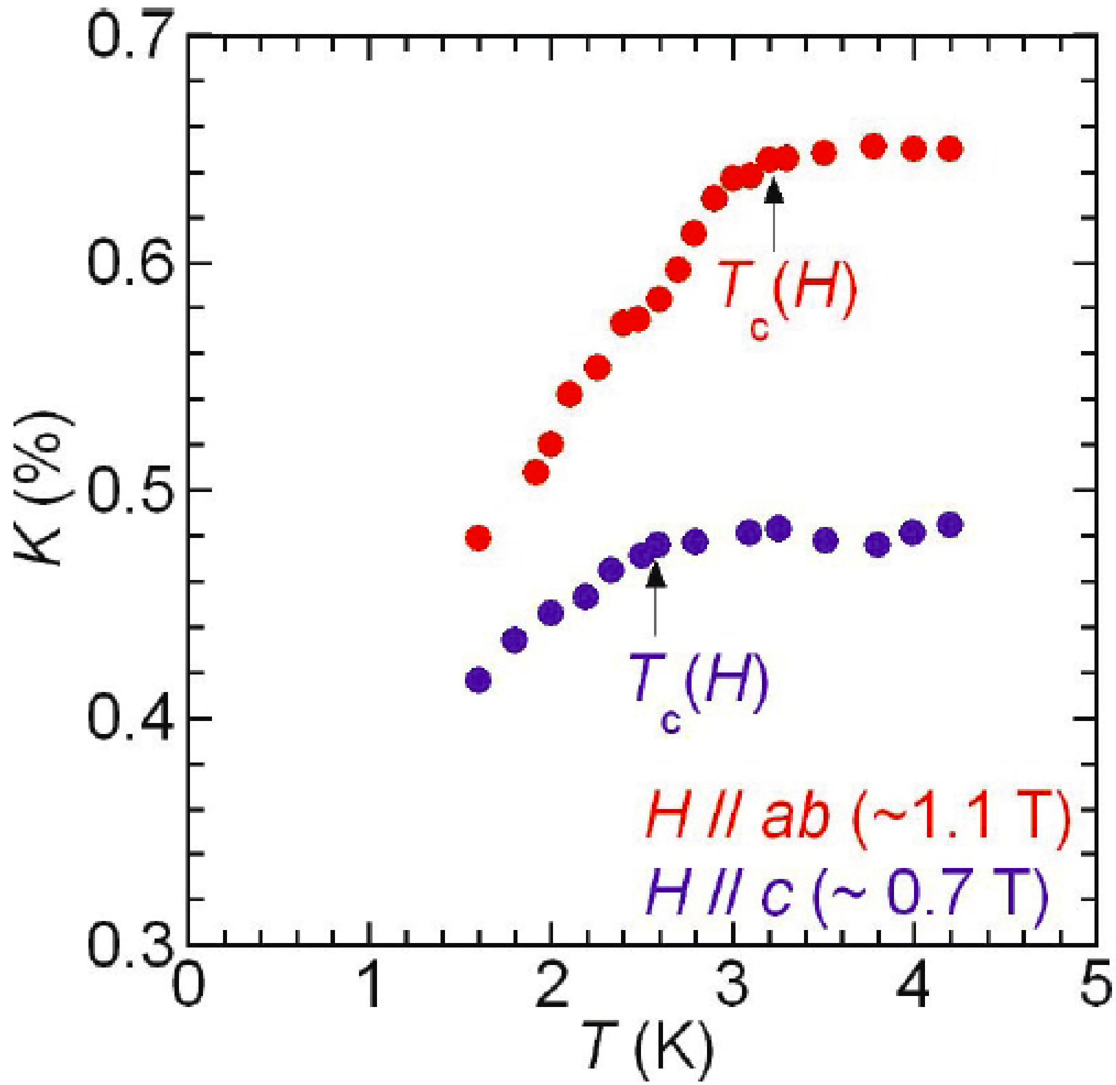
Order parameters and spectrum





Okazaki et.al.
Science (2012)

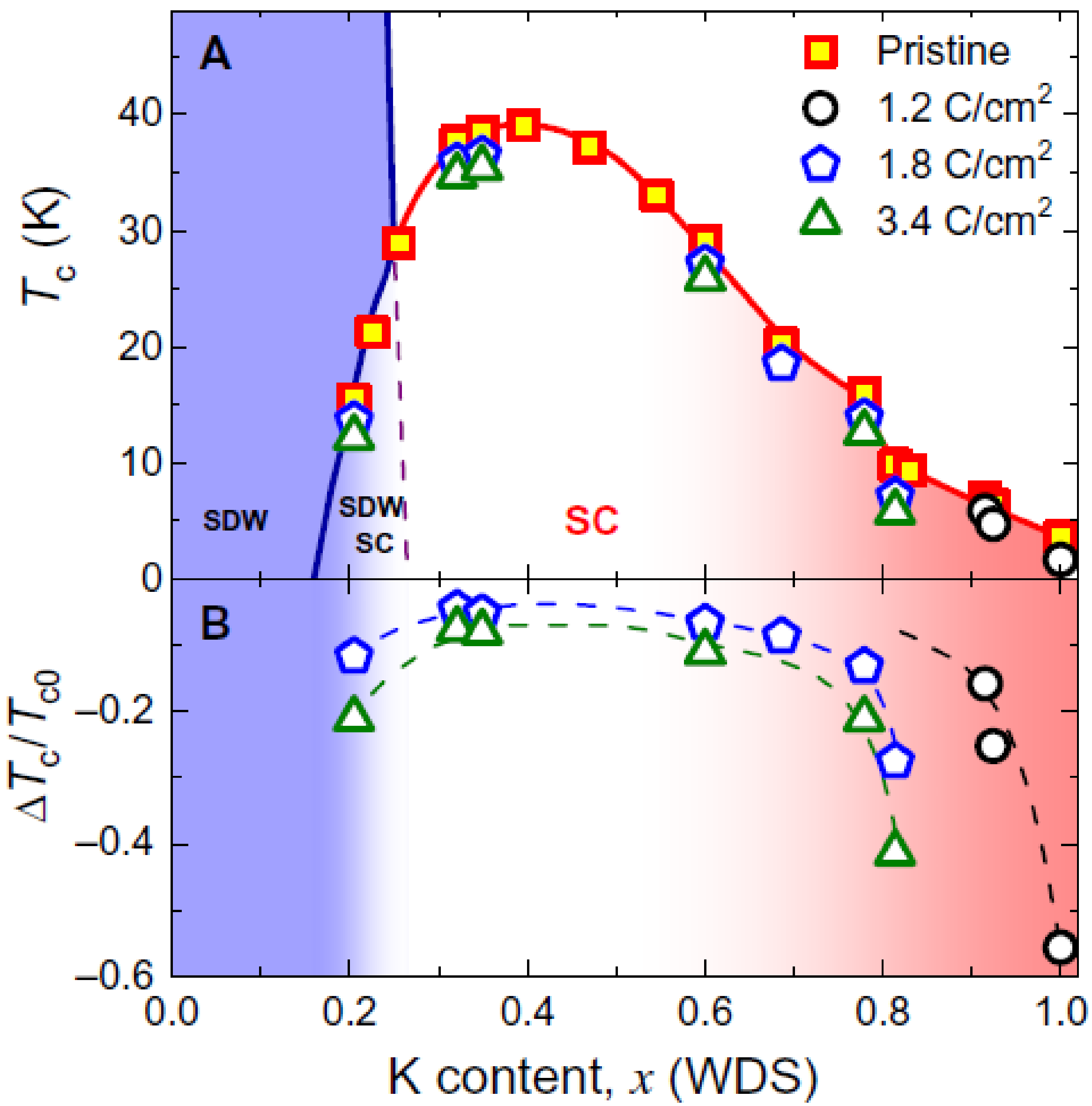
Knight shift KFe_2As_2



Fukuzawa et.al. J. Phys. Soc. Jpn **80** (2011)

$Ba_{1-x}K_xFe_2As_2$

$$T_c \sim e^{-\frac{\mu^2}{\lambda^2}\frac{1}{N_0(J-U')}}$$



Cho et.al. Sci.Adv. (2016)

Open questions

- How to (reliably) determine the parameters in the low energy effective Hamiltonian from first principles?
- Under what conditions do we achieve $J_{eff}>U_{eff}'$? Phonons?
- Interplay of hole and electron pockets?
- How to incorporate the additional ordering tendencies at smaller doping?