Shadowed Triplet Pairing in Hund's metal with Spin-Orbit Coupling

Hae-Young Kee
University of Toronto

Canadian Institute for Advanced Research

NSERC CRSNG

CENTER FOR QUANTUM MATERIALS

KITP Correlated Systems with Multicomponent Local Hilbert Spaces,
2020 November 10

Austin Lindquist **Jonathan Clepkens** **Christoph Puetter**

References

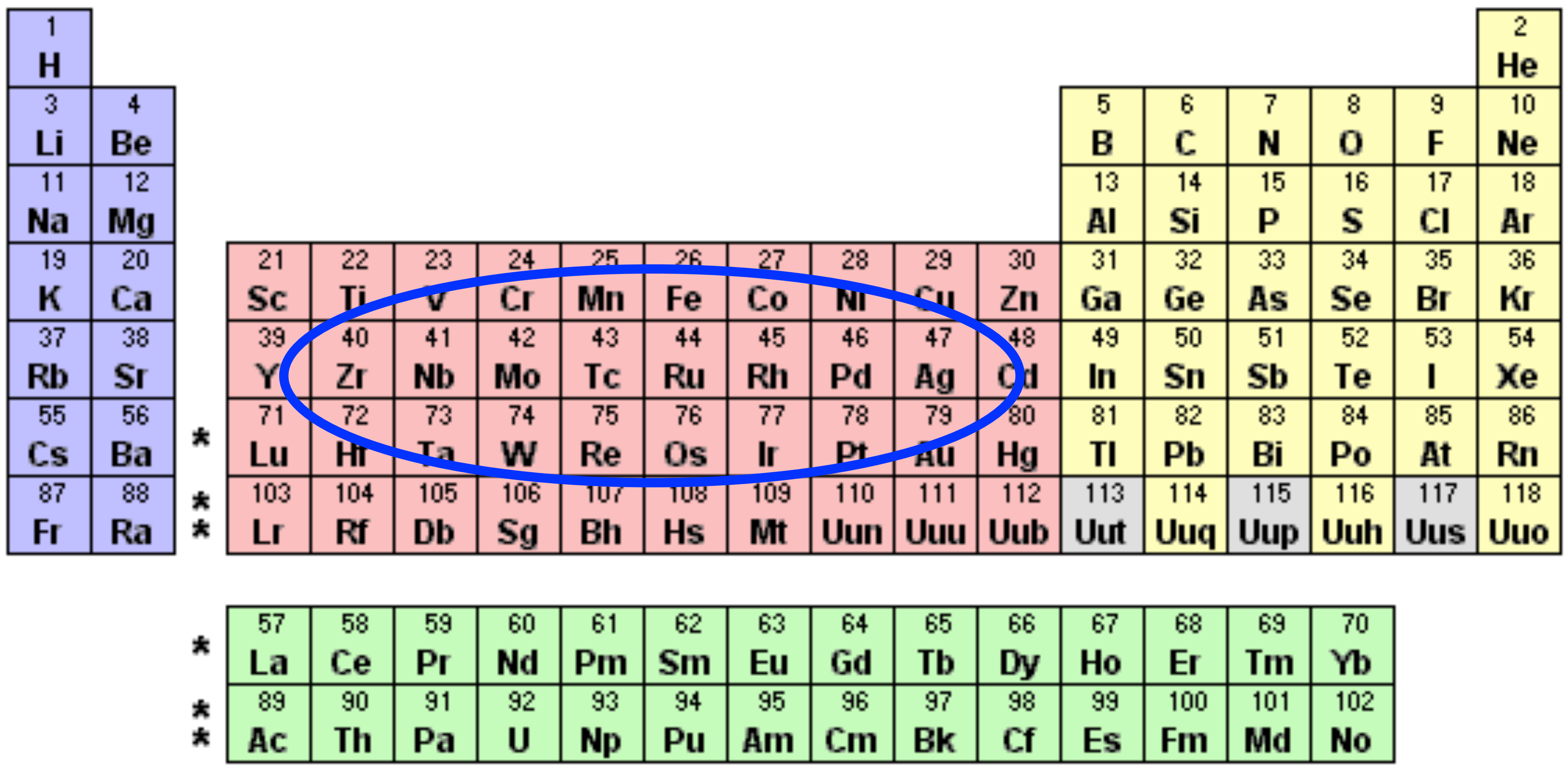
arXiv:2009.08597
Shadowed Triplet Pairings in Hund's Metals with Spin-Orbit Coupling
J. Clepkens, A. Lindquist, HYK

arXiv:1912.02215
Distinct reduction of Knight shift in superconducting state of Sr2RuO4 under uniaxial strain, PRR 2, 320 (2020).
A. Lindquist, HYK

arXiv:1101.4656
Identifying spin-triplet pairing in spin-orbit coupled multi-band superconductors, EPL 98, 27010 (2012).
C. Puetter, HYK

C. M. Puetter, PhD Thesis, Univ. of Toronto (2012).

Significant spin-orbit coupling (SOC)
Importance of Hund's coupling



Sr2RuO4

SOC < bandwidth; $4d^4$

SOC & Hund's

RuCl3

SOC > bandwidth (honeycomb); $4d^5$

Kitaev & Gamma interaction from SOC & Hund's

Outline

- Sr_2RuO_4; spin-triplet vs. singlet?
- Even-parity spin-triplet pairing and SOC: Shadowed triplet
- Applying to Sr_2RuO_4
- Proposed experiment

Sr2RuO4

	Sr_2RuO_4	$Sr_3Ru_2O_7$	$SrRuO_3$
	superconductor ($T_c = 1.5$ K)	paramagnetic metal	ferromagnetic metal ($T_c = 165$ K)
n	1	2	∞
space group	tetragonal I4/mmm	orthorhombic Bbcb (# 68)	orthorhombic
lattice parameters	$a = 3.862$ Å, $c = 12.729$ Å, $\theta = \phi = 0°$	$a = b = 5.5006$ Å, $c = 20.725$ Å, $\theta = 6.8°, \phi = 0°$	$a = 5.56$ Å, $b = 5.53$ Å, $c = 7.84$ Å, $\theta \neq 0, \phi \neq 0$
ρ_c/ρ_{ab}	$\gtrsim 400$	~ 300	~ 1.1
γ	$38 \frac{\text{mJ}}{\text{Ru mol K}^2}$	$110 \frac{\text{mJ}}{\text{Ru mol K}^2}$	$29 \frac{\text{mJ}}{\text{Ru mol K}^2}$
m^*/m_0	~ 4	—	$\sim 3 - 3.4$
R_W	$1.7 - 1.8$	$\gtrsim 10$	—
μ	—	—	$1.1\mu_B$/Ru (in-plane)

Rice and Sigrist, JPCM (1995): spin triplet with

$\vec{d}(\mathbf{p}) = \hat{z}(p_x + ip_y)$ - analog He3 A-phase

Spin Triplet

A theoretical description of the new phases of liquid ^{3}He

Anthony J. Leggett   Rev. Mod. Phys., Vol. 47, No. 2, April 1975

Cooper pair explicitly in the form

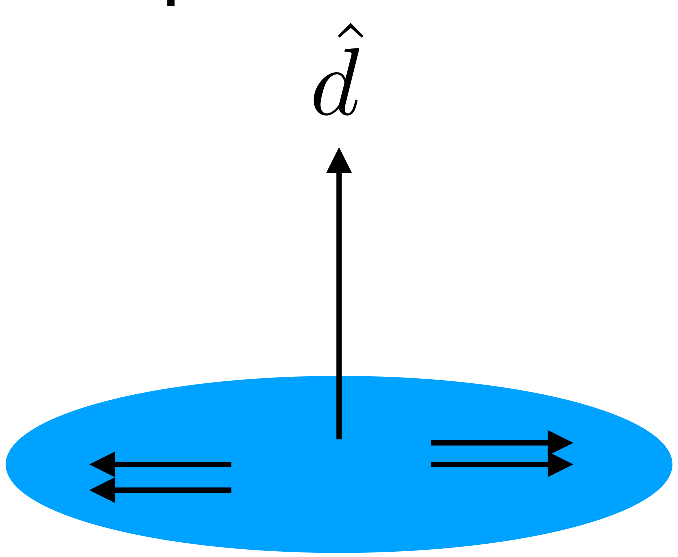
$$\Psi(\sigma_1\sigma_2:\mathbf{n}) = \Psi_{\uparrow\uparrow}(\mathbf{n})\,|\uparrow\uparrow\rangle + \Psi_{\uparrow\downarrow}(\mathbf{n})\,|\uparrow\downarrow + \downarrow\uparrow\rangle + \Psi_{\downarrow\downarrow}(\mathbf{n})\,|\downarrow\downarrow\rangle \quad (7.38)$$

and then verify explicitly that for real $\mathbf{d}(\mathbf{n})$ we have the *operator* relation

$$\mathbf{d}(\mathbf{n})\cdot\hat{\mathbf{S}}\Psi(\sigma_1\sigma_2:\mathbf{n}) \equiv 0, \quad (7.39)$$

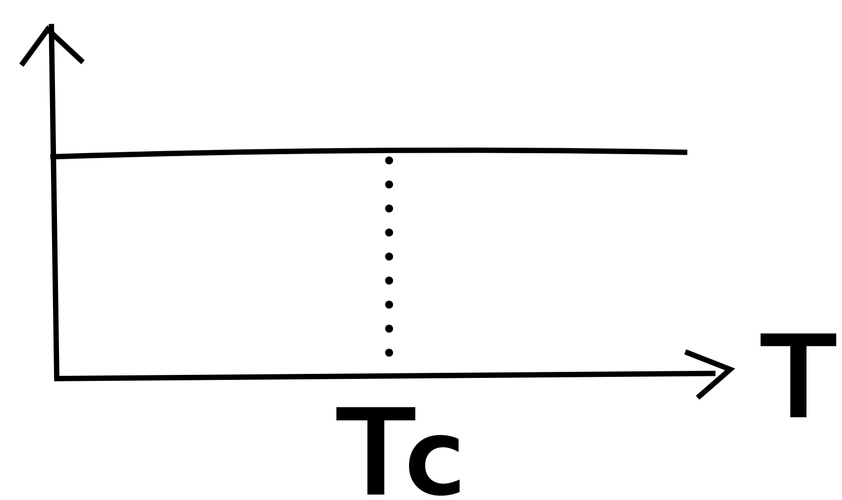
Introducing d-vector

pairs are condensed in the eigenstates of S=1 and S_z =0



H//plane

Knight shift

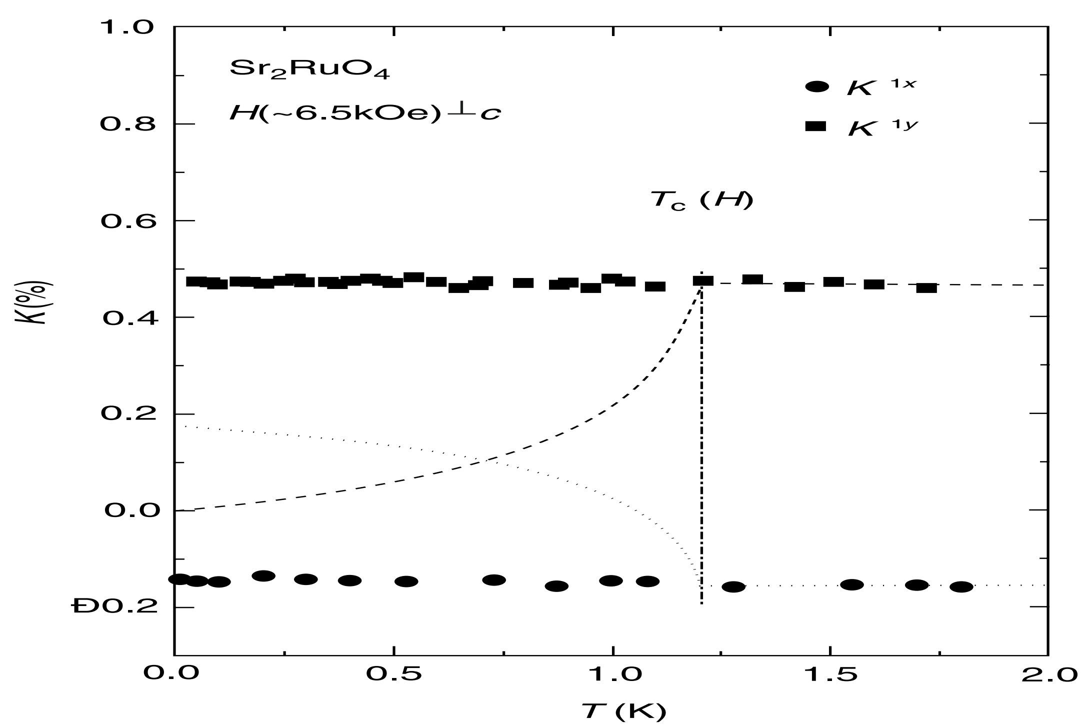


Review

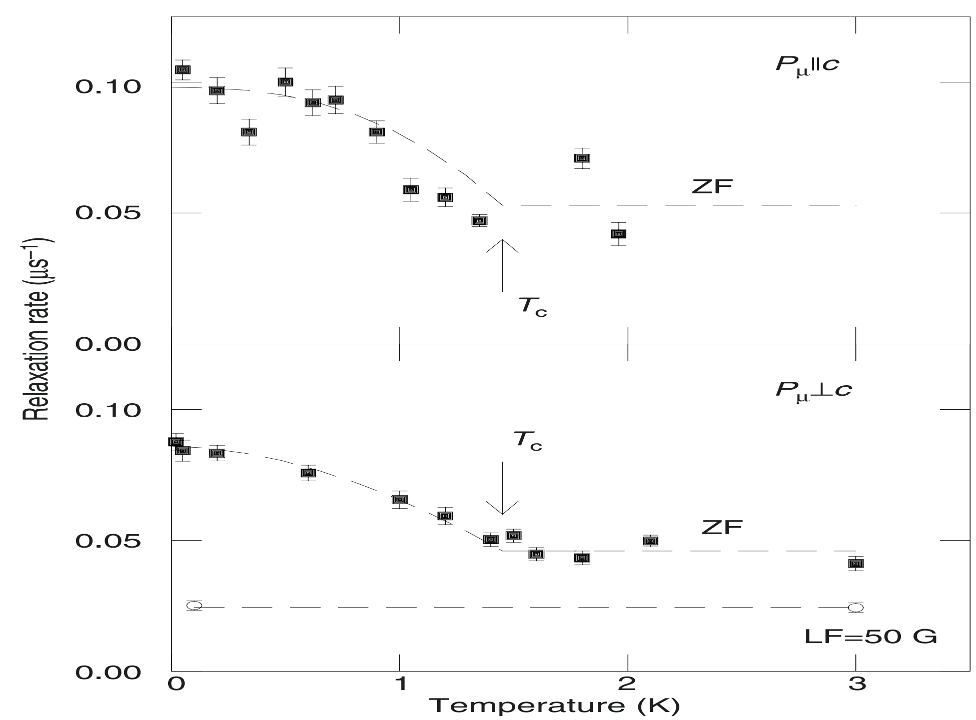
Discovery of SC, Y. Maeno et al , Nature (1994)

Rice and Sigrist, JPCM (1995): spin triplet with

$$\vec{d}(\mathbf{p}) = \hat{z}(p_x + ip_y)$$ - analog He3 A-phase



K. Ishida et al, Nature (1998)



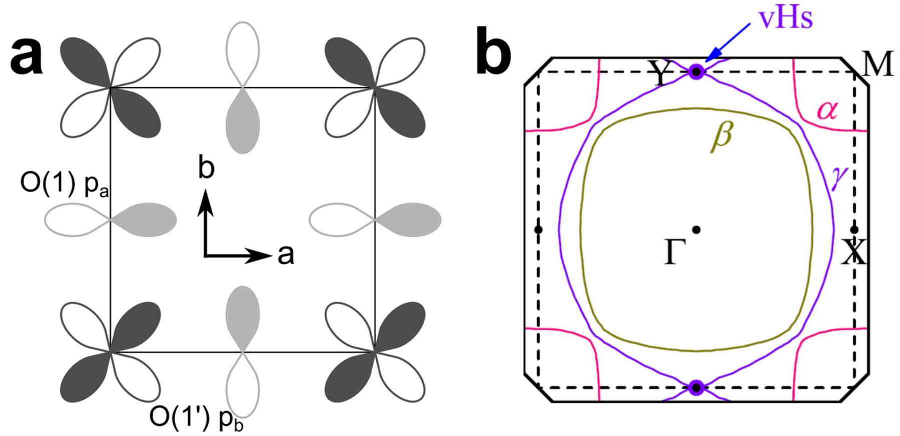
G. Luke et al, Nature (1998)

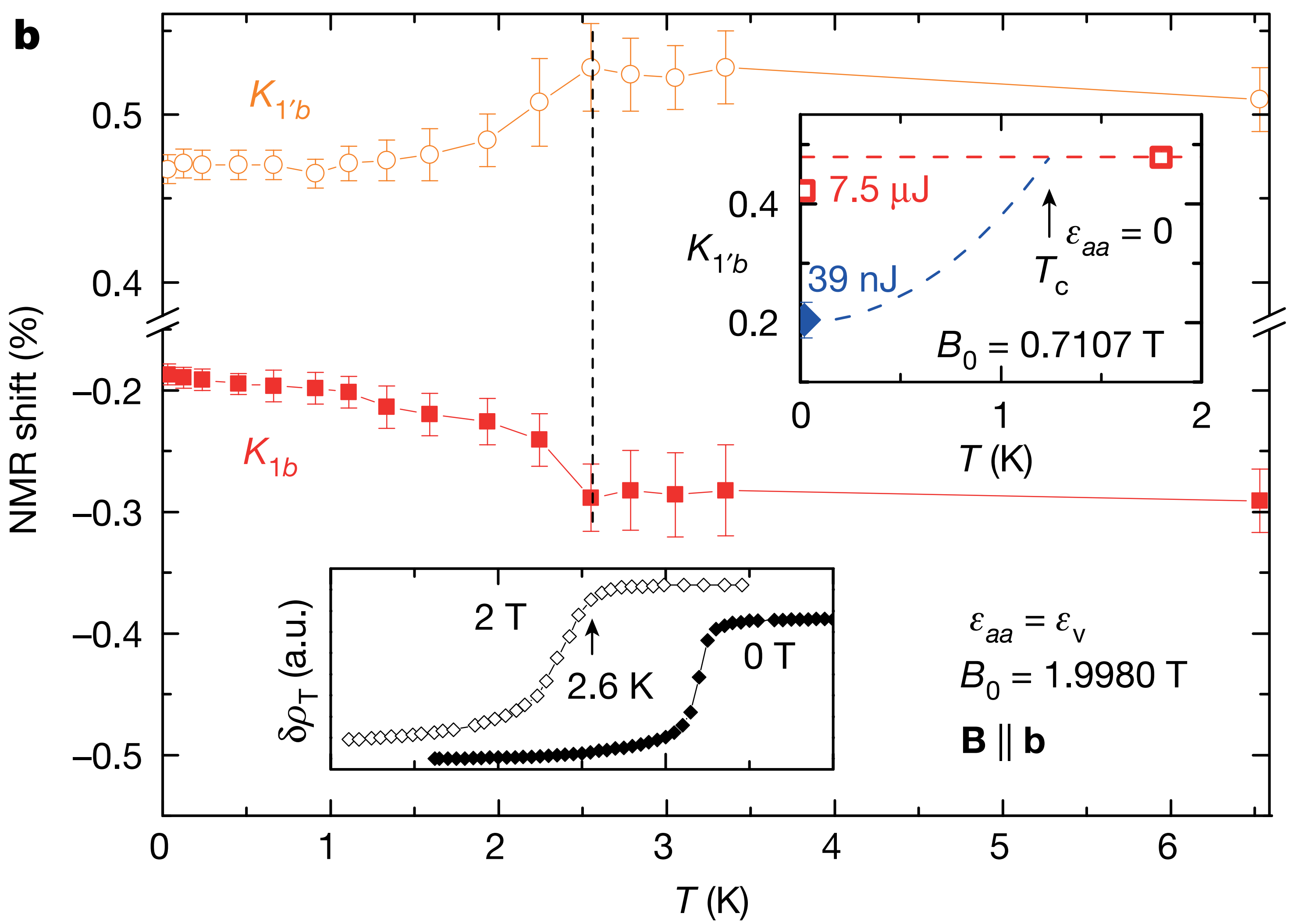
Summer Seminars for Correlated Electrons
and Frustrated Magnets
Zoom Link

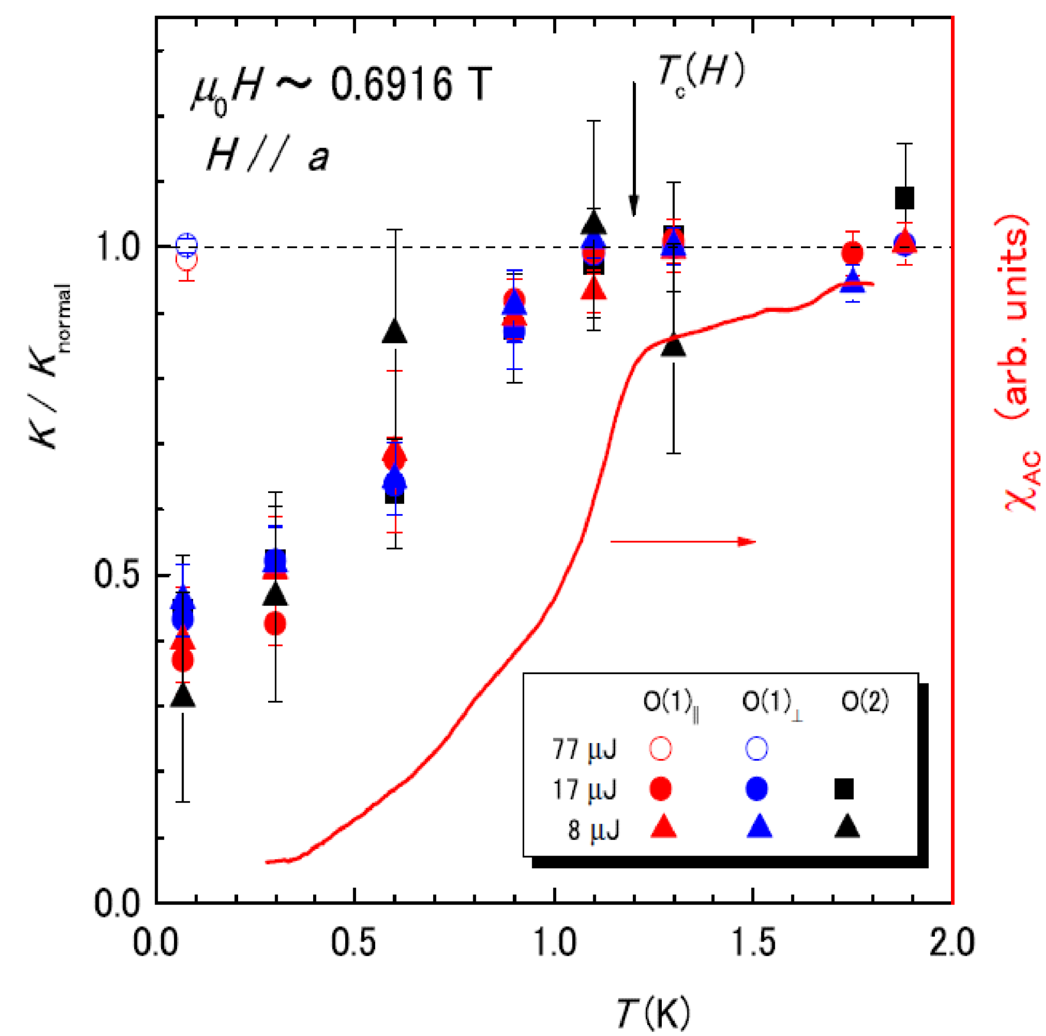
https://sites.google.com/umn.edu/cm-weekly-seminar/home

update on Sr2RuO4: A. Mackenzie

NMR: Knight shift



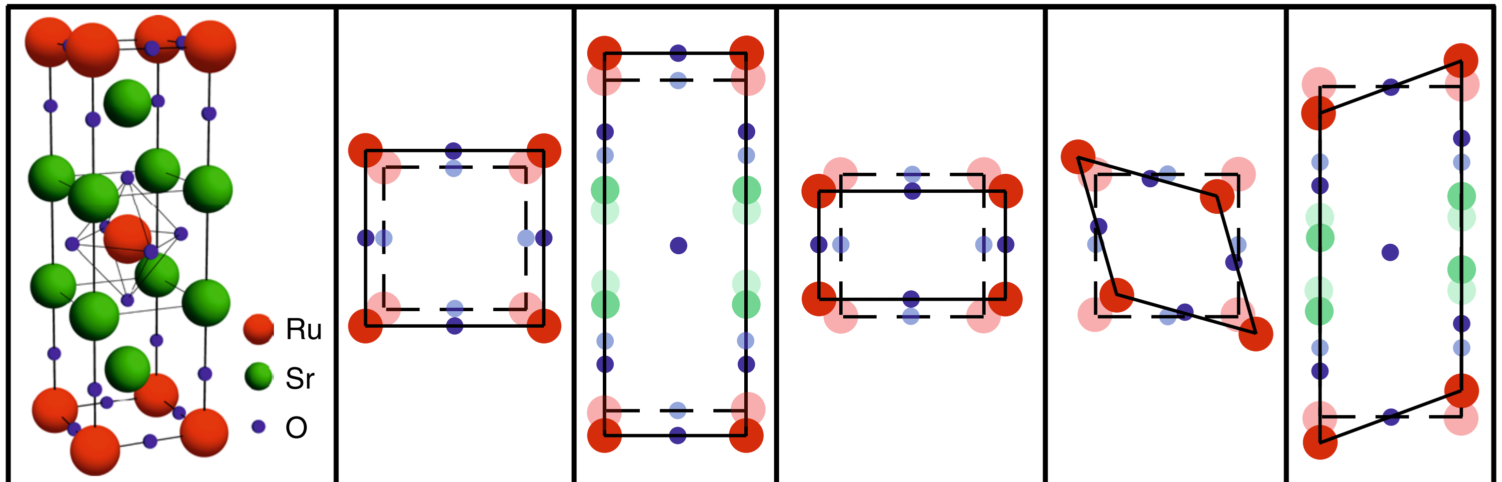




A. Pustogow et al, Nature (2019)

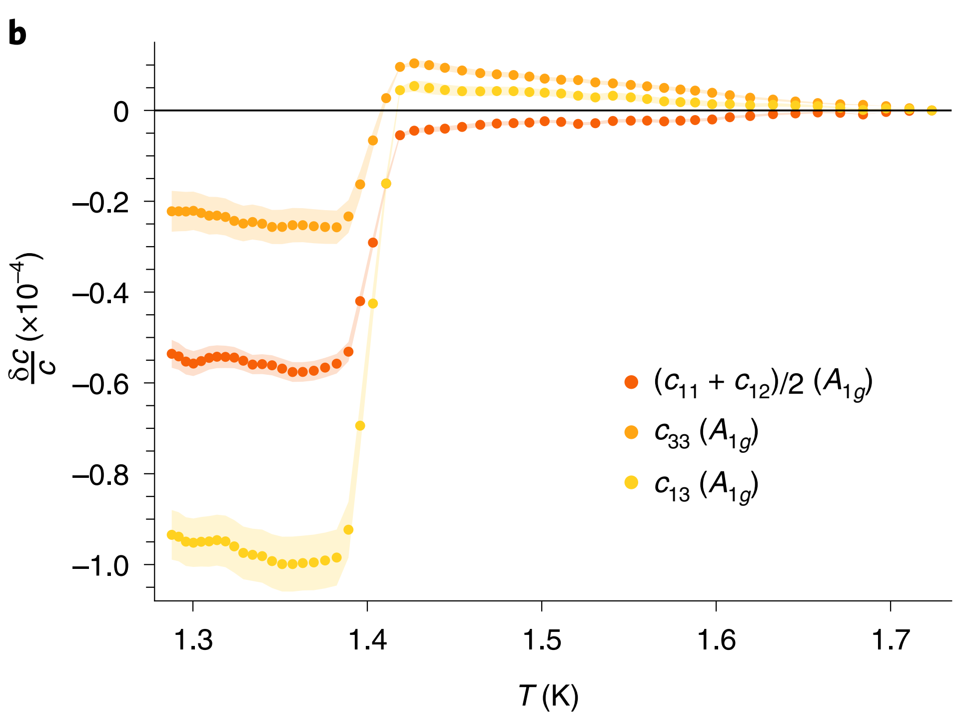
K. Ishida et al, JPSJ 89, 034712 (2020)

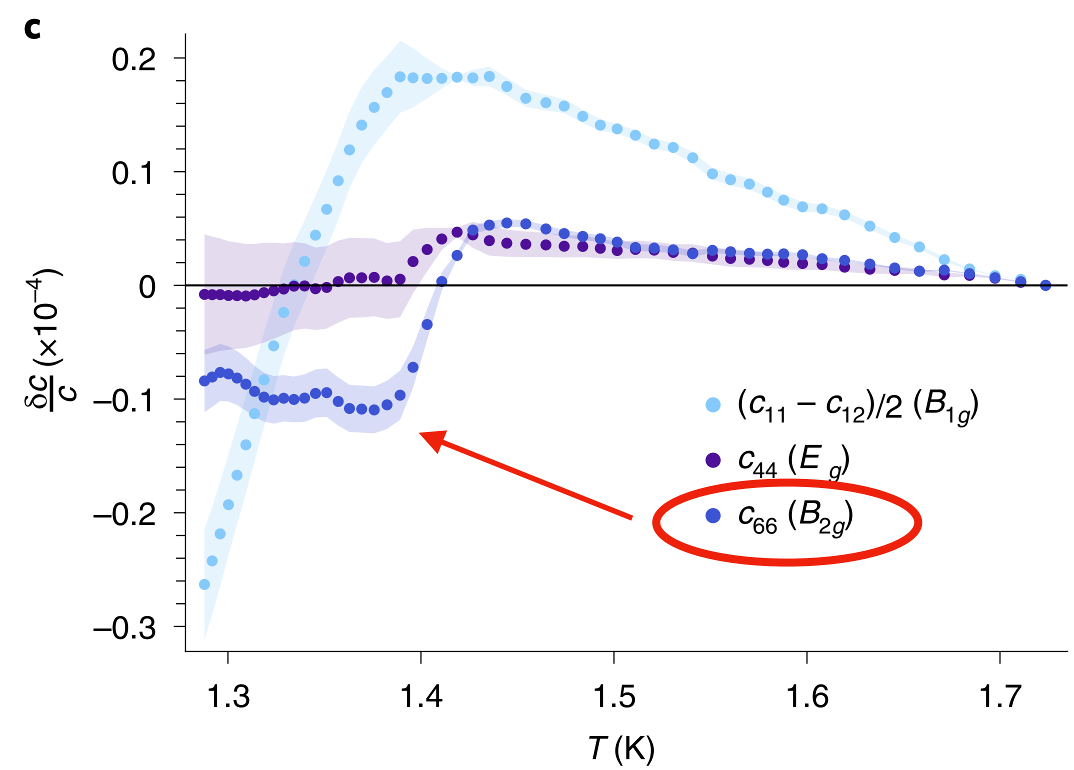
resonant ultrasound spectroscopy



Coupling to order parameter		Compression		Shear		
	Representation	A_{1g}		B_{1g}	B_{2g}	E_g
	Elastic modulus	$(c_{11}+c_{12})/2$	c_{33}	$(c_{11}-c_{12})/2$	c_{66}	c_{44}
Coupling to order parameter	One-component e.g. *d*-wave $\eta \approx d_{x^2-y^2}$	✓ $\epsilon_{A_{1g}}\eta^2$		✗	✗	✗
Coupling to order parameter	Two-component e.g. *p*-wave $\eta \approx (p_x, p_y)\hat{z}$	✓ $\epsilon_{A_{1g}}(\eta_x^2+\eta_y^2)$		✓ $\epsilon_{B_{1g}}(\eta_x^2-\eta_y^2)$	✓ $\epsilon_{B_{2g}}(\eta_x\eta_y)$	✗

two-component order parameter

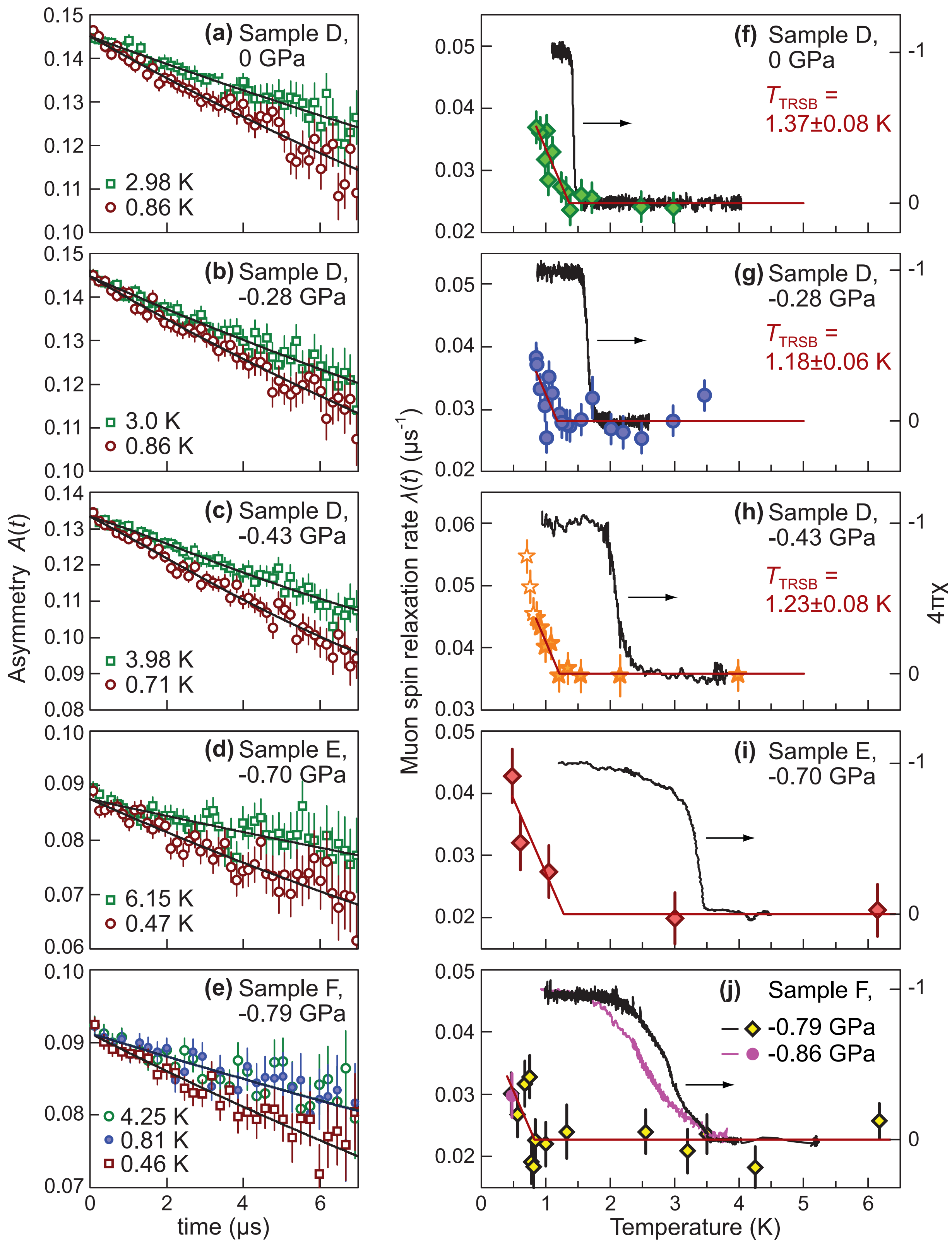




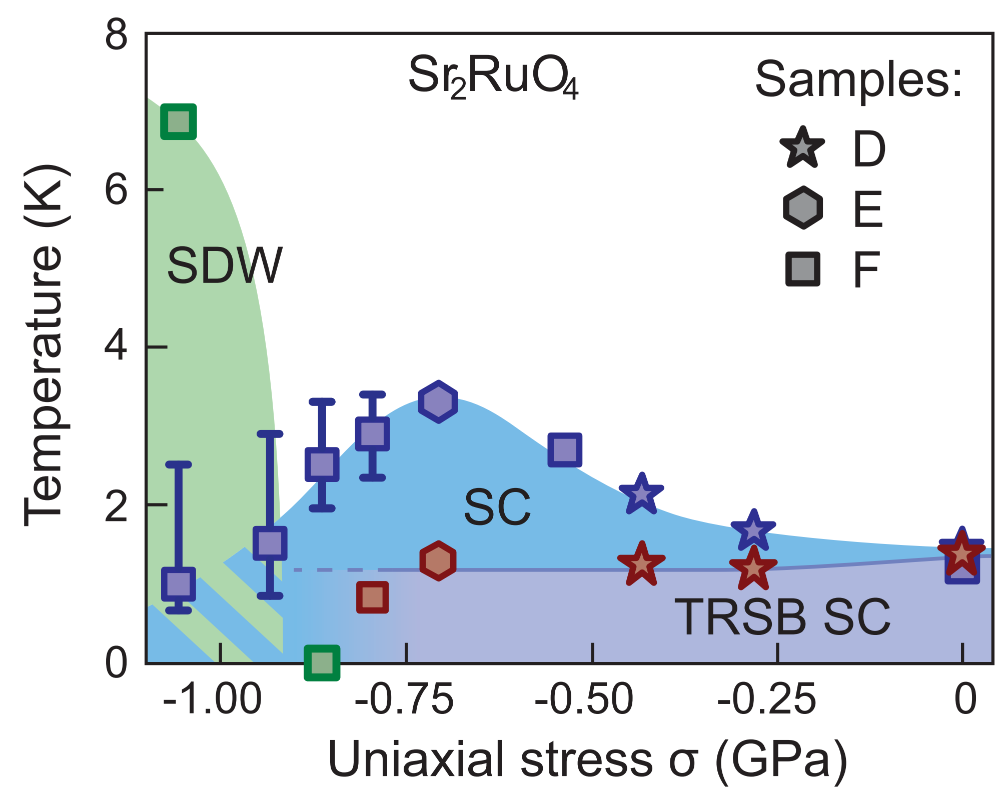
ultrasound: C. Lupien PhD thesis 2002

S. Gohsh et al, Nature Physics (2020)

muSR under strain

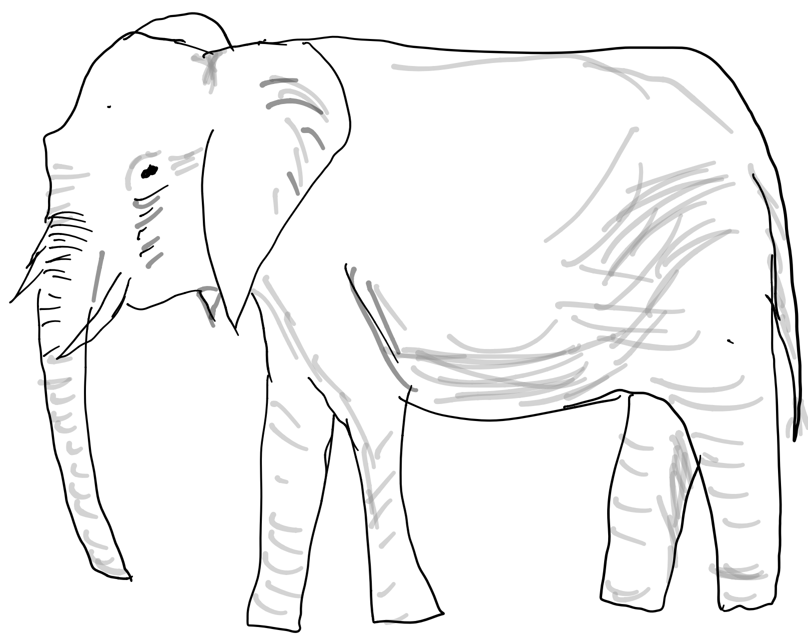


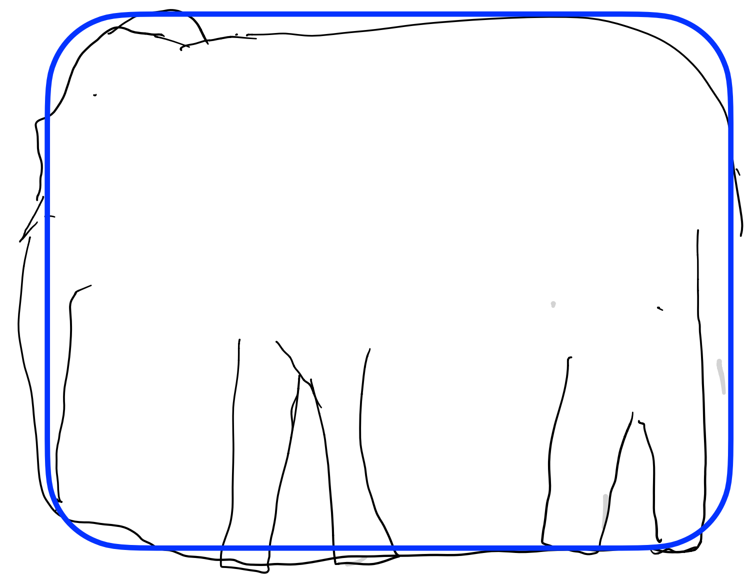
time reversal symmetry broken SC



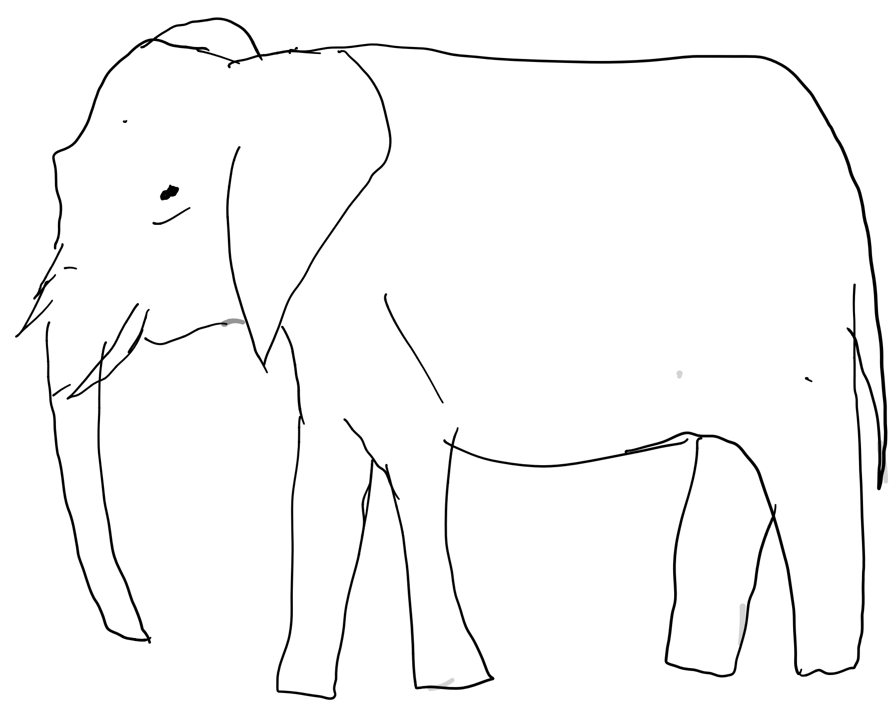
V. Grinenko et al, arXiv:2001.08152

reality vs. beauty of simplicity



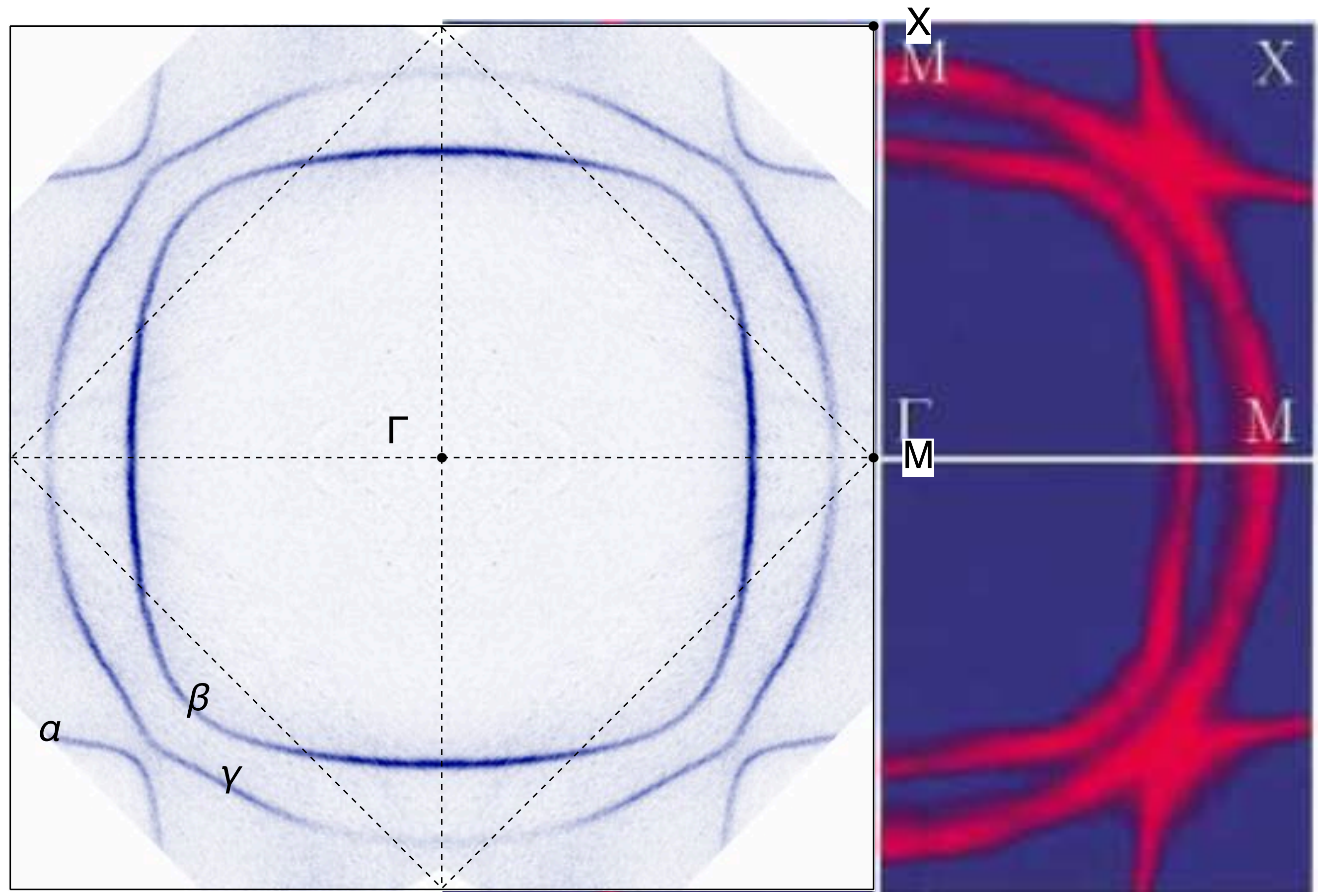


topology = ball = trivial



Reality of multi-orbital systems

Fermi Surface



A. Tamai et al, PRX (2019)

A. Mackenzie et al, PRL 76, 3786 (1996);
C. Bergemann et al, PRL 84, 2662 (2000);
A. Damascelli et al, PRL 85, 5194 (2000);

Orbitals are mixed

SOC: spin direction changes along k-space

Antisymmetric wave-function condition

$$\vec{d}(\mathbf{k}) = -\vec{d}(-\mathbf{k})$$

Single band/orbitals
odd-parity pairing;
example p-wave, sin(kx) or sin(ky)

Multi-orbital/bands
even-parity triplet pairing is allowed;
orbital (a,b) antisymmetric

$$\vec{d}(\mathbf{k}) = \vec{d}(-\mathbf{k})$$

eg: $\langle c^{\dagger}_{\mathbf{k},\sigma,a} c^{\dagger}_{-\mathbf{k},\sigma,b} - c^{\dagger}_{\mathbf{k},\sigma,b} c^{\dagger}_{-\mathbf{k},\sigma,a} \rangle$

Multi-orbital Interaction

$$
\begin{aligned}
H_{int} =& \frac{U}{2} \sum_{i,a,\sigma\neq\sigma'} n_{a,i\sigma} n_{a,i\sigma'} + \frac{U'}{2} \sum_{i,a\neq b,\sigma\sigma'} n_{a,i\sigma} n_{b,i\sigma'} \\
&+ \frac{J_H}{2} \sum_{i,a\neq b,\sigma\sigma'} c^\dagger_{a,i\sigma} c^\dagger_{b,i\sigma'} c_{a,i\sigma'} c_{b,i\sigma} \\
&+ \frac{J_H}{2} \sum_{i,a\neq b,\sigma\neq\sigma'} c^\dagger_{a,i\sigma} c^\dagger_{a,i\sigma'} c_{b,i\sigma'} c_{b,i\sigma},
\end{aligned}
$$

$\longrightarrow$

$$
\begin{aligned}
H_{int} =& \frac{4U}{N} \sum_{a,\mathbf{k}\mathbf{k}'} \hat{\Delta}^{s\dagger}_{a,\mathbf{k}} \hat{\Delta}^{s}_{a,\mathbf{k}'} \\
&+ \frac{2(U' - J_H)}{N} \sum_{\{a\neq b\},\mathbf{k}\mathbf{k}'} \hat{\mathbf{d}}^\dagger_{a/b,\mathbf{k}} \cdot \hat{\mathbf{d}}_{a/b,\mathbf{k}'} \\
&+ \frac{4J_H}{N} \sum_{a\neq b,\mathbf{k}\mathbf{k}'} \hat{\Delta}^{s\dagger}_{a,\mathbf{k}} \hat{\Delta}^{s}_{b,\mathbf{k}'} \\
&+ \frac{2(U' + J_H)}{N} \sum_{a\neq b,\mathbf{k}\mathbf{k}'} \hat{\Delta}^{s\dagger}_{a/b,\mathbf{k}} \hat{\Delta}^{s}_{a/b,\mathbf{k}'},
\end{aligned}
$$

spin triplet

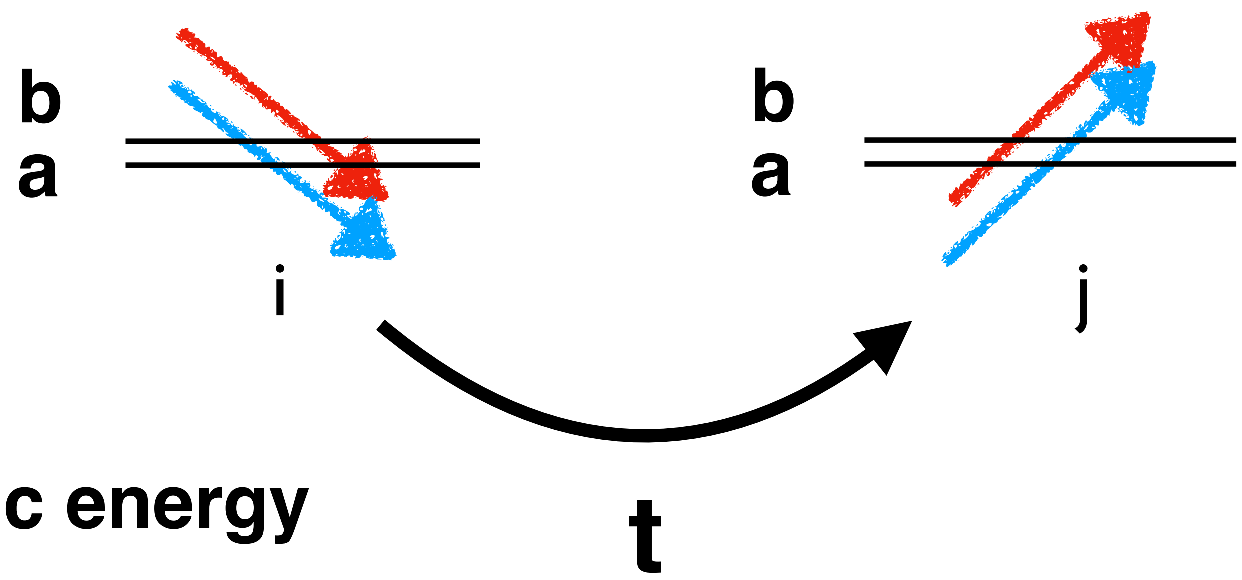
$$
\hat{\mathbf{d}}_{a/b,\mathbf{k}} = \frac{1}{4} \sum_{\sigma\sigma'} [i\sigma^y \boldsymbol{\sigma}]_{\sigma\sigma'} \left(c_{a,\mathbf{k}\sigma} c_{b,-\mathbf{k}\sigma'} - c_{b,\mathbf{k}\sigma} c_{a,-\mathbf{k}\sigma'} \right)
$$

$$
\hat{\Delta}^{s}_{a/b,\mathbf{k}} = \frac{1}{4} \sum_{\sigma\sigma'} [i\sigma^y]_{\sigma\sigma'} \left(c_{a,\mathbf{k}\sigma} c_{b,-\mathbf{k}\sigma'} + c_{b,\mathbf{k}\sigma} c_{a,-\mathbf{k}\sigma'} \right)
$$

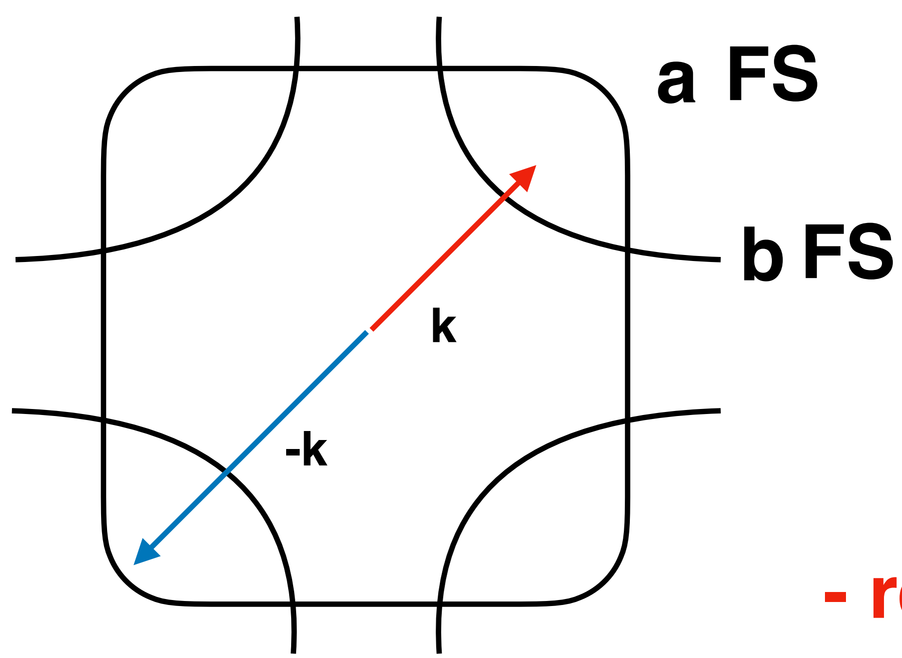
$$
\hat{\Delta}^{s}_{a,\mathbf{k}} = \frac{1}{4} \sum_{\sigma\sigma'} [i\sigma^y]_{\sigma\sigma'} c_{a,\mathbf{k}\sigma} c_{a,-\mathbf{k}\sigma'},
$$

C. Puetter, HYK, EPL 98, 27010 (2012) ; arXiv:1101.4656

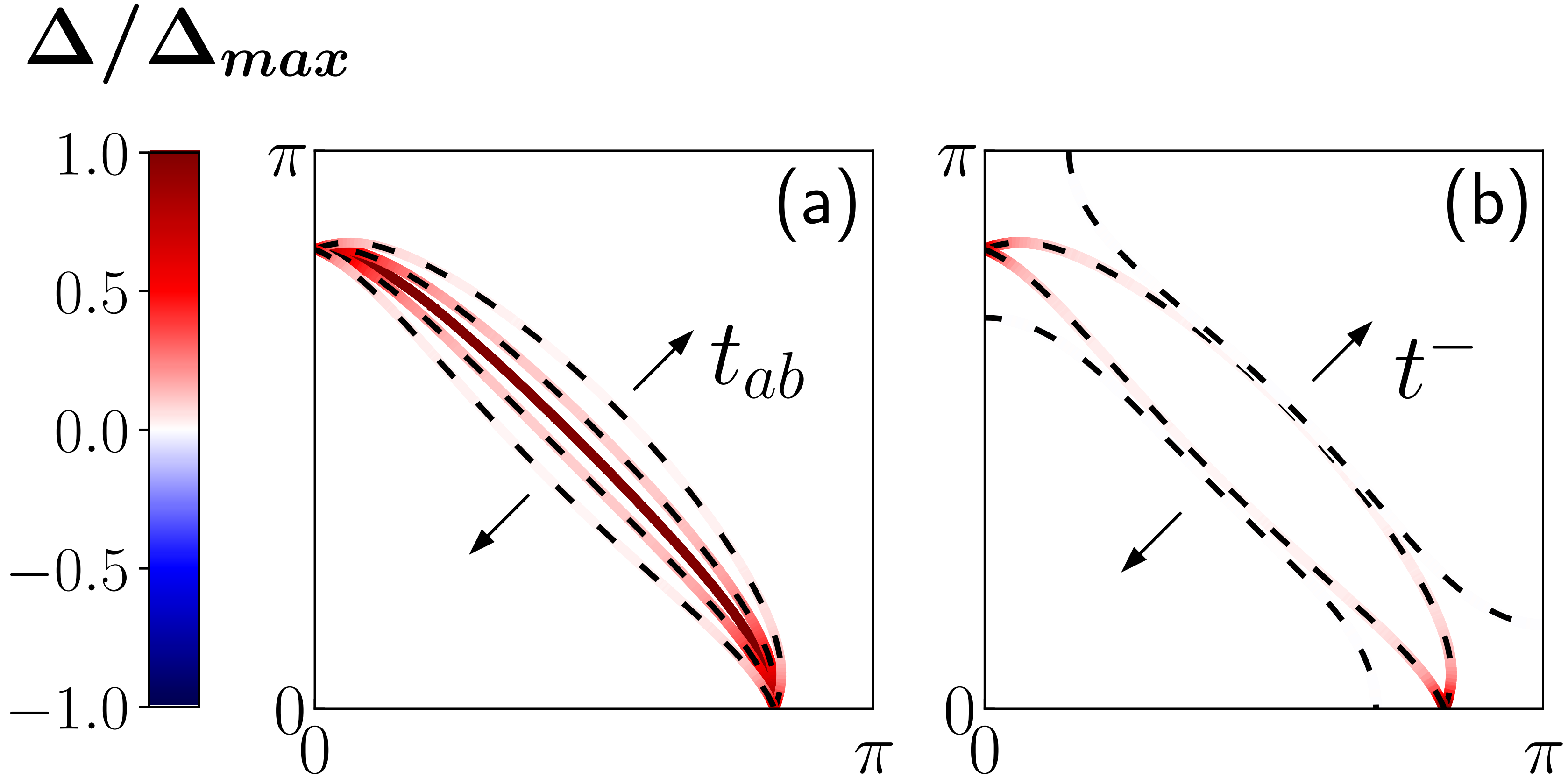
Pairing is local: $U' < J_H$



Kinetic energy



However, it is fragile
- requires degeneracy of bands



$$t_{ab} c_i^{a\dagger} c_j^b$$

Orbital hybridization

$$t^-(c_i^{a\dagger} c_j^a - c_i^{b\dagger} c_j^b)$$

Orbital hopping difference

Hund's rule coupling as the microscopic origin of the spin-triple tpairing in a correlated and degenerate band system, A. Klejnberg, J. Spalek, JPCMP 11, 6553 (1999);
X. Dai et al, PRL (2008) on Pnictides

SOC!

C. Puetter, HYK, EPL 98, 27010 (2012); O.Vafek, A.V. Chubukov, PRL (2017); …………..

Effects of SOC: 2-orbital model

$$H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \big(H_0(\mathbf{k}) + H_{\mathrm{SOC}}^{z}(\mathbf{k}) + H_{\mathrm{pair}}(\mathbf{k}) \big) \Psi_{\mathbf{k}}$$

$$\Psi_{\mathbf{k}}^{\dagger} = \left(\psi_{\mathbf{k}}^{\dagger}, T\psi_{\mathbf{k}}^{T} T^{-1} \right) \quad \psi_{\mathbf{k}}^{\dagger} = (c_{\mathbf{k}\uparrow}^{a\dagger}, c_{\mathbf{k}\uparrow}^{b\dagger}, c_{\mathbf{k}\downarrow}^{a\dagger}, c_{\mathbf{k}\downarrow}^{b\dagger})$$

$$H_0(\mathbf{k}) = \rho_3 \Big(\frac{\xi_{\mathbf{k}}^{+}}{2} \sigma_0 \tau_0 + \frac{\xi_{\mathbf{k}}^{-}}{2} \sigma_0 \tau_3 + t_{\mathbf{k}} \sigma_0 \tau_1 \Big)$$

$\xi_{\mathbf{k}}^{\pm} = \xi_{\mathbf{k}}^{a} \pm \xi_{\mathbf{k}}^{b}$, $\quad t_{\mathbf{k}} c_{\mathbf{k}}^{a\dagger} c_{\mathbf{k}}^{b}$ **: orbital hybridization**

$H_{\mathrm{SOC}}^{z}(\mathbf{k}) = -\lambda_{\mathbf{k}} \rho_3 \sigma_3 \tau_2$ **momentum dep. SOC**

$$H_{\mathrm{pair}} = -d_{a/b}^{z} \rho_2 \sigma_3 \tau_2 .$$

$d_{a/b}^{z} \equiv (U' - J_H) \frac{1}{N} \sum_{\mathbf{k}} \langle \hat{d}_{a/b,\mathbf{k}}^{z} \rangle$. **spin-triplet**

---

change to band basis

$$\begin{pmatrix} c_{\mathbf{k}\sigma}^{a} \\ c_{\mathbf{k}\sigma}^{b} \end{pmatrix} = \begin{pmatrix} \frac{\eta_\sigma + 1}{2} f_{\mathbf{k}} - \frac{\eta_\sigma - 1}{2} f_{\mathbf{k}}^{*} & -g_{\mathbf{k}} \\ g_{\mathbf{k}} & \frac{\eta_\sigma + 1}{2} f_{\mathbf{k}}^{*} - \frac{\eta_\sigma - 1}{2} f_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k},s} \\ \beta_{\mathbf{k},s} \end{pmatrix}$$

In the band basis

two bands α, β

pseudo-spin singlet (intra-band)

$$\tilde{H}_{\rm pair}(\mathbf{k}) = i\Delta^s(\mathbf{k})\big[(\alpha^\dagger_{\mathbf{k},+}\alpha^\dagger_{-\mathbf{k},-} - \alpha^\dagger_{\mathbf{k},-}\alpha^\dagger_{-\mathbf{k},+}) - (\beta^\dagger_{\mathbf{k},+}\beta^\dagger_{-\mathbf{k},-} - \beta^\dagger_{\mathbf{k},-}\beta^\dagger_{-\mathbf{k},+})\big]$$
$$+i\Delta^s_{\alpha\beta}(\mathbf{k})\big[(\alpha^\dagger_{\mathbf{k},+}\beta^\dagger_{-\mathbf{k},-} - \alpha^\dagger_{\mathbf{k},-}\beta^\dagger_{-\mathbf{k},+}) + (\beta^\dagger_{\mathbf{k},+}\alpha^\dagger_{-\mathbf{k},-} - \beta^\dagger_{\mathbf{k},-}\alpha^\dagger_{-\mathbf{k},+})\big]$$
$$+d^z_{\alpha\beta}(\mathbf{k})\big[(\alpha^\dagger_{\mathbf{k},+}\beta^\dagger_{-\mathbf{k},-} + \alpha^\dagger_{\mathbf{k},-}\beta^\dagger_{-\mathbf{k},+}) - (\beta^\dagger_{\mathbf{k},+}\alpha^\dagger_{-\mathbf{k},-} + \beta^\dagger_{\mathbf{k},-}\alpha^\dagger_{-\mathbf{k},+})\big].$$

pseudo-spin triplet (inter-band)

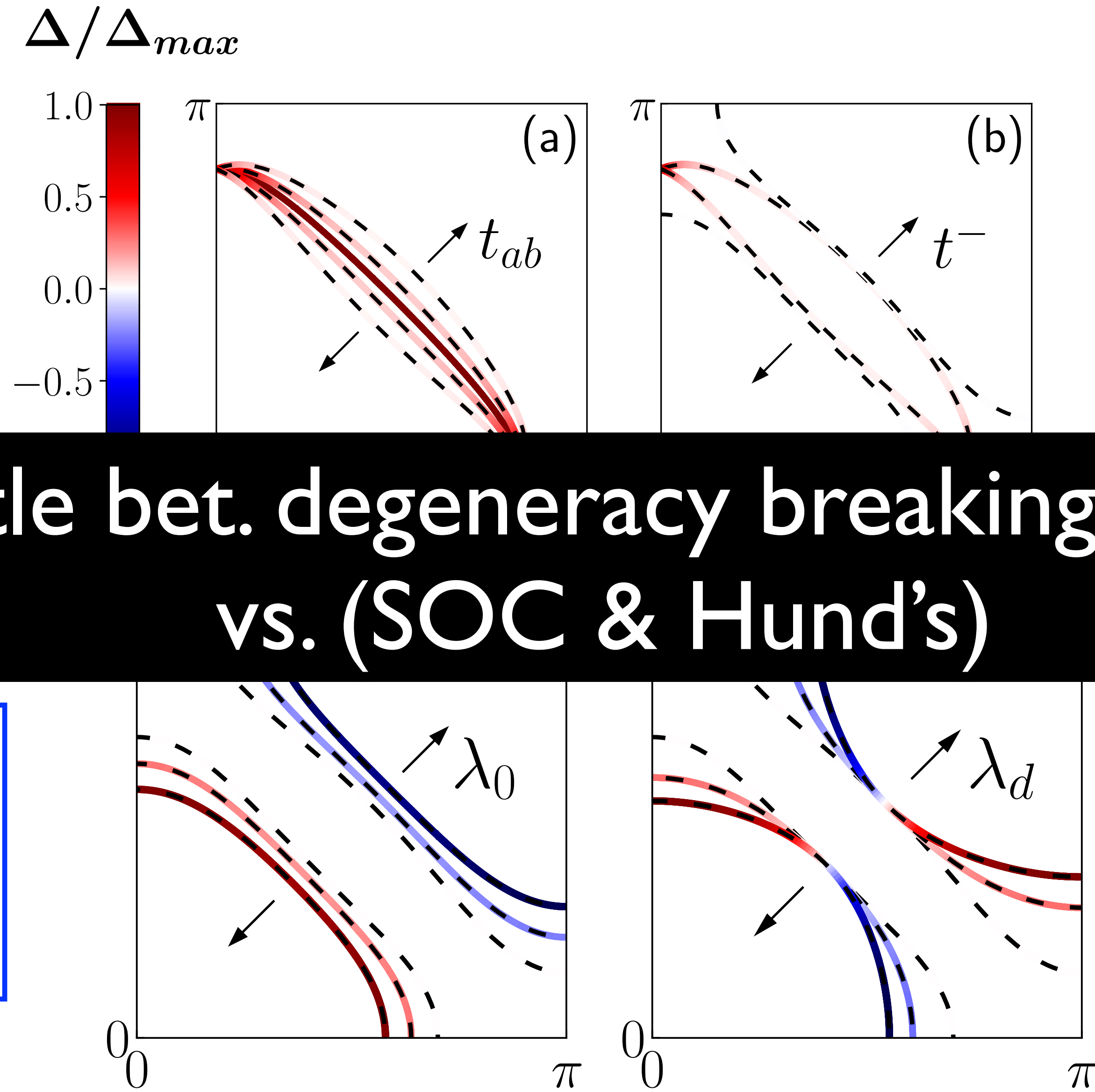
$$\Delta^s(\mathbf{k}) = -2d^z_{a/b}\mathrm{Im}(f_\mathbf{k})g_\mathbf{k} = \frac{-2d^z_{a/b}\lambda_\mathbf{k}}{\sqrt{\xi_\mathbf{k}^{-2} + 4(t^2_\mathbf{k} + \lambda^2_\mathbf{k})}}$$

spin-triplet

$$\Delta^s_{\alpha\beta}(\mathbf{k}) = -d^z_{a/b}\mathrm{Im}(f^2_\mathbf{k}) = -2d^z_{a/b}|f_\mathbf{k}|^2\frac{t_\mathbf{k}\lambda_\mathbf{k}}{t^2_\mathbf{k} + \lambda^2_\mathbf{k}}$$

$$d^z_{\alpha\beta}(\mathbf{k}) = d^z_{a/b}(g^2_\mathbf{k} + \mathrm{Re}(f^2_\mathbf{k})) = d^z_{a/b}\big(g^2_\mathbf{k} + |f_\mathbf{k}|^2\frac{t^2_\mathbf{k} - \lambda^2_\mathbf{k}}{t^2_\mathbf{k} + \lambda^2_\mathbf{k}}\big).$$

Significance of SOC on the pairing $\Delta^s(\mathbf{k})$



battle bet. degeneracy breaking terms vs. (SOC & Hund's)

$$-\frac{2d^z_{a/b}\lambda_{\mathbf{k}}}{\sqrt{\xi^{-2}_{\mathbf{k}} + 4(t^2_{\mathbf{k}} + \lambda^2_{\mathbf{k}})}}$$

SOC enhances pairing

SOC determines pairing symmetry

$$i(\cos k_x - \cos k_y)\left(\sigma^z_{\sigma\sigma'} c^{a\dagger}_{\mathbf{k}\sigma} c^b_{\mathbf{k}\sigma'}\right)$$

Figure from arXiv:2009.08597, J. Clepkens, A. Lindquist, HYK

Back to Sr2RuO4: t2g orbitals

Energy Scale

Crys

t2g ba , 1.5) eV

Correlated metal

Correlation

U ~ 2 - 3 eV

J ~ 0.4 - 0.7eV

orbital degeneracy breaking terms,
e.g, orbital hybridization ~ 0.01 - 0.1 eV

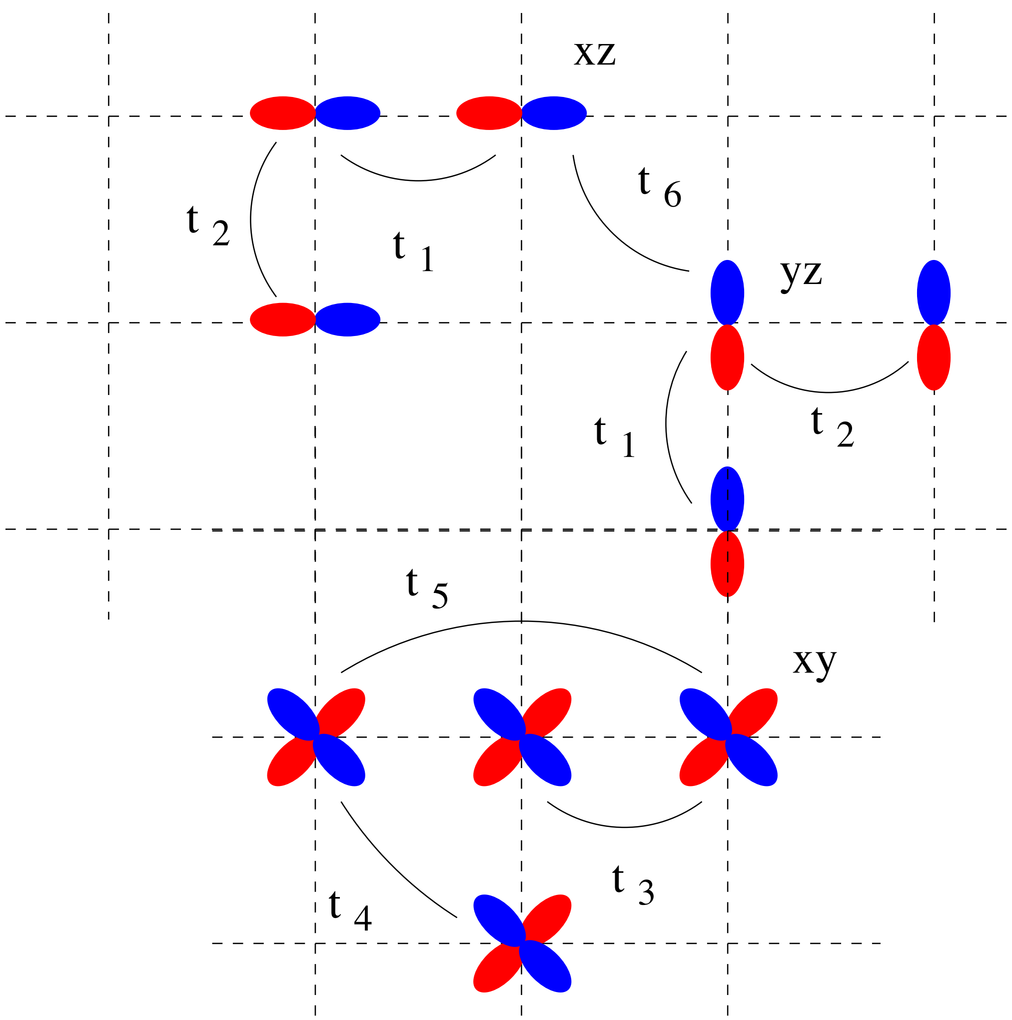
SOC ~ 0.05 - 0.16 eV

crystal field: dxy - dxz/yz ~ 0.08 eV

Tc ~ 1.5 - 3K

H = Hint + Hkin + Hsoc

$$H_{\rm kin} + H_{\rm SO} = \sum_{\mathbf{k},\sigma} C^{\dagger}_{\mathbf{k}\sigma} \begin{pmatrix} \varepsilon^{yz}_{\mathbf{k}} & \varepsilon^{1d}_{\mathbf{k}} + i\lambda & -\lambda \\ \varepsilon^{1d}_{\mathbf{k}} - i\lambda & \varepsilon^{xz}_{\mathbf{k}} & i\lambda \\ -\lambda & -i\lambda & \varepsilon^{xy}_{\mathbf{k}} \end{pmatrix} C_{\mathbf{k}\sigma}, \quad C^{\dagger}_{\mathbf{k}\sigma} = \left(c^{yz\dagger}_{\mathbf{k}\sigma}, c^{xz\dagger}_{\mathbf{k}\sigma}, c^{xy\dagger}_{\mathbf{k}-\sigma}\right)$$



$$\varepsilon^{yz}_{\mathbf{k}} = -2t_1 \cos k_y - 2t_2 \cos k_x - \mu_{\rm 1D},$$

$$\varepsilon^{xz}_{\mathbf{k}} = -2t_1 \cos k_x - 2t_2 \cos k_y - \mu_{\rm 1D},$$

$$\varepsilon^{xy}_{\mathbf{k}} = -2t_3\left(\cos k_x + \cos k_y\right) - 4t_4 \cos k_x \cos k_y - 2t_5\left(\cos(2k_x) + \cos(2k_y)\right) - \mu_{\rm xy},$$

$$t_{\mathbf{k}} = -4t_{ab} \sin k_x \sin k_y$$

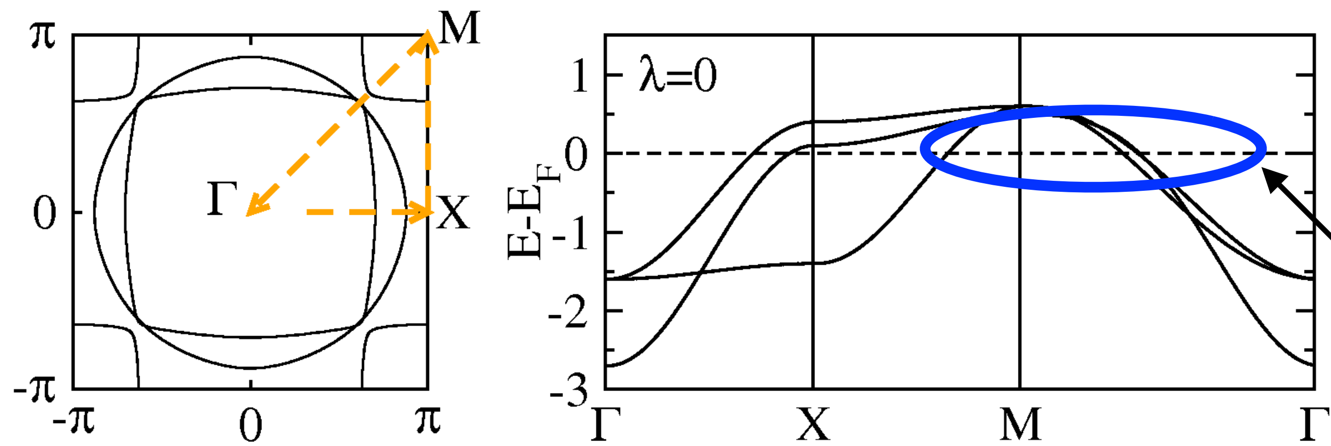
λ **atomic spin-orbit coupling (SOC)**

μ_{1D}

μ_{xy} **atomic potential**

Spin-Orbit Coupling

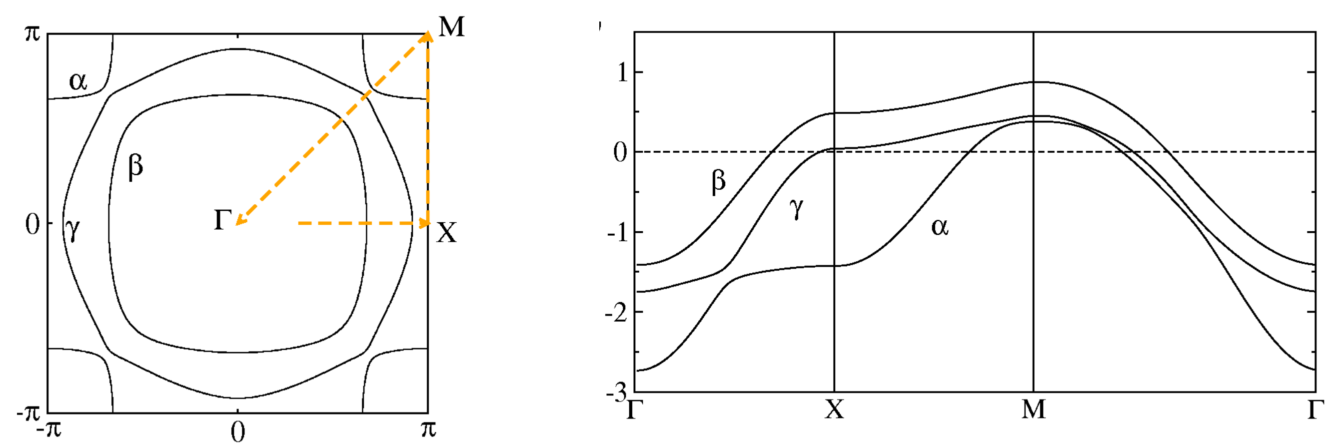
SOC ~ 0.05 - 0.16 eV



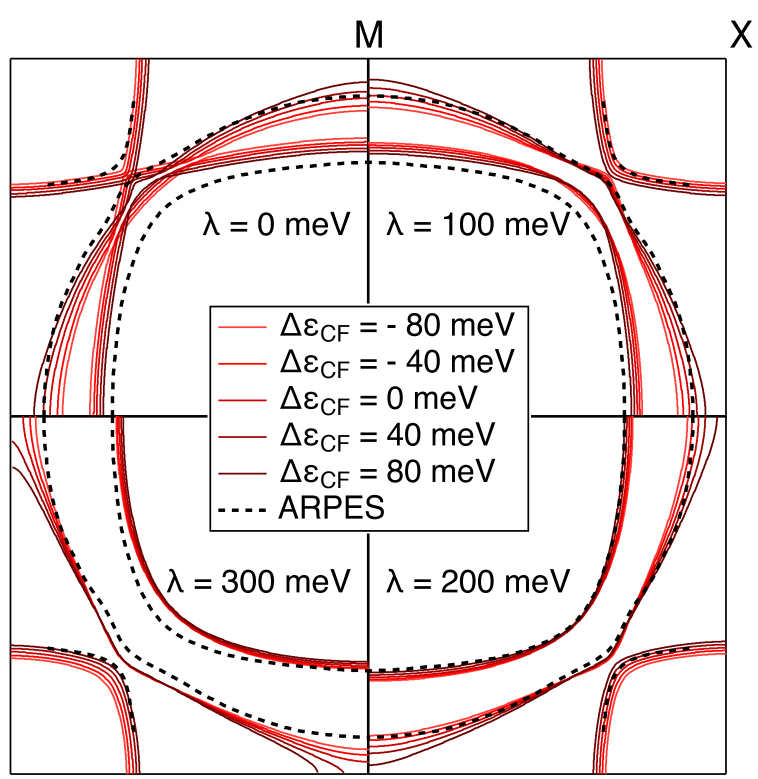
almost degenerate

degeneracy breaking vs. SOC

SOC



C. M. Puetter, PhD Thesis (2012).



effective SOC > SOC$_{LDA}$

A. Tamai et al, PRX (2019)

Multi-orbital Interaction

$$H_{int} = \frac{U}{2} \sum_{i,a,\sigma\neq\sigma'} n_{a,i\sigma} n_{a,i\sigma'} + \frac{U'}{2} \sum_{i,a\neq b,\sigma\sigma'} n_{a,i\sigma} n_{b,i\sigma'}$$
$$+ \frac{J_H}{2} \sum_{i,a\neq b,\sigma\sigma'} c^\dagger_{a,i\sigma} c^\dagger_{b,i\sigma'} c_{a,i\sigma'} c_{b,i\sigma}$$
$$+ \frac{J_H}{2} \sum_{i,a\neq b,\sigma\neq\sigma'} c^\dagger_{a,i\sigma} c^\dagger_{a,i\sigma'} c_{b,i\sigma'} c_{b,i\sigma},$$

$\longrightarrow$

$$H_{int} = \frac{4U}{N} \sum_{a,\mathbf{kk}'} \hat{\Delta}^{s\dagger}_{a,\mathbf{k}} \hat{\Delta}^{s}_{a,\mathbf{k}'}$$
$$+ \frac{2(U'-J_H)}{N} \sum_{\{a\neq b\},\mathbf{kk}'} \hat{\mathbf{d}}^\dagger_{a/b,\mathbf{k}} \cdot \hat{\mathbf{d}}_{a/b,\mathbf{k}'}$$
$$+ \frac{4J_H}{N} \sum_{a\neq b,\mathbf{kk}'} \hat{\Delta}^{s\dagger}_{a,\mathbf{k}} \hat{\Delta}^{s}_{b,\mathbf{k}'}$$
$$+ \frac{2(U'+J_H)}{N} \sum_{a\neq b,\mathbf{kk}'} \hat{\Delta}^{s\dagger}_{a/b,\mathbf{k}} \hat{\Delta}^{s}_{a/b,\mathbf{k}'},$$

spin triplet

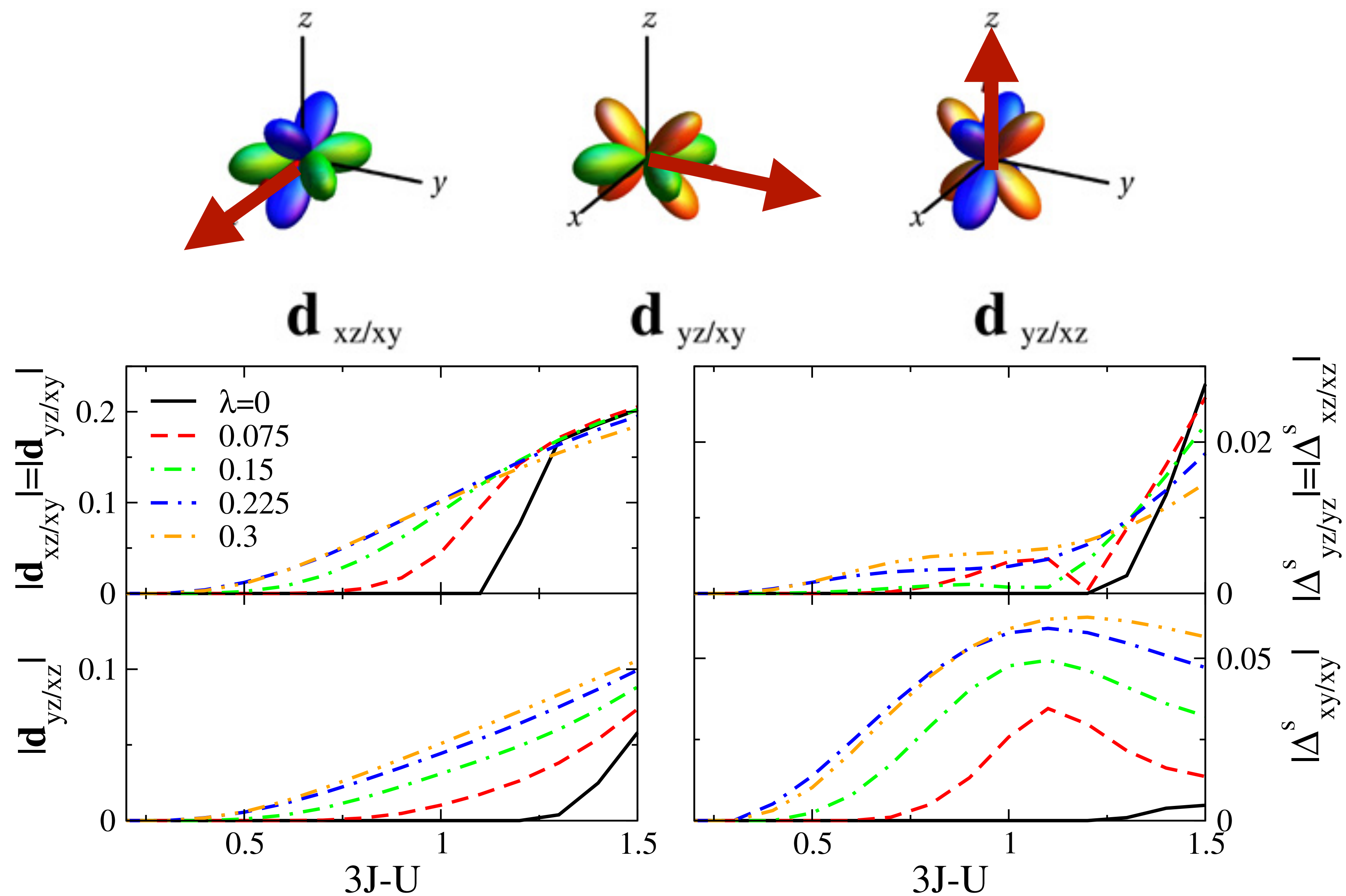
$$\hat{\mathbf{d}}_{a/b,\mathbf{k}} = \frac{1}{4} \sum_{\sigma\sigma'} [i\sigma^y \boldsymbol{\sigma}]_{\sigma\sigma'} \left(c_{a,\mathbf{k}\sigma} c_{b,-\mathbf{k}\sigma'} - c_{b,\mathbf{k}\sigma} c_{a,-\mathbf{k}\sigma'} \right)$$
$$\hat{\Delta}^s_{a/b,\mathbf{k}} = \frac{1}{4} \sum_{\sigma\sigma'} [i\sigma^y]_{\sigma\sigma'} \left(c_{a,\mathbf{k}\sigma} c_{b,-\mathbf{k}\sigma'} + c_{b,\mathbf{k}\sigma} c_{a,-\mathbf{k}\sigma'} \right)$$
$$\hat{\Delta}^s_{a,\mathbf{k}} = \frac{1}{4} \sum_{\sigma\sigma'} [i\sigma^y]_{\sigma\sigma'} c_{a,\mathbf{k}\sigma} c_{a,-\mathbf{k}\sigma'},$$

C. Puetter, HYK, EPL 98, 27010 (2012) ; arXiv:1101.4656

Identifying spin-triplet pairing in spin-orbit coupled multi-band superconductors

EPL 98, 27010 (2012) arXiv:1101.4656.

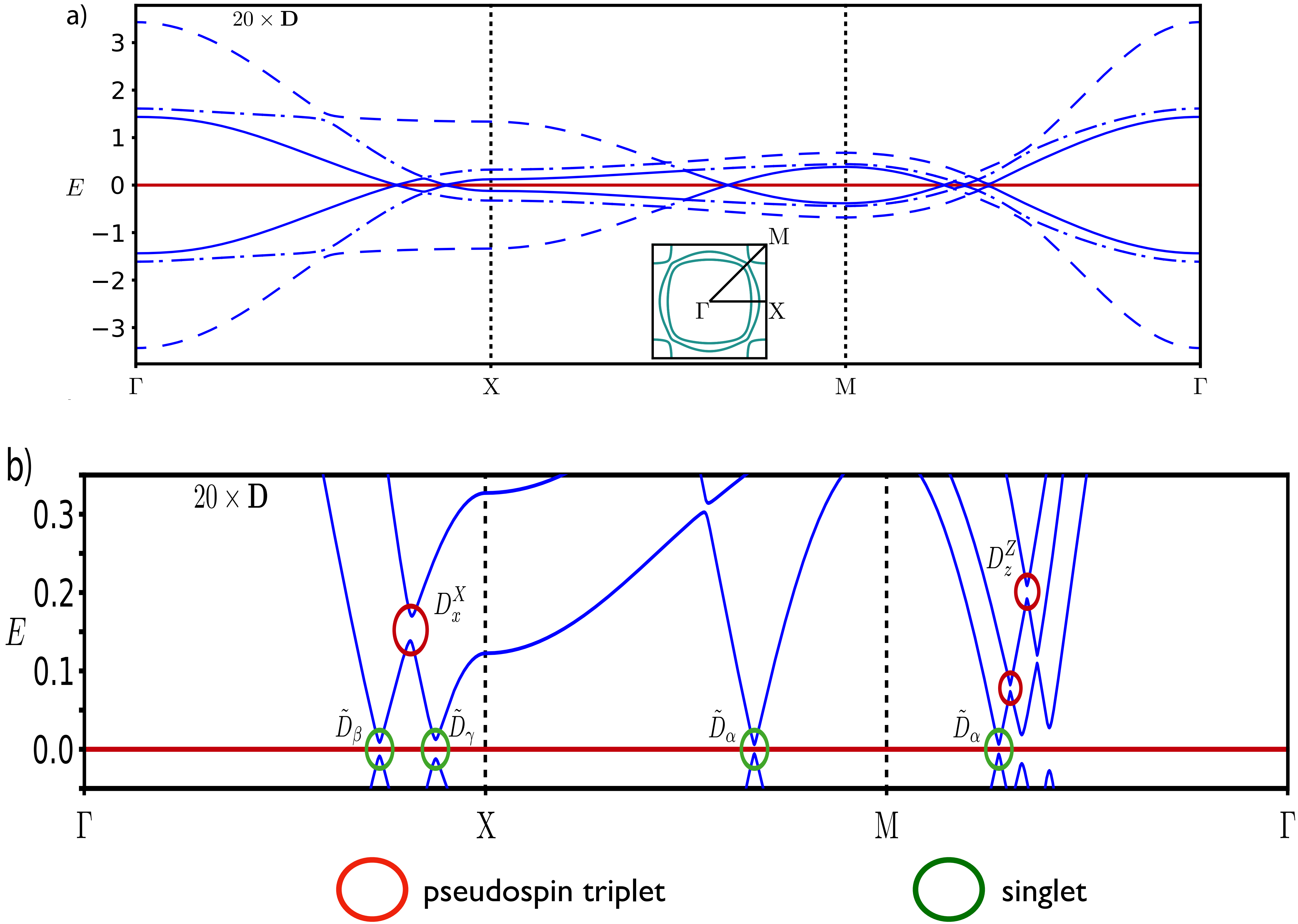
CHRISTOPH M. PUETTER[1] and HAE-YOUNG KEE[1,2(a)]



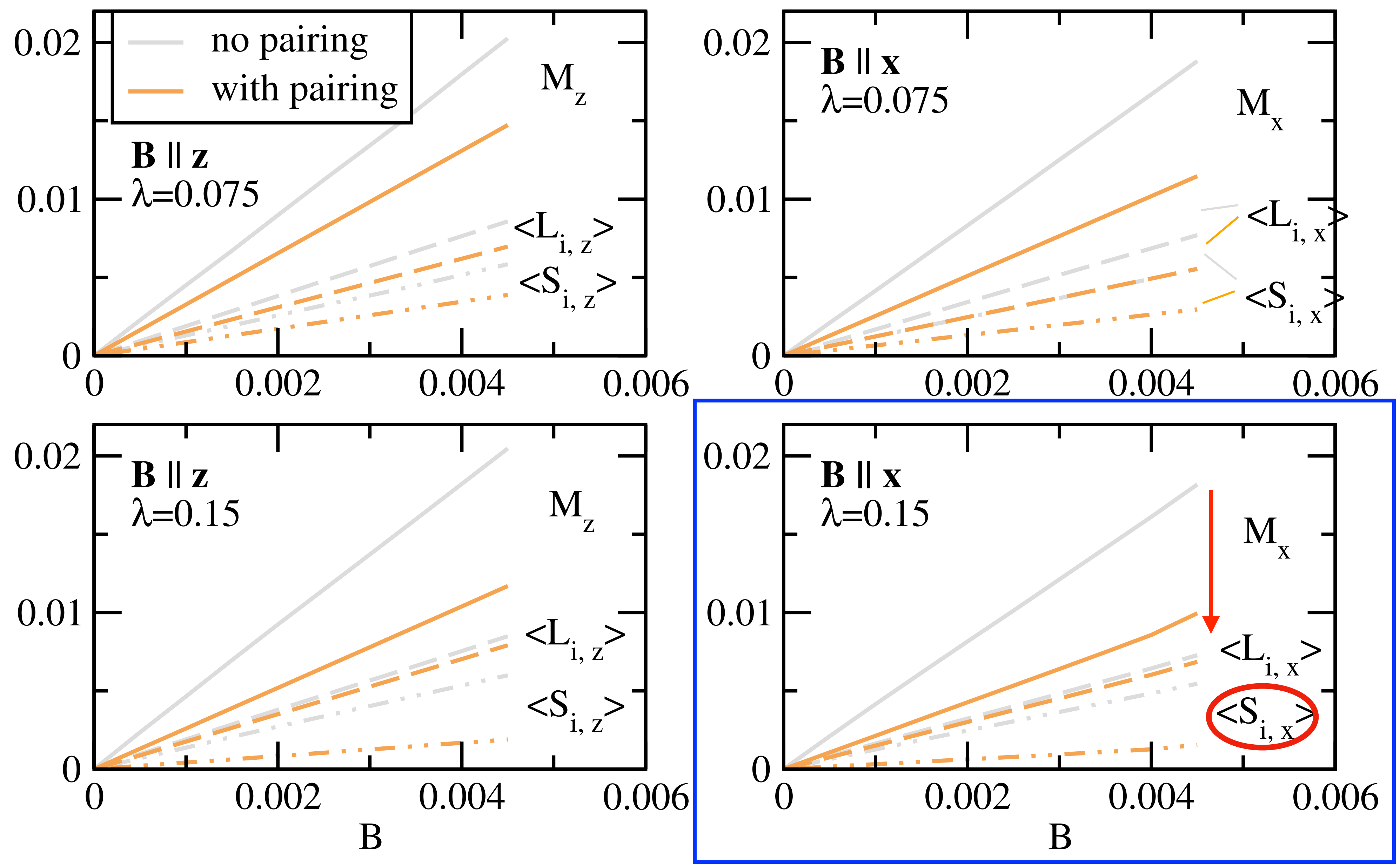
SOC enhances inter-orbital (orbital-singlet) even-parity spin-triplet & pins d-vector direction (varies in momentum space)

atomic SOC: anisotropic S-wave

QP dispersion



magnetization



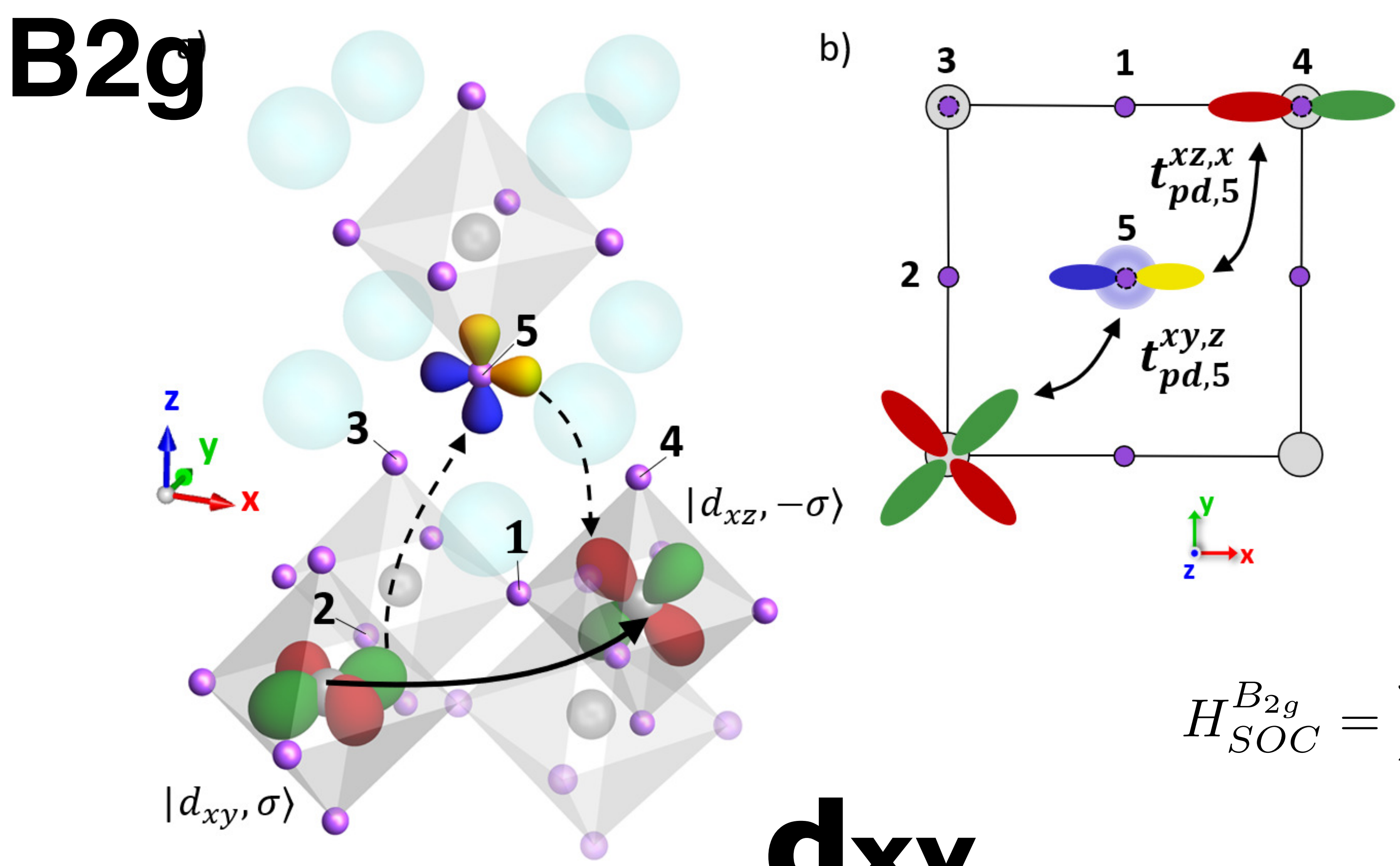
C. Puetter, HYK, EPL 98, 27010 (2012) ; arXiv:1101.4656

Deduction of Knight shift for all field directions

How to get two-component OP?

momentum dependent SOC
beyond atomic SOC

momentum-dependent SOC: $\lambda(\mathbf{k})$



$$H^{B_{2g}}_{SOC} = \sum_{p_\pm} \frac{H^0|p_\pm\rangle\langle p_\pm|H^0}{E_d - E_{p_\pm}},$$

dxy

$$-8i\lambda^{B2g} \sum_{\mathbf{k}\sigma\sigma'} \sin k_x \sin k_y \left(\sigma^y_{\sigma\sigma'} c^{xz\dagger}_{\mathbf{k}\sigma} c^{xy}_{\mathbf{k}\sigma'} - \sigma^x_{\sigma\sigma'} c^{yz\dagger}_{\mathbf{k}\sigma} c^{xy}_{\mathbf{k}\sigma'}\right) + h.c.$$

$$\lambda^{B_{2g}} = \frac{\lambda_p}{(E_{pd} + \frac{\lambda_p}{2})(E_{pd} - \lambda_p)} \sum_i t^{a_i}_{pd,i} t^{b_i}_{pd,i}$$

SOC determines pairing; $\Delta^s(\mathbf{k}) \propto d_{a/b} \times \lambda(\mathbf{k})$

When atomic λ & momentum-dep. SOC $\lambda^{B_{2g}}$ present

pseudo-spin singlet $\boxed{s + id_{xy}}$

$$s \propto d^{x}_{xz/yz}\lambda,\ d^{y}_{yz/xy}\lambda,\ d^{z}_{xz/yz}\lambda$$

$$d_{xy} \propto d^{x(y)}_{yz(xz)/xy}(\sin k_x \sin k_y)\ \lambda^{B2g}$$

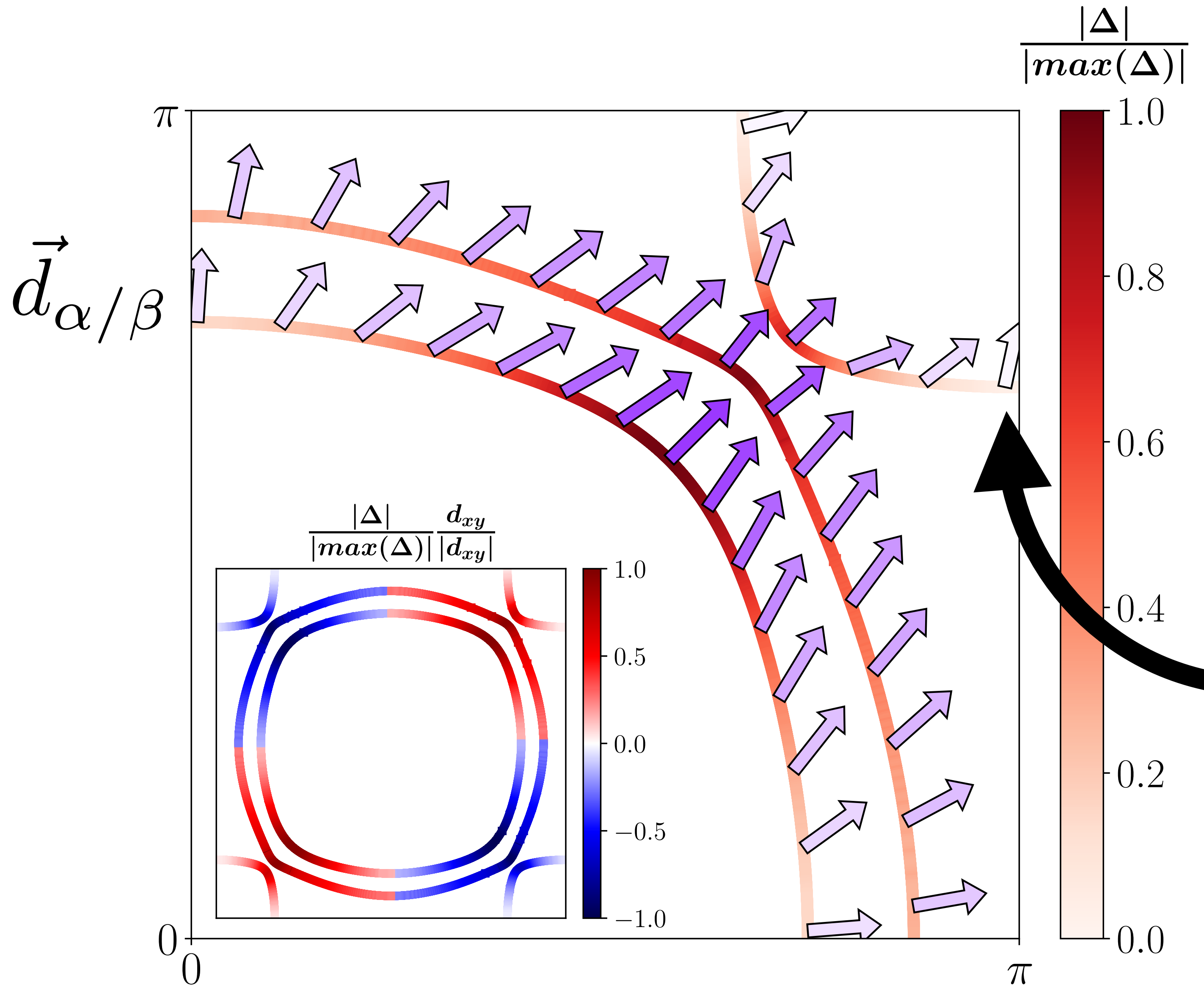
$J_H - U' = 0.7$ $\lambda = 0.05$ $\lambda^{B2g} = 0.038$ $\lambda^{Eg} = 0.005$

t_1	t_2	t_3	t_4	t_{ab}	μ_{1d}	μ_{xy}
0.45	0.05	0.5	0.2	0.025	0.54	0.64

Shadowed Triplet Pairing

$s + id_{xy}$ pseudo-spin singlet

$\vec{d}_{\alpha/\beta}$ pseudo-spin triplet pairing finite away from the Fermi energy



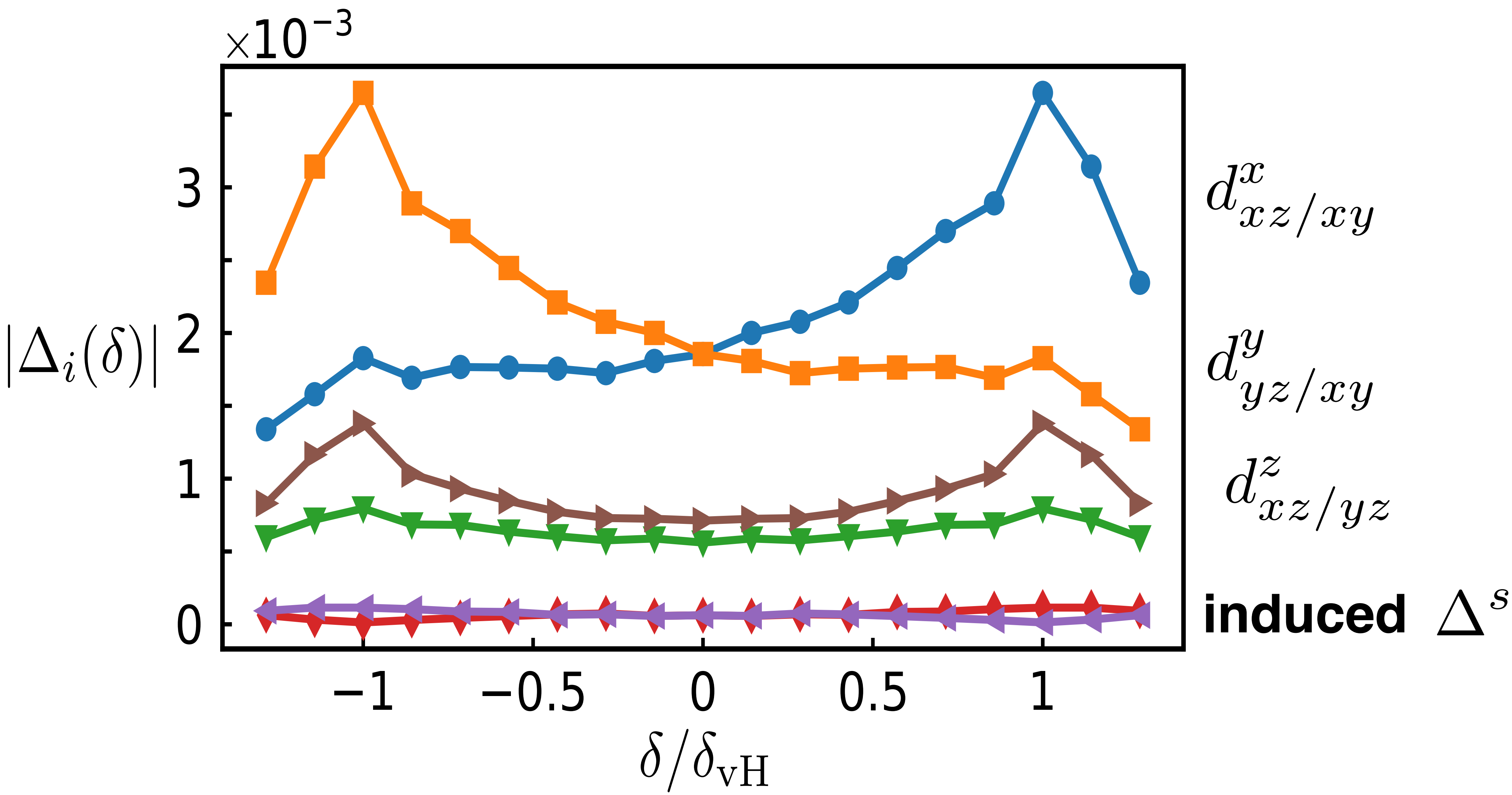
$\Delta_{max} = 2 \times 10^{-4}$

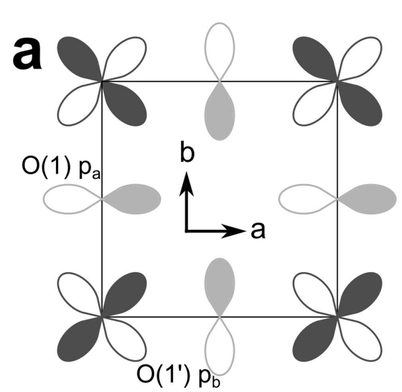
$\Delta_{min} \sim 10^{-6}$

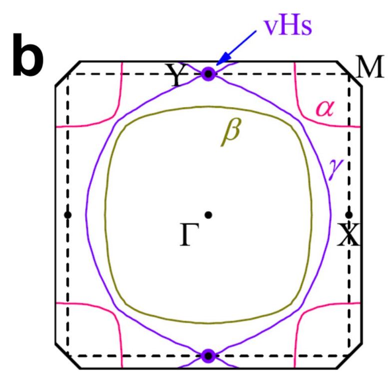
~ O(1) mK

arXiv:2009.08597, J. Clepkens, A. Lindquist, HYK

Effects of Strain





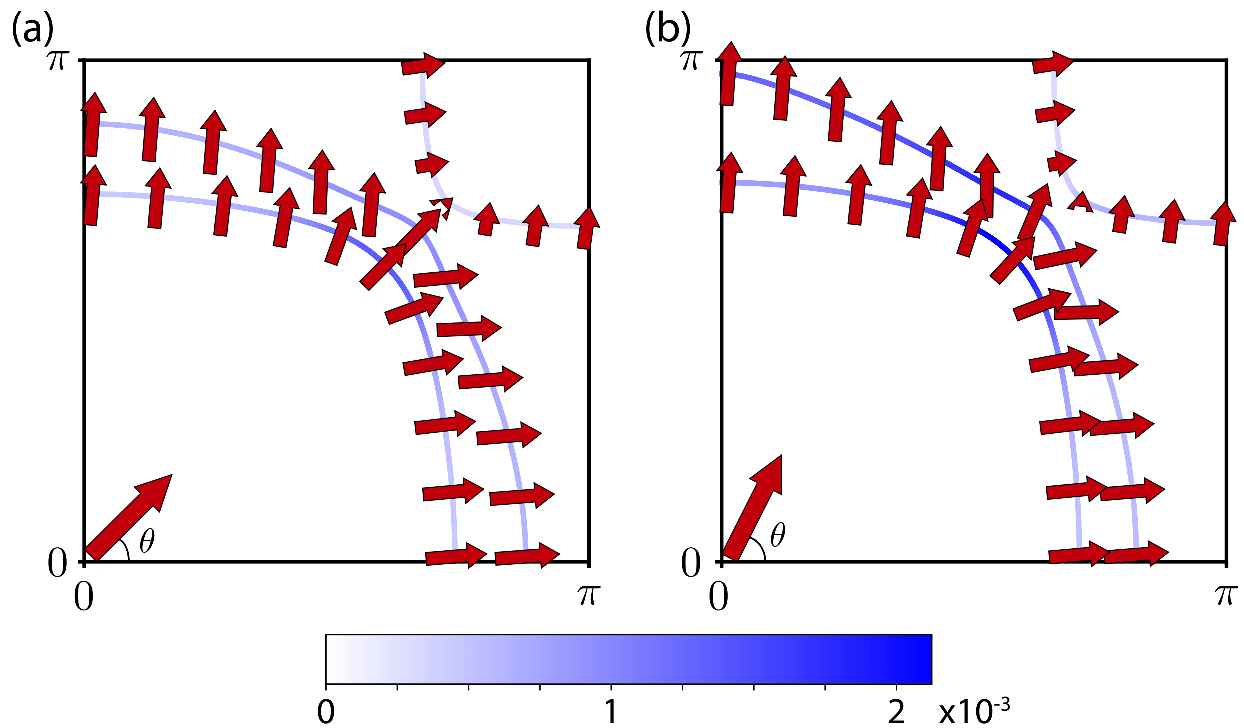


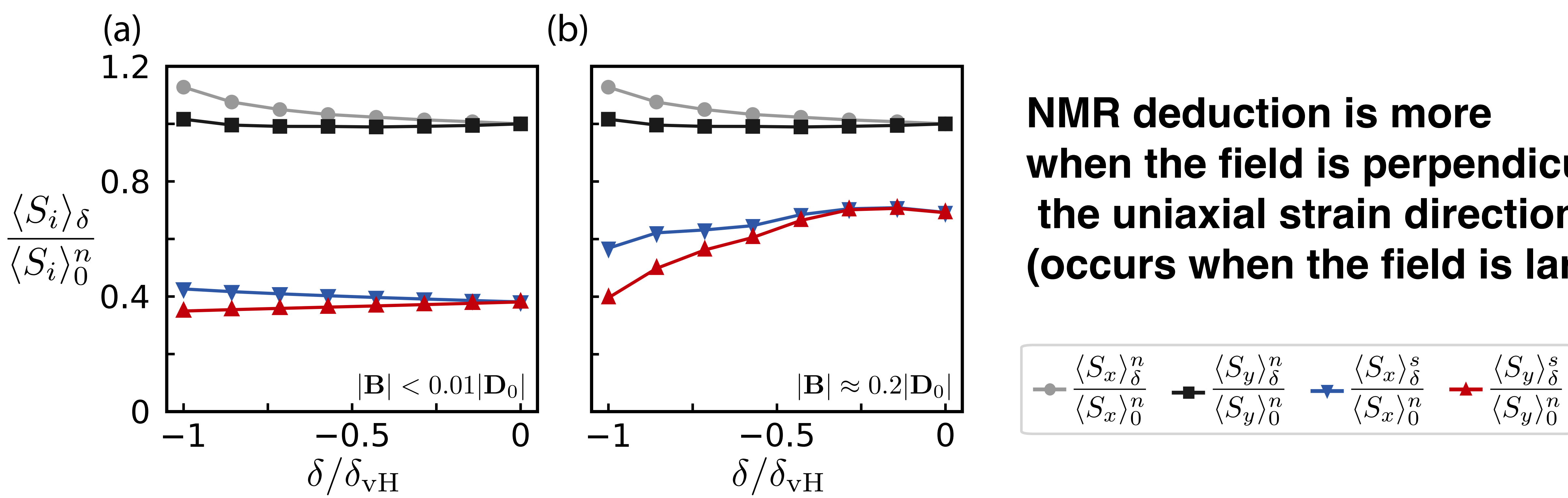
A. Lindquist, HYK, PRR 2, 320 (2020)

Proposal to test the theory

NMR under strain

Uniaxial strain along a-axis

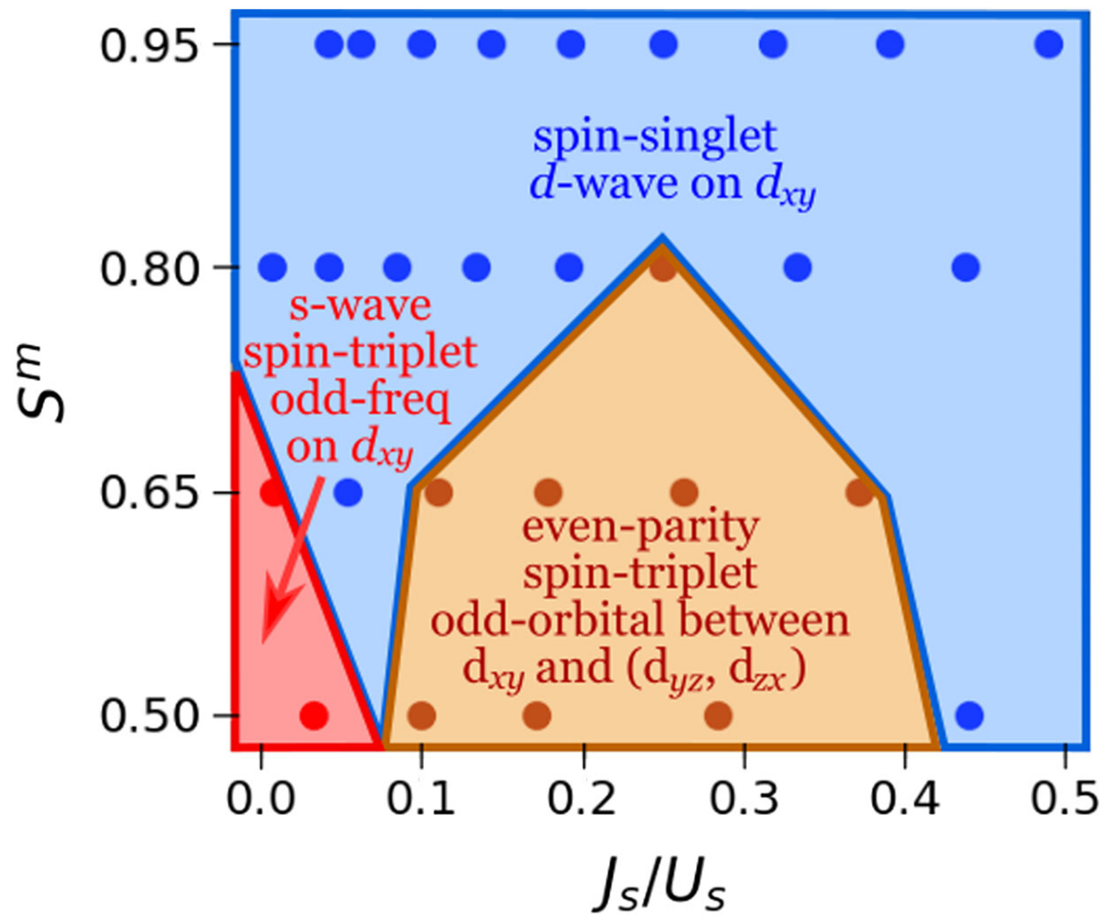




NMR deduction is more when the field is perpendicular to the uniaxial strain direction (occurs when the field is large)

A. Lindquist, HYK, PRR 2, 320 (2020)

Beyond MF



LDA+ DMFT: O. Gingras et al, PRL 123, 217005 (2019)

Application to Pnictides

O.Vafek, A.V. Chubukov, PRL (2017); Hund's + SOC on 2-orbitals

Conclusion

Within a MF of Kanamori + t2g + SOC: applicable Hund's metal with SOC

- SOC determines the gap size and k-dependence of pairing
- pseudospin singlet + pseudospin triplet + i induced singlet
- d-vector changes in k-space
- For Sr2RuO4: s+ i d (TRSB SC) & pseudospin triplet & induced singlet

beyond on-site interaction? Tc? HQV?