ETH zürich

# Identification of detrimental effects to multi-band superconductivity: Application to $Sr_2RuO_4$

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**SPS Meeting - Geneva - August 24th 2017**

# Outline

1) What we already know:
   - BCS Theory, Symmetries and Anderson's Theorems

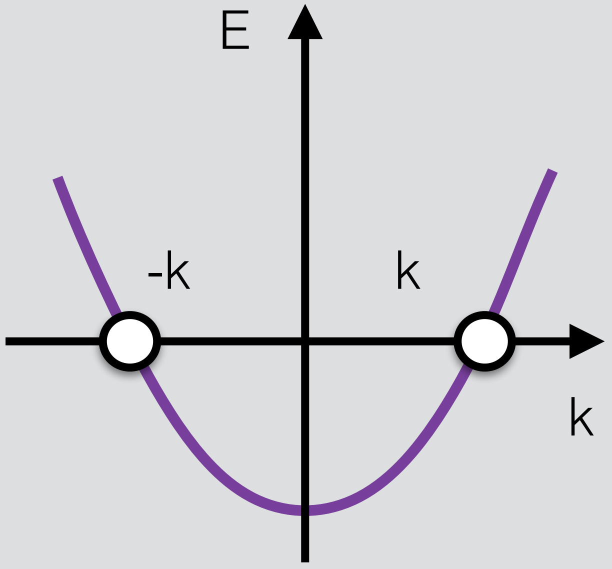
2) Orbital x Band Basis:
   - Introducing the concept of "SC Fitness"

3) Sanity check:
   - 1 band + key symmetry breaking fields

4) Application to $Sr_2RuO_4$:
   - The most compatible order parameter
   - New mechanism for suppression of SC

5) Final remarks

# What we already know:

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Robust instability: $T_c \sim \omega_c e^{-1/v_{eff}N(0)}$

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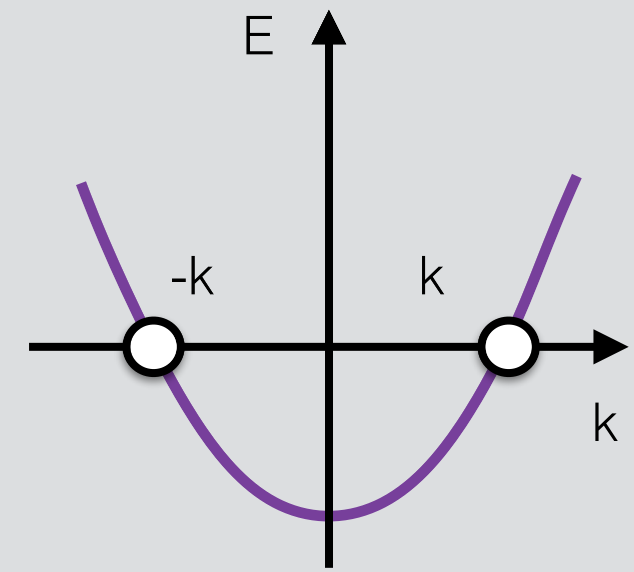


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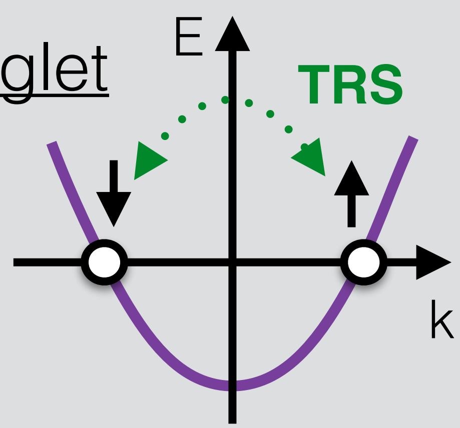
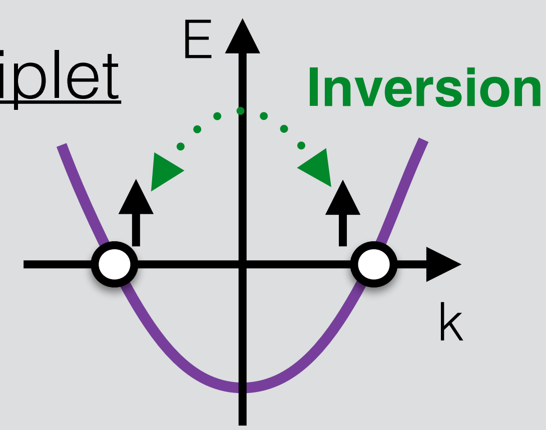
Singlet




Triplet

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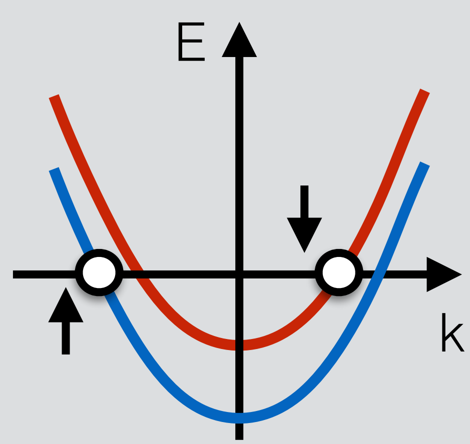


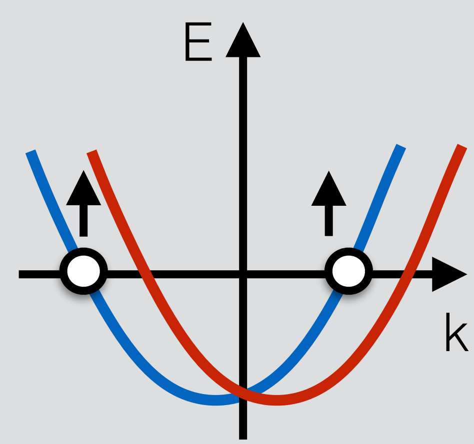

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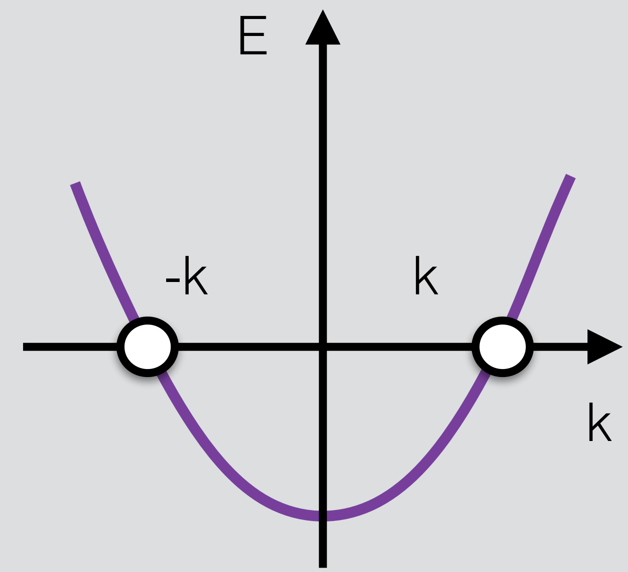


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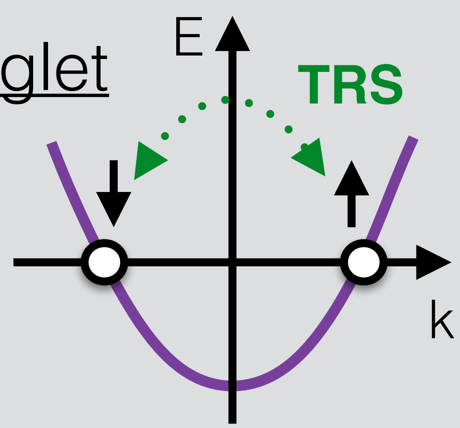


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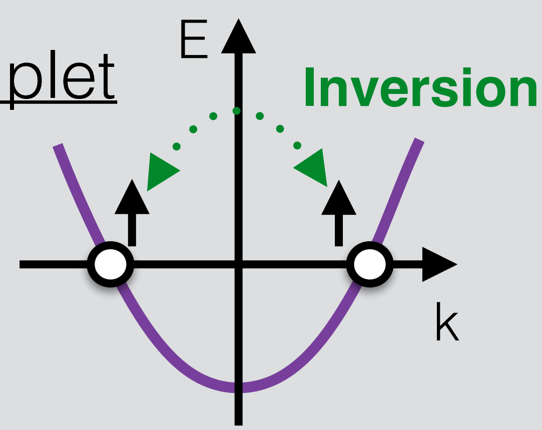


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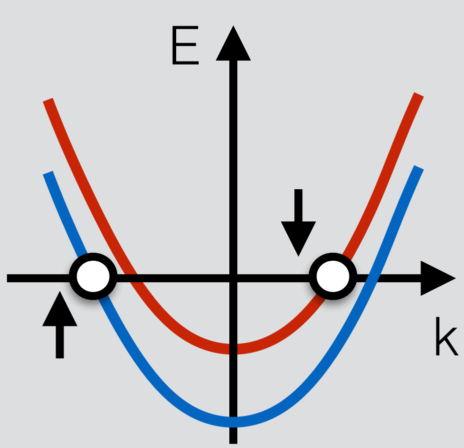
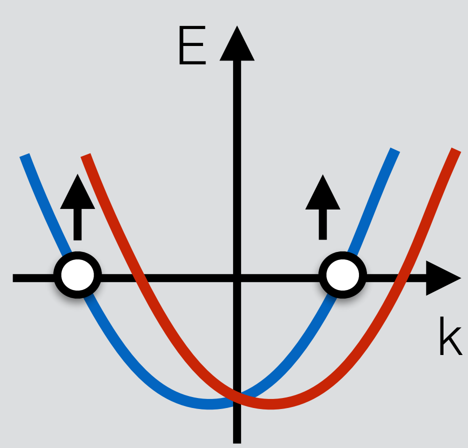
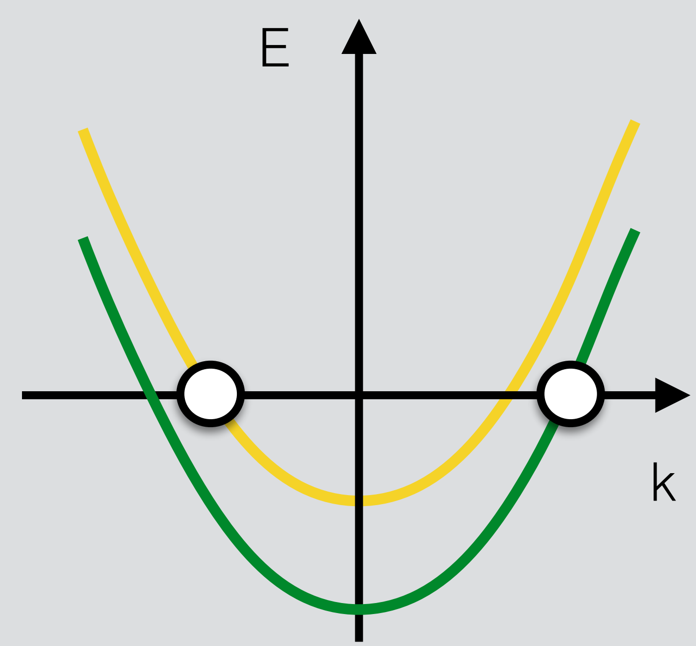



Multi-Band Systems




**"Inter-band pairing is NOT robust"**

# From the orbital to the band basis…

The MF Hamiltonian for a multi-orbital system:

$$H_{MF} = \sum_{\mathbf{k}} \Psi^{\dagger}_{\mathbf{k}} \begin{pmatrix} H_0(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^{\dagger}(\mathbf{k}) & -H_0^*(-\mathbf{k}) \end{pmatrix} \Psi_{\mathbf{k}},$$

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(Inter-orbital hopping, SOC,…)

Unitary transformation to the band basis:

$$H_0^B(\mathbf{k}) = U_{\mathbf{k}} H_0(\mathbf{k}) U_{\mathbf{k}}^{\dagger}$$

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# …and back to the orbital basis:

Key symmetries+
Only intra-band pairing

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**Q: What condition it imposes in the orbital basis?**

$$H_0(\mathbf{k})\Delta(\mathbf{k}) - \Delta(\mathbf{k})H_0^*(-\mathbf{k}) = 0,$$

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In general this condition won't be satisfied and this modified commutator is finite, so we introduce the concept of **"SC Fitness":**

$$H_0(\mathbf{k})\Delta(\mathbf{k}) - \Delta(\mathbf{k})H_0^*(-\mathbf{k}) = F(\mathbf{k})(i\sigma_2)$$

**Measure of INcompatibility of the gap and underlying electronic structure.**

$$\begin{cases} F(\mathbf{k}) = 0 & \textbf{Compatible} \\ F(\mathbf{k}) \neq 0 & \textbf{Not Compatible/ Detrimental} \end{cases}$$

# Sanity check:

Single band problem under external perturbation:

$$H_0(\mathbf{k})\Delta(\mathbf{k}) - \Delta(\mathbf{k})H_0^*(-\mathbf{k}) = F(\mathbf{k})(i\sigma_2)$$

$$H_0(\mathbf{k}) \to H_0(\mathbf{k}) + \delta H(\mathbf{k})$$

| "SC Fitness" $F(\mathbf{k})$ | TRS breaking $\delta H_{TR} = -\mathbf{h}\cdot\boldsymbol{\sigma}$ | Inv breaking $\delta H_{Inv}(\mathbf{k}) = \mathbf{g}(\mathbf{k})\cdot\boldsymbol{\sigma}$ |
|---|---|---|
| Singlet $\Delta_S(\mathbf{k}) = d_0(\mathbf{k})(i\sigma_2)$ | | |
| Triplet $\mathbf{z} = \lvert S_z=0\rangle = \frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\rangle + \lvert\downarrow\uparrow\rangle)$, $\mathbf{x} = \lvert S_x=0\rangle = \frac{1}{\sqrt{2}}(-\lvert\uparrow\uparrow\rangle + \lvert\downarrow\downarrow\rangle)$, $\mathbf{y} = \lvert S_y=0\rangle = \frac{1}{\sqrt{2}}(\lvert\uparrow\uparrow\rangle + \lvert\downarrow\downarrow\rangle)$, $\Delta_T(\mathbf{k}) = (\mathbf{d}_T(\mathbf{k})\cdot\boldsymbol{\sigma})(i\sigma_2)$ | | |

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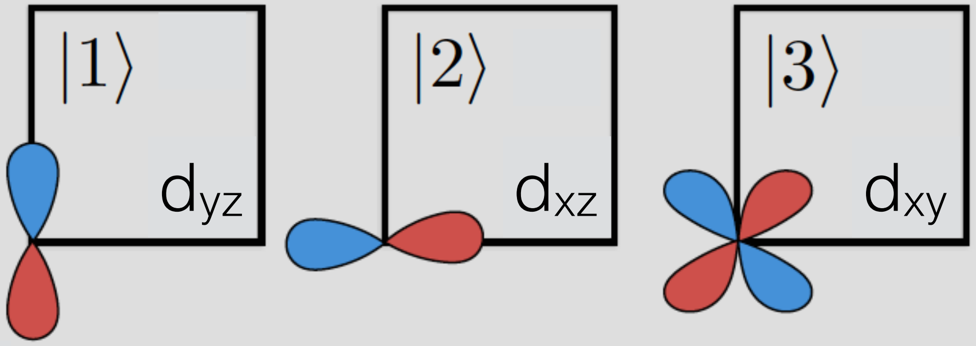
**Unified closed form for the effect of perturbations on the critical temperature:**

$$T_c \sim T_c^0\left(1 - \frac{7\xi(3)}{64(\pi T_c^0)^2}\left\langle Tr|\hat{F}(\mathbf{k})|^2\right\rangle_{FS}\right)$$

* perturbative in the external symmetry breaking fields

# Application to $Sr_2RuO_4$:

Basic ingredients:




Hamiltonian including Inter-orbital hopping (IOH) and Spin-orbit coupling (SOC)

$$H_{SRO}(\mathbf{k}) = \begin{pmatrix} \epsilon_{1\mathbf{k}} I_2 & t_{\mathbf{k}} I_2 + i\eta\sigma_3 & -i\eta\sigma_2 \\ t_{\mathbf{k}} I_2 - i\eta\sigma_3 & \epsilon_{2\mathbf{k}} I_2 & i\eta\sigma_1 \\ i\eta\sigma_2 & -i\eta\sigma_1 & \epsilon_{3\mathbf{k}} I_2 \end{pmatrix}$$

in the orbital basis:

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The gap matrix (only intra-orbital pairing):

$$\Delta_a(\mathbf{k}) = \begin{cases} d_{a0}(\mathbf{k})(i\sigma_2) \\ \mathbf{d}_a(\mathbf{k}) \cdot \boldsymbol{\sigma}(i\sigma_2) \end{cases}$$

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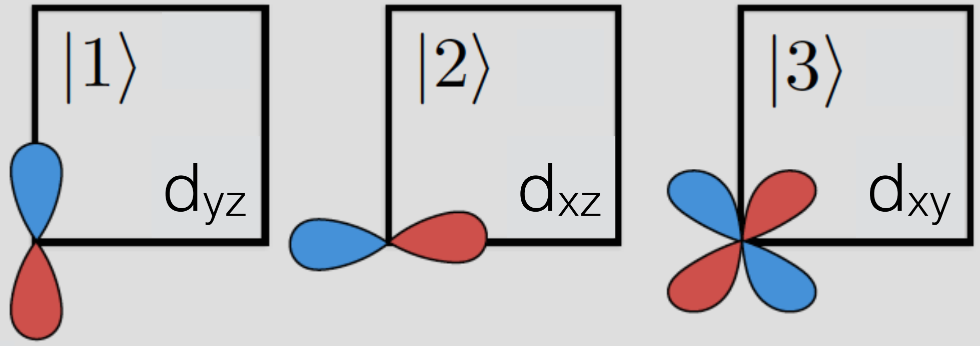


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**Q: How IOE shape the SC state?**

$$[H_0(\mathbf{k}) + \delta H(\mathbf{k}), \hat{\Delta}(\mathbf{k})]^* = \hat{F}(\mathbf{k})(i\sigma_2)$$

**Example: IOH**

$$\hat{F}_{IOH} = it(\hat{d}_{1j} - \hat{d}_{2j})\lambda_2 \otimes \sigma_j$$

$$j = 0, x, y, z$$

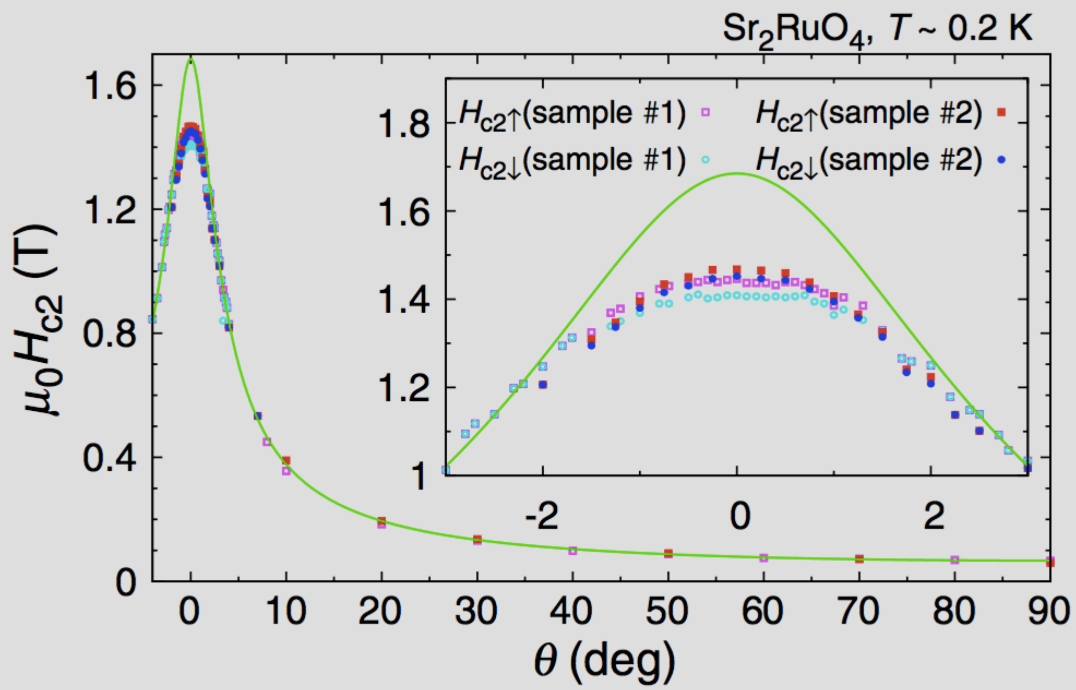
| $F(\mathbf{k})$ | **IOH** | **SOC** | **IOH +SOC** |
|---|---|---|---|
| $\Delta_S$ | $\hat{d}_{10} = \hat{d}_{20}$ | $\hat{d}_{10} = \hat{d}_{20} = \hat{d}_{30}$ | ✓ |
| $\Delta_{Tx}$ | $\hat{d}_{1x} = \hat{d}_{2x}$ | $-\hat{d}_{1x} = \hat{d}_{2x} = \hat{d}_{3z}$ | ✗ |
| $\Delta_{Ty}$ | $\hat{d}_{1y} = \hat{d}_{2y}$ | $\hat{d}_{1y} = -\hat{d}_{2y} = \hat{d}_{3y}$ | ✗ |
| $\Delta_{Tz}$ | $\hat{d}_{1z} = \hat{d}_{2z}$ | $\hat{d}_{1z} = \hat{d}_{2z} = -\hat{d}_{3z}$ | ✓ |

**Only compatible triplet state: d-vector in the z-direction!**

Yonezawa et al., PRL 110, 077003 (2013)
Yonezawa et al., J. Phys. Soc. Jpn. 83, 083706 (2014)

# $Sr_2RuO_4$: upper critical field

## I) Anisotropy:




**Effective mass model (EMM):**

$$h_{c2,EMM}(\theta) = \frac{h_{c2}(90^o)}{\sqrt{\sin^2\theta + \cos^2\theta/\Gamma^2}},$$

$$\Gamma = \sqrt{M/m} \approx 25$$

**Deviations from EMM for angles within 2º from the plane.**

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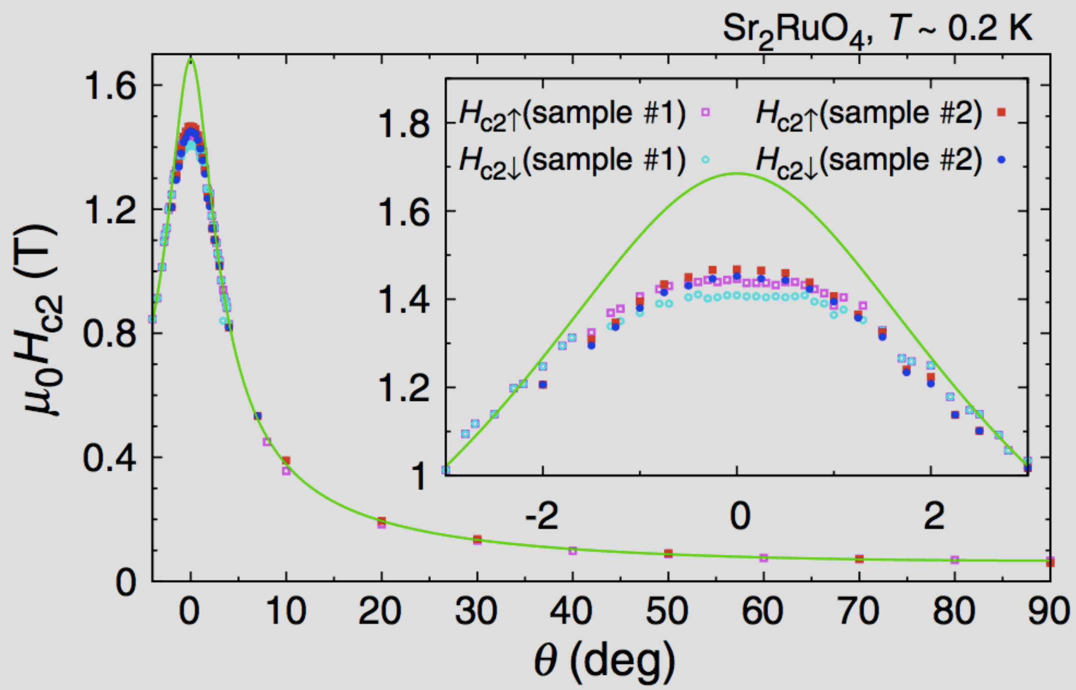


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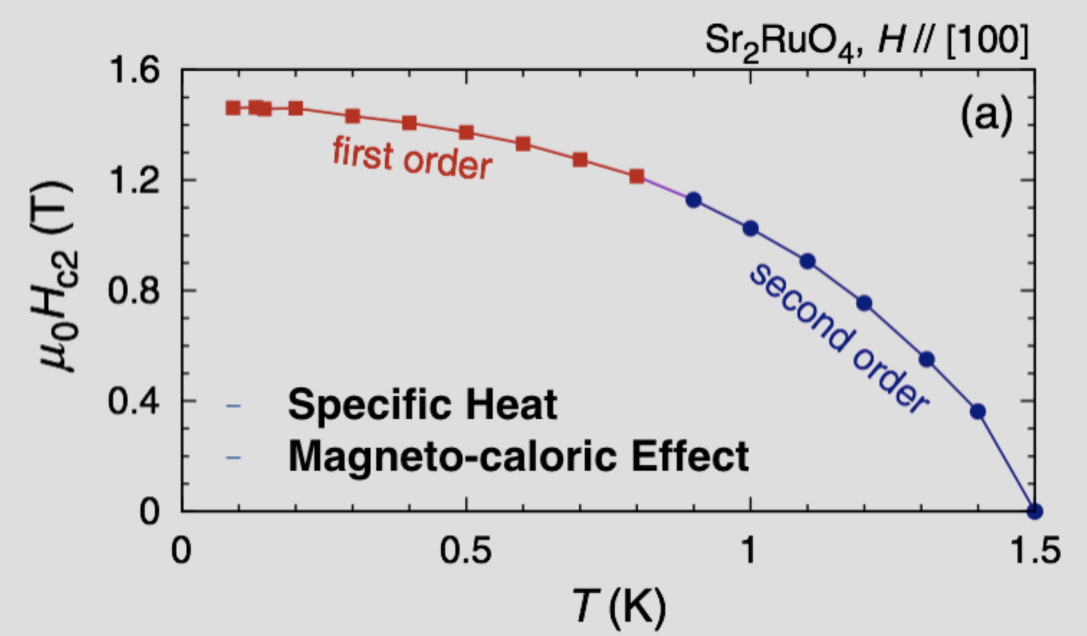
## II) Transition 2nd ➔ 1st order:




For in plane fields transition becomes **1st order** below 0.8K.

**1st order ➔ Pauli limiting effect? NO:**
**d-vector is along z-direction.**
**No change in the Knight shift across Tc.**

**New mechanism?!**

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Given a multi-orbital system:

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$$\hat{F}_{Orb} = -2i h_{ox} d_z \lambda_7 \otimes \sigma_3$$

**Now in plane magnetic is also detrimental to d-vector along z-direction due to IOE.**

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**Now in plane magnetic is also detrimental to d-vector along z-direction due to IOE.**

**Qualitative distinct from the single-band scenario:**

$$\hat{F}_{Spin} \;=\; -2\mathbf{h} \cdot \mathbf{d}_T I_2$$

# Under magnetic field:

Given a multi-orbital system:

$$\delta H_{Orb} = -\mathbf{L}\cdot\mathbf{h}_o$$

Evaluating the **"SC Fitness"** for:

$$\begin{cases} \mathbf{h}_o // \hat{x} \\ \hat{d}_{z1} = \hat{d}_{z2} = -\hat{d}_{z3} = d_z \end{cases}$$

$$\hat{F}_{Orb} \;=\; -2ih_{ox}d_z\lambda_7 \otimes \sigma_3$$

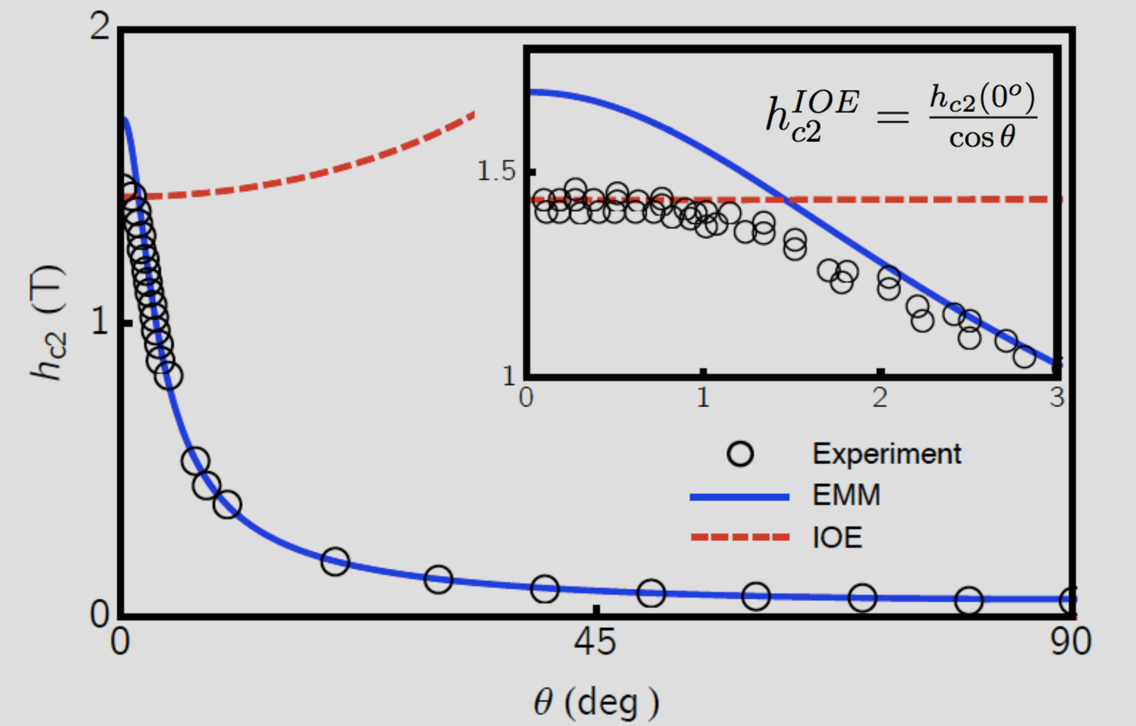
**Now in plane magnetic is also detrimental to d-vector along z-direction due to IOE.**

**Qualitative distinct from the single-band scenario:**

$$\hat{F}_{Spin} \;=\; -2\mathbf{h}\cdot\mathbf{d}_T I_2$$

# INTER ORBITAL EFFECT

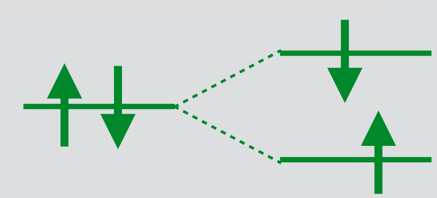
- **Change in anisotropy**
- **1st order transition**

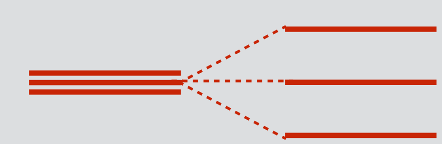



$$E_C = -\frac{N(0)|\Delta|^2}{2}$$

$$E_M = -\frac{\Delta\chi_{Orb}h_x^2}{2}$$

$$h_{c2}^{IOE} \approx \sqrt{\frac{N(0)}{\Delta\chi_{Orb}}}\frac{T_c^0}{\cos\theta}$$





**Pauli PM Limiting** **IOE Limiting**

Phys. Rev. B **94**, 104501 (2016)
Journal of Physics: Conf. Series **807**, 052011 (2017)

# Final Remarks

- We developed the concept of **SC Fitness**:

$$H_0(\mathbf{k})\Delta(\mathbf{k}) - \Delta(\mathbf{k})H_0^*(-\mathbf{k}) = F(\mathbf{k})(i\sigma_2)$$

  - Measure of the **instability of the SC state** in presence of symmetry breaking fields;

- **Application to $Sr_2RuO_4$:**
  - Find the **interplay of IOH and SOC** favours the **d-vector along the z-direction**;
  - Find **new mechanism** to suppress SC in multi-orbital systems: **Inter-Orbital Effect**;

- **Future work:**
  - Detailed microscopic calculation for the IOE;
  - Application to other materials and model systems;

**SC Fitness 2.0: Useful tool for engineering the normal state in order to obtain the desired (exotic/topological) SC state.**