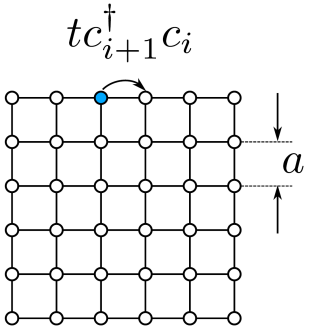
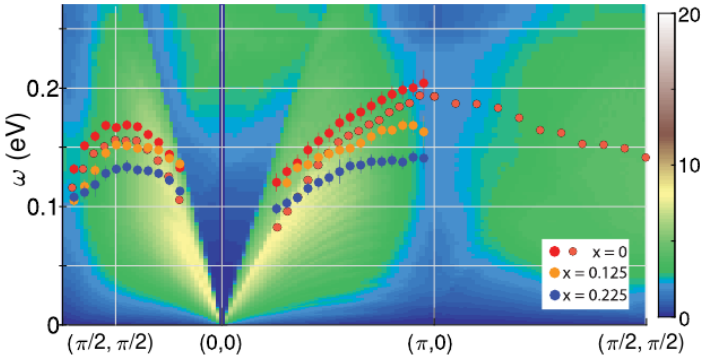
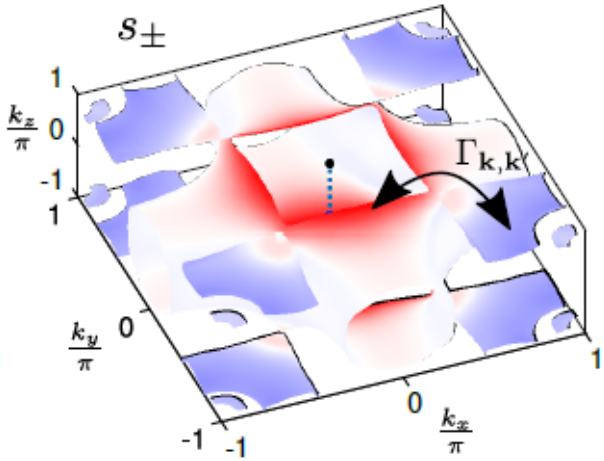
Magnetic fluctuations for superconductivity: From itinerant to localized picture

Andreas Kreisel
Niels Bohr Institute, University of Copenhagen

$$H_0 = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}$$

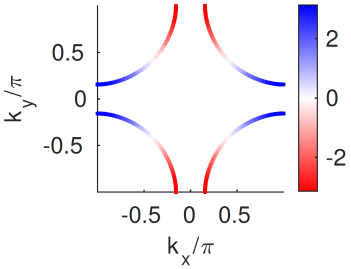






Theory of superconductivity: In a nutshell

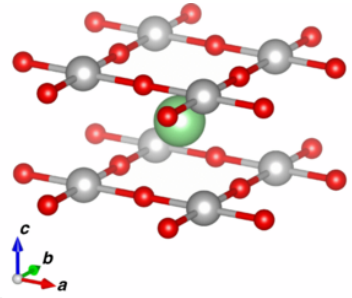
- Superconducting order parameter $\Delta(\mathbf{k})$



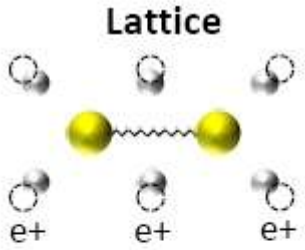
- Theoretical question: Calculate order parameter from given pairing interaction

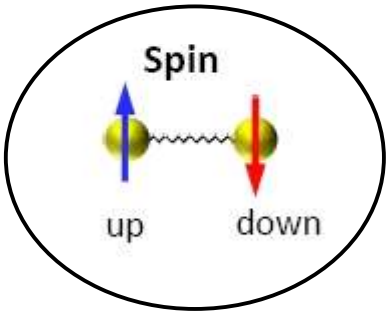
$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} \Gamma(\mathbf{k}-\mathbf{k}') \frac{\tanh(\frac{E_{\mathbf{k}'}}{2k_BT})}{2E_{\mathbf{k}'}} \Delta(\mathbf{k}') \qquad \text{BCS gap equation}$$

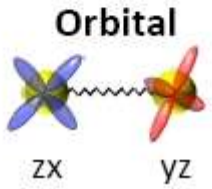
- Preliminary question: Are the spin fluctuations used for the calculations the "right ones" for a given material?



?



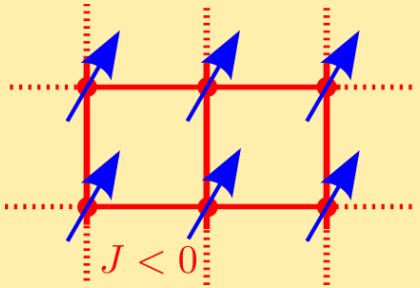


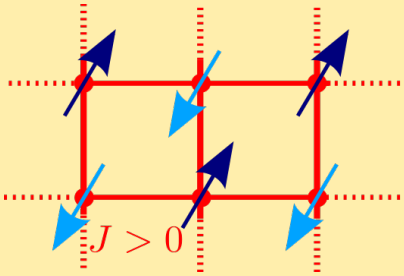


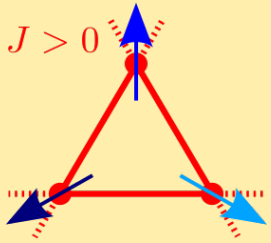
$$\Gamma_{\text{Spin}}(\mathbf{q}) \sim \frac{3}{2}(U + U^2\chi(\mathbf{q}))$$

Quantum magnetism

Localized picture

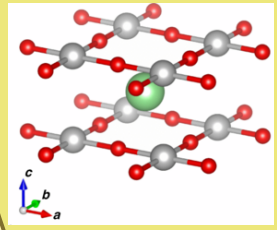




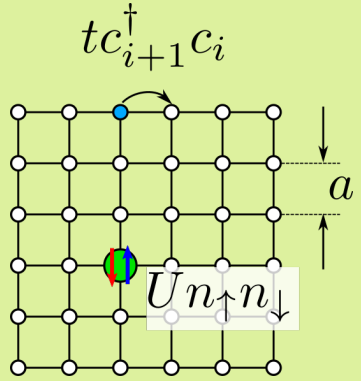


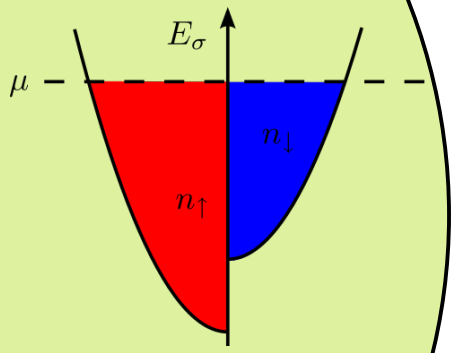
$$H = \frac{1}{2}\sum_{ij} J_{ij}\vec{S}_i \cdot \vec{S}_j$$

unconventional superconductors



Itinerant picture

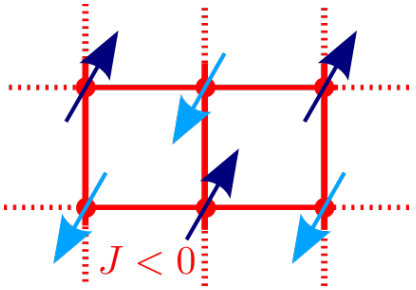




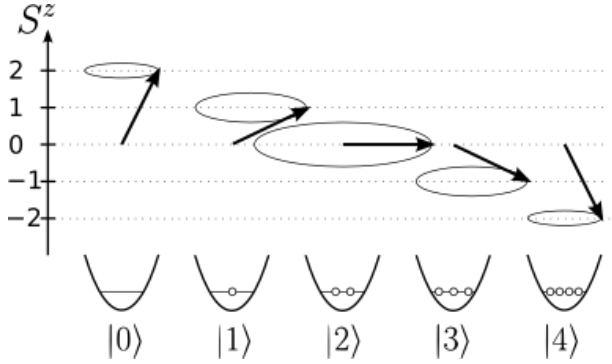
$$H = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Localized picture: Heisenberg (like) models

- Heisenberg model $H = \frac{1}{2}\sum_{ij} J_{ij}\vec{S}_i \cdot \vec{S}_j$

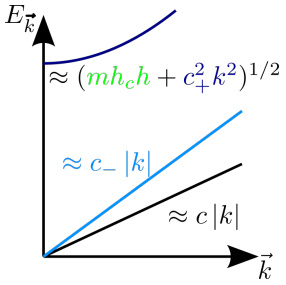


- Spin-wave approach: map to bosons

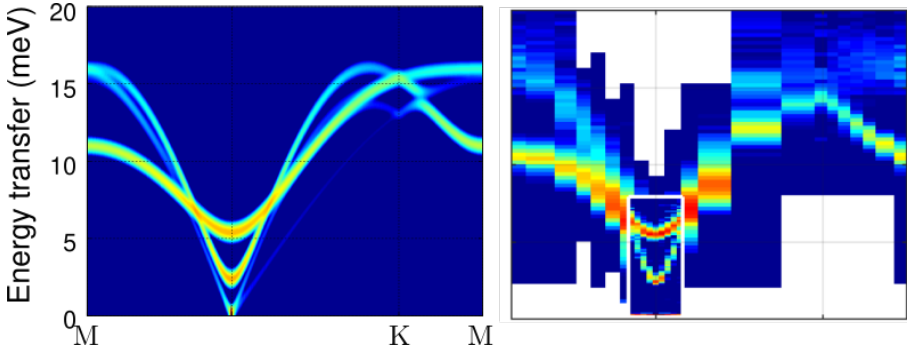


- Solve dynamical matrix for eigenvalues

$$D_{\mathbf{k}} = \begin{pmatrix} A_{\mathbf{k}} & B_{\mathbf{k}} \\ B^*_{-\mathbf{k}} & -A^T_{-\mathbf{k}} \end{pmatrix}$$



Analytical+interactions:
AK, et al., Phys. Rev. B **78**, 035127 (2008)

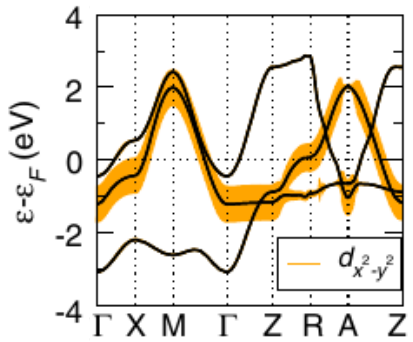


numerical:
Holm, AK, et al., Phys. Rev. B **97**, 134304 (2018)

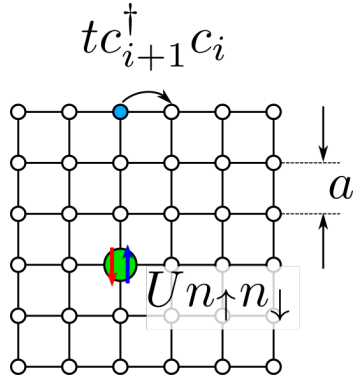
Spin

Itinerant picture: conduction electrons and Coulomb interaction

- Electronic band structure

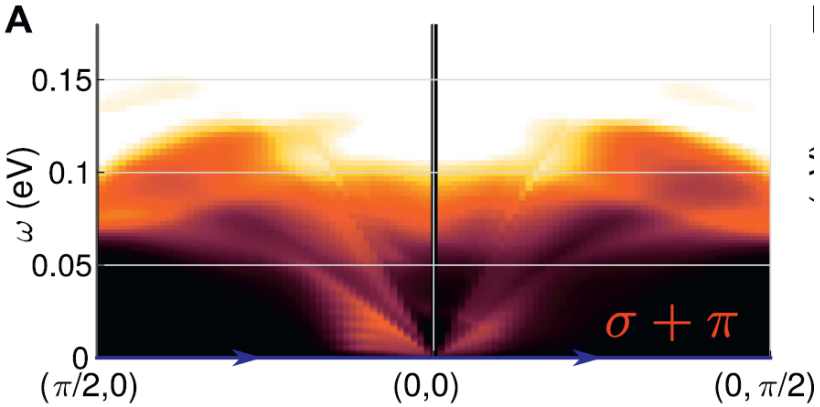


$$\chi_0(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}} \frac{f(\xi_{\mathbf{k}+\mathbf{q}}) - f(\xi_{\mathbf{k}})}{\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}}$$



- Interactions (for example in RPA)

$$\chi_{RPA}(\mathbf{q}) = \frac{\chi_0(\mathbf{q})}{1 - U\chi_0(\mathbf{q})}$$

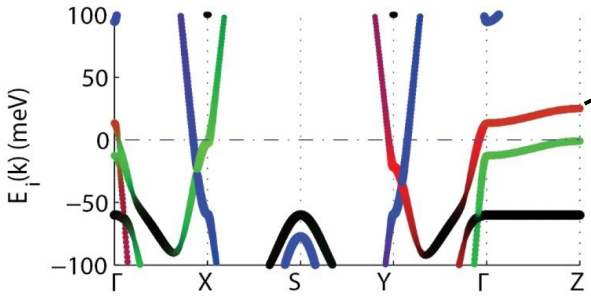


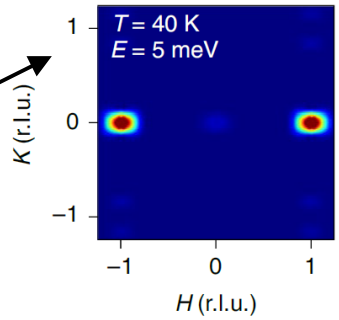
"paramagnon" bands → compare to experimental data INS, RIXS...

AK, et al, Frontiers in Physics **10**, 859424 (2022)

Examples: Pairing glue in FeSe

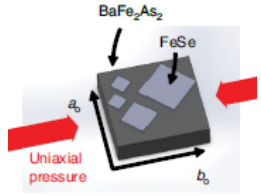
- "simplest crystal structure for Fe-based SC

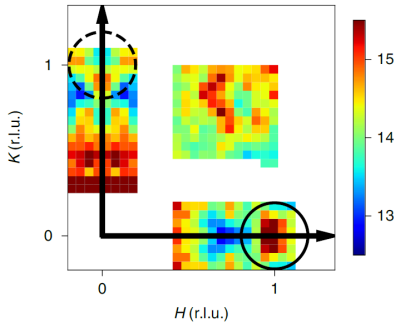




$$H = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}$$

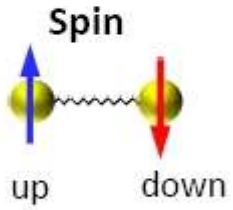
$$\chi_{RPA}(\mathbf{q}) = \frac{\chi_0(\mathbf{q})}{1 - U\chi_0(\mathbf{q})}$$





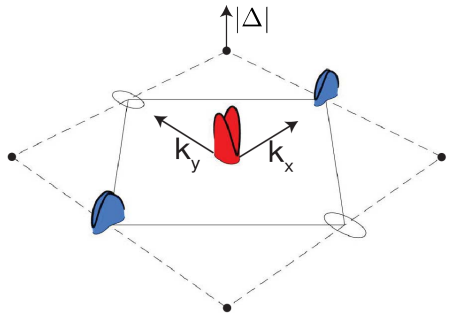
Strongly anisotropic spin fluctuations → verified by INS on mosaic of FeSe single crystals
Chen, AK, et al., Nat. Mater. **18**, 709 (2019)

- Calculation of superconducting order parameter



$$\Gamma_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}') = \left[\frac{3}{2}\bar{U}^s\chi_1^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^s + \frac{1}{2}\bar{U}^s - \frac{1}{2}\bar{U}^c\chi_0^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^c + \frac{1}{2}\bar{U}^c\right]_{\ell_1\ell_2\ell_3\ell_4}$$

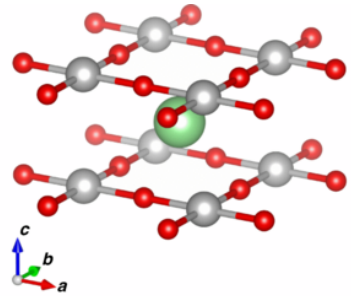
$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'}\Gamma(\mathbf{k}-\mathbf{k}')\frac{\tanh(\frac{E_{\mathbf{k}'}}{2k_BT})}{2E_{\mathbf{k}'}}\Delta(\mathbf{k}')$$

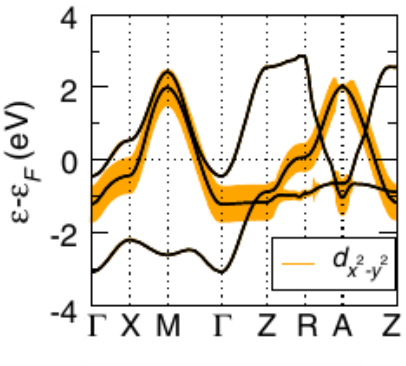


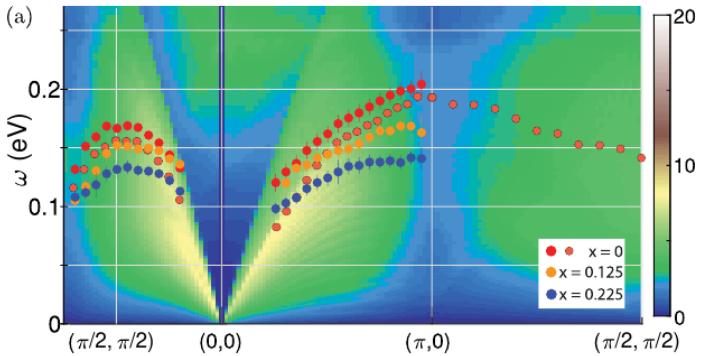
Strongly anisotropic order parameter
Sprau, … AK, et al., Science, **357**, 75 (2017)

Examples: infinite layer nickelates

- Cuprate analog of high T_c superconductors?



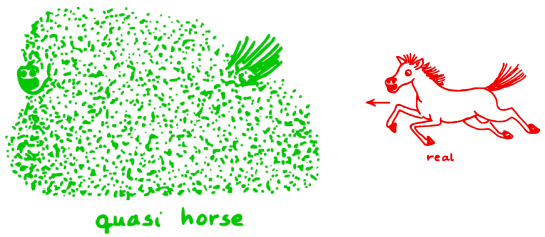


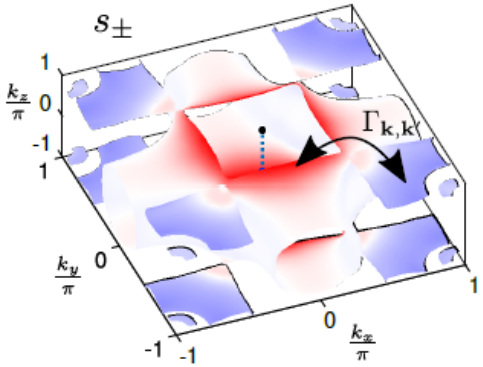


Only thin films, so comparison to RIXS !

H. Lu, M. Rossi, A. Nag, et al., Science **373**, 213 (2021)

- Calculation of superconducting order parameter



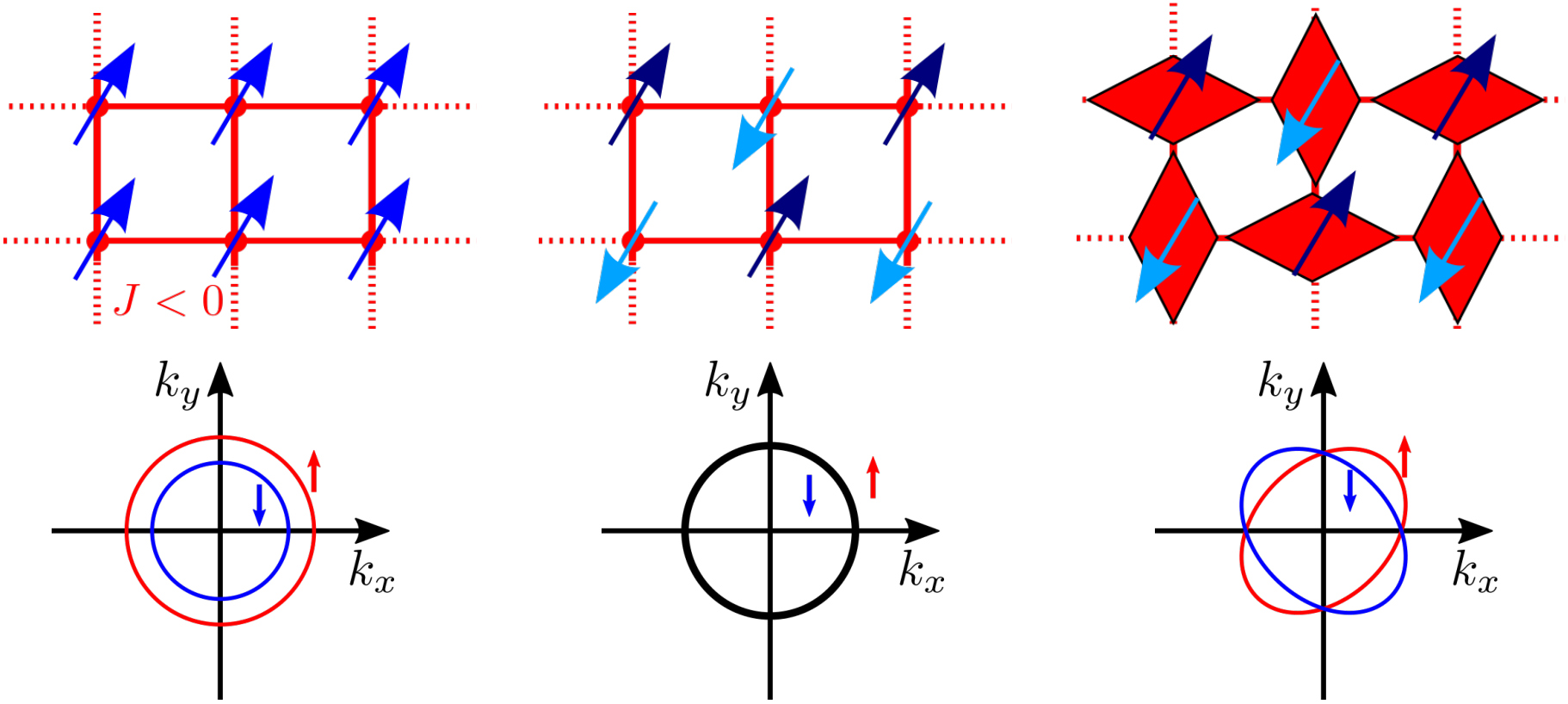


S-wave symmetry → more similar to multiband iron-based superconductors!

AK, et al, Phys. Rev. Lett. **129**, 077002 (2022)

Current projects

- Ferromagnetism antiferromagnetism altermagnetism



- Question: Mechanism for altermagnetism, superconducting pairing?

Šmejkal, et al, PRX **12**, 040501 (2022), PRX **12** 031042 (2022)