Spin-dependent Masses in High Magnetic Field: Minimal Model for *CeCoIn*$_5$

- Andrzej P. Kądzielawa[1,2], Dominik Legut[2], Maciej Fidrysiak[1], and Józef Spałek[1]

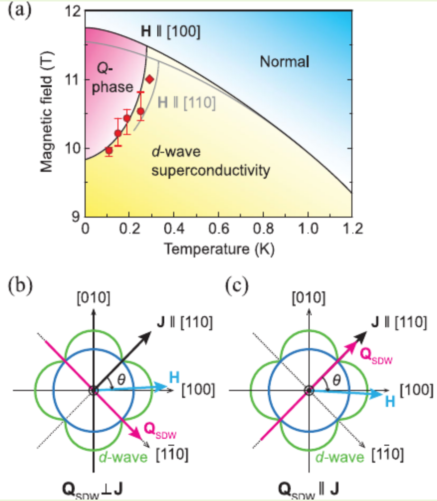
[1]Marian Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland
[2]IT4Innovations, Vysoká škola báňská - Technical University of Ostrava, Ostrava, Czech Republic
`andrzej.piotr.kadzielawa@vsb.cz`

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

Regensburg, April 3, 2019

Motivation

Superconductivity



D.-Y. Kim, *et al.*, Phys. Rev. X **6**, 041059 (2016).

Properties

- d-wave superconductivity ($\sim 2\ GPa$);
- Q-phase for "small" magnetic field;
- spin-split of effective mass for "large" magnetic field;

Spin-split masses

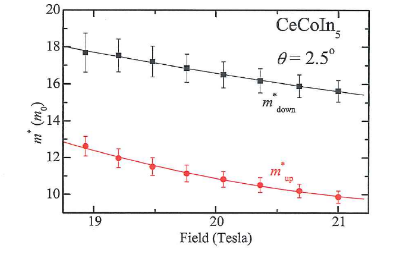


Figure 2.26: Effective masses of both spin components of the α_1-orbit in $CeCoIn_5$ as a function of field applied at 2.5° from [001] to [100] direction. Lines are guide for the eye.

Ilya Sheikin, *Quantum oscillations in f-electron compounds*, École Doctorale de Physique, Université Joseph Fourier, Grenoble (2011).

Main points

1. Introduction
   - Motivation
2. Methods
   - Band calculations
   - Mean-field
   - Hamiltonian
3. Results
   - Conclusions

Slater-Koster

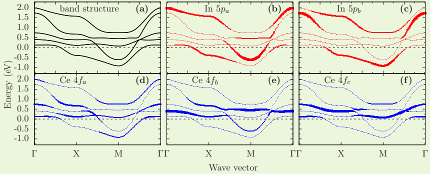
Characteristics of approach

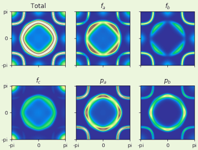
- treatment of localized electrons
- electronic correlations either omitted or included with double-counting
- complexity of the model
- band structure and density of states as output

5 orbital model

$$|p_{a\uparrow}\rangle = -|l = 1, s = \uparrow\rangle,$$
$$|p_{a\downarrow}\rangle = |l = -1, s = \downarrow\rangle,$$
$$|p_{b\uparrow}\rangle = -|l = -1, s = \uparrow\rangle,$$
$$|p_{b\downarrow}\rangle = |l = 1, s = \downarrow\rangle,$$
$$|f_{a\uparrow}\rangle = |j = 5/2, j^z = -5/2\rangle,$$
$$|f_{a\downarrow}\rangle = |j = 5/2, j^z = 5/2\rangle,$$
$$|f_{b\uparrow}\rangle = |j = 5/2, j^z = -1/2\rangle,$$
$$|f_{b\downarrow}\rangle = |j = 5/2, j^z = 1/2\rangle,$$
$$|f_{c\uparrow}\rangle = |j = 5/2, j^z = 3/2\rangle,$$
$$|f_{c\downarrow}\rangle = |j = 5/2, j^z = -3/2\rangle.$$

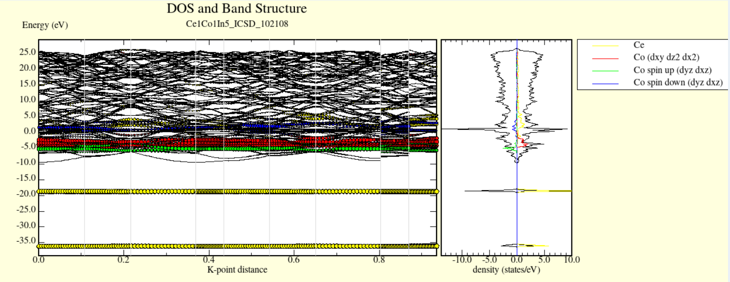
Slater-Koster Methods



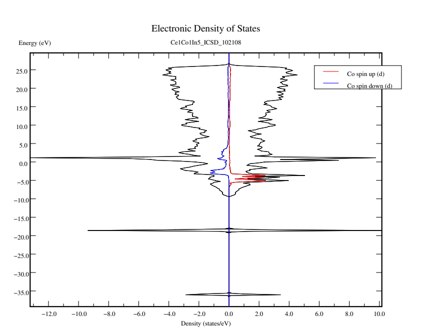


TOP: Slater-Koster band structure; density of 1.8 $\frac{el.}{f.u.}$; T = 0.01 $\frac{eV}{kB}$. **LEFT**: Fermi surface.

GGA + U: Band structure



Density of States



Remarks on physics for the toy model

- We used $U = 7\ eV$
- Two partially filled bands Co-$\downarrow$
- Two filled bands Co-$\uparrow$
- Four Ce bands $\sim -1.5\ eV$ below Fermi surface.
- Bandwidth of partially filled Co-$\downarrow$is $\sim 1\ eV$.
- We can use this data a the starting values to a many-paramter toy model.

Gutzwiller Approximation

Treatment of correlations

$$|\Psi\rangle \equiv \mathcal{C}^{\mathbf{G}} |\Psi_0\rangle ,$$

$$\mathcal{C}^{\mathbf{G}} = \prod_i \left(1 - (1-g)\, \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\right) |\Psi_0\rangle ,$$

general $\mathcal{C}^{\mathbf{G}} = \prod_i \sum_\Gamma \lambda_{i\Gamma} |\Gamma\rangle \langle\Gamma| ,$

where $|\Psi_0\rangle$ is uncorrelated state, g a variational parameter, $\hat{n}_i$ a particle number operator, $\{\Gamma\}$ set of local states, and $\lambda_{i\Gamma}$ variational parameters.

Basic scheme

We start with second quantization Hamiltonian $\mathcal{H}$

- $\hookrightarrow$ obtain effective Hamiltonian
- $\hookrightarrow$ diagonalize effective Hamiltonian
- $\hookrightarrow$ optimize variational parameters

Wide range of applications

- unconventional superconductivity
  Phys. Rev. B **95**, 024506 (2017);
  Phys. Rev. B **96**, 054511 (2017).
- heavy fermions - Kondo physics
  J. Phys.: Condesed Matter **24**, 205602 (2012).
- magnetism and quantum criticality
  Phys. Rev. B **90**, 081114(R) (2014);
  Phys. Rev. B **91**, 081108(R) (2015).
- coexistance of magnetism and sc superconductivity
  J. Phys.: Condensed Matter **29**, 36 (2017);
  Phys. Rev. B **97**; 224519 (2018);
  arXiv:**1902.08444** (2019).

? spin-split masses
  this work

Periodic Anderson Model

Working Hamiltonian 1+1 model

$$\hat{\mathcal{H}} = \sum_{\langle i,j\rangle\sigma} t\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \sum_{\langle\langle i,j\rangle\rangle\sigma} t'\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} - \sum_{i\sigma}\sigma h\hat{n}_{i\sigma}$$
$$+ \sum_{i\sigma}(\epsilon_f - \sigma h)\hat{n}^{f}_{i\sigma} + U\sum_{i}\hat{n}^{f}_{i\uparrow}\hat{n}^{f}_{i\downarrow} + \sum_{i\sigma} V(\hat{c}^{\dagger}_{i\sigma}\hat{f}_{i\sigma} + h.c.),$$

$\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}\hat{f}^{\dagger}_{i\sigma}\hat{f}_{i\sigma}$ - creators and annihilators of conducting and f electrons i.o.; $\epsilon_f < 0$. t, t' - hoppings; V - $c-f$ hybridization; U - onsite f-electron repulsion

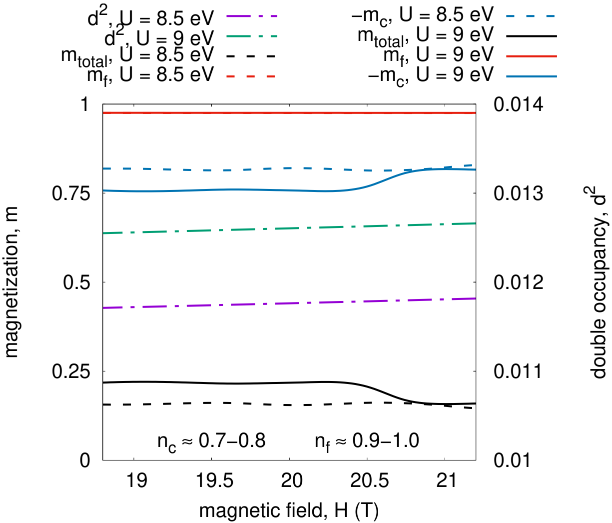
$$E_G \equiv \frac{\langle\Psi|\hat{\mathcal{H}}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi_0|\mathcal{C}^{\mathbf{G}}\hat{\mathcal{H}}\mathcal{C}^{\mathbf{G}}|\Psi_0\rangle}{\langle\Psi_0|\mathcal{C}^{\mathbf{G}}\mathcal{C}^{\mathbf{G}}|\Psi_0\rangle}$$

Effective Hamiltonian

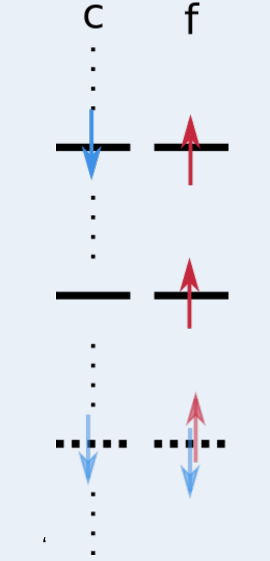
$$\hat{\mathcal{H}}_{\mathrm{eff}} \equiv \sum_{\mathbf{k}\sigma} \begin{pmatrix} \hat{c}^{\dagger}_{\mathbf{k}\sigma} & \hat{f}^{\dagger}_{\mathbf{k}\sigma} \end{pmatrix} \begin{pmatrix} \epsilon^{c}_{\mathbf{k}} - \sigma h - \mu & \sqrt{q_\sigma}V \\ \sqrt{q_\sigma}V & \epsilon_f - \sigma(h + \lambda^{f}_{m}) - \lambda^{f}_{n} - \mu \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\sigma} \\ \hat{f}_{\mathbf{k}\sigma} \end{pmatrix}$$
$$+ \Lambda(Ud^2 + \lambda^{f}_{n}n_f + \lambda^{f}_{m}m_f),$$

$\sqrt{q_\sigma} \equiv \frac{\sqrt{2d^2}\sqrt{n+\sigma m-2d^2}+\sqrt{2-2n+2d^2}\sqrt{n-\sigma m-2d^2}}{\sqrt{2-n-\sigma m}\sqrt{n+\sigma m}}$: band narrowing factors

Mean fields



Scheme



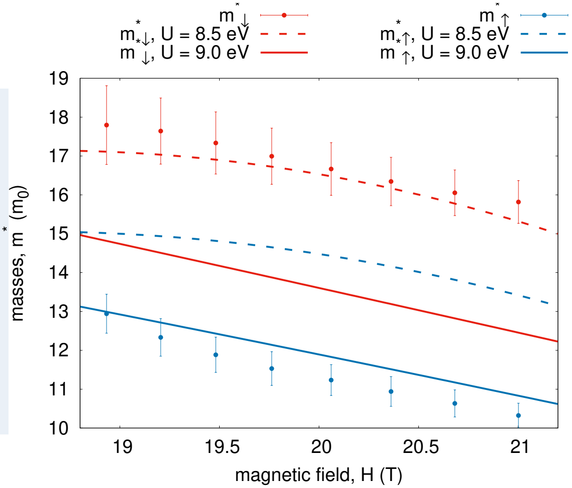
Spin-split masses

Definition of effective mass in model with correlator

$$m_\sigma^* \equiv \frac{\left\langle \Psi_0 \middle| \hat{c}_{i\sigma}^\dagger \hat{f}_{i\sigma} \middle| \Psi_0 \right\rangle}{\left\langle \Psi \middle| \hat{c}_{i\sigma}^\dagger \hat{f}_{i\sigma} \middle| \Psi \right\rangle}$$

$$\equiv \frac{\left\langle \Psi_0 \middle| \hat{c}_{i\sigma}^\dagger \hat{f}_{i\sigma} \middle| \Psi_0 \right\rangle}{\left\langle \Psi_0 \middle| \mathcal{C}^{\mathrm{G}} \hat{c}_{i\sigma}^\dagger \hat{f}_{i\sigma} \mathcal{C}^{\mathrm{G}} \middle| \Psi_0 \right\rangle}$$

$$\stackrel{\text{by def.}}{\equiv} \frac{1}{\sqrt{q_\sigma}}$$



Conclusion

1+1 orbital model provides us with qualitative behavior of spin-split masses in $CeCoIn_5$.

Conclusions

Physics of hydrogen planes

- on-site repulsion of f electrons, coupled with $c-f$ hybridization causes spin-split of effective masses
- Gutzwiller approximation gives proper qualitative behavior (smaller m^*'s with rising H), but not quantitatively.
- There is a need of calculations on larger model.
- Three different methods (DFT, S-K, and GA) provide us with consistent, complementary results.
- There is a need for computationally quick methods to treat specific physical phenomena.

Advertisement

Two immediately open post-doc positions till **end of 2021** in modeling of condensed matter physics from first-principles and beyond at **Czech National Supercomputing Center IT4Innovations**, Technical University of Ostrava, Czechia (€1600-2000).