Ferromagnetism and spin triplet superconductivity in UGe_2

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Introduction

- In 2000 Saxena *et al.* reported on a superconductivity inside the ferromagnetic phase of UGe_2
- Coexistence with ferromagnetism implies spin-triplet superconductivity, unlike in the BCS theory
- Until today only three ferromagnetic superconductors have been discovered: UGe_2, $UCoGe$, $URhGe$
- All of them are so called heavy-fermion compounds
- The key ingredient in understanding their physics are unfilled $5f$ levels of the uranium atoms
- I will discuss a possible effective microscopic model for magnetism and superconductivity in UGe_2

Crystal structure

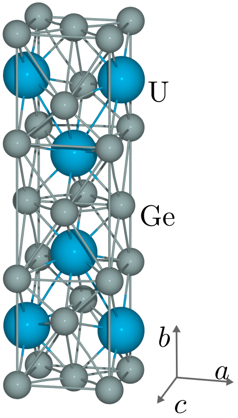

Figure: Primitive cell of UGe_2

- primitive cell size $(a, b, c) = (0.40, 1.51, 0.41)$Å
- orthorhombic centrosymmetric crystal system
- spontaneous magnetization along a axis
- $[U] = [Rn]\,5f^3\,3d^1\,7s^2$
- $[Ge] = [Ar]\,3d^{10}\,4s^2\,4p^2$

Phase diagram

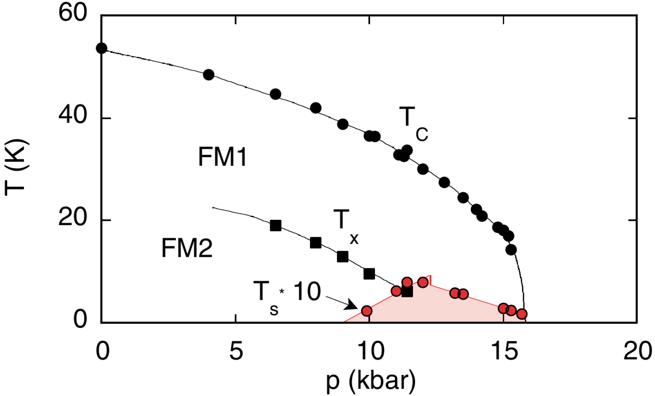

Figure: Pressure-temperature phase diagram (Pfleiderer 2002)

For $p = 1.2\,\mathrm{GPa}$: $T_{sc} = 0.8\,\mathrm{K}, T_C = 30\,\mathrm{K}$

Magnetization

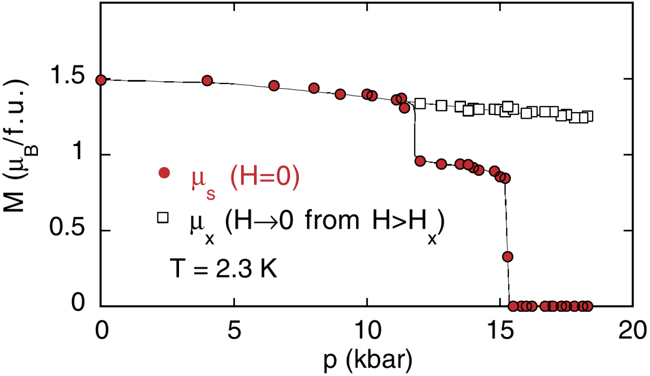

Figure: Magnetization vs. pressure (Pfleiderer 2002)

Band structure

- Band structure calculations can explain the ordered moment
- However they fail to properly describe the Fermi surface

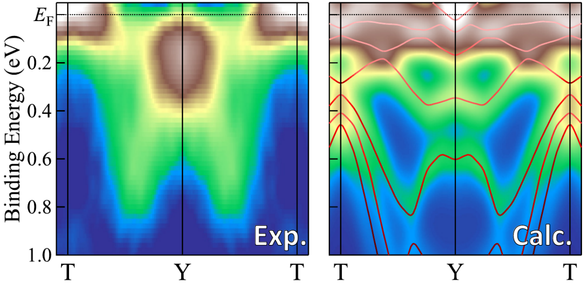

Figure: Angle-resolved photoemission spectroscopy results (Fujimori 2015)

- De Haas - van Alphen oscillation experiments indicate quasi 2-dimensional character

Anderson lattice model

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \epsilon_f \sum_{i\sigma} \hat{n}^f_{i\sigma} + U \sum_i \hat{n}^f_{i\uparrow} \hat{n}^f_{i\downarrow}$$
$$+ \sum_{i\sigma} \left(V c^\dagger_{i\sigma} f_{i\sigma} + V^* f^\dagger_{i\sigma} c_{i\sigma} \right)$$

- Effective model describing hybridization of initially localized f-electrons with mobile conduction electrons
- Strong Coulomb interaction between f electrons "pins" magnetic moments to f-levels
- Popular model for heavy-fermion compounds explaining the origin of large effective masses due to peaks in the density of states

Gutzwiller approximation

- Ansatz wavefunction

$$|\Psi_G\rangle = \prod_i \hat{P}_i |\Psi_0\rangle$$

$$\hat{P}_i = 1 - (1-g)\hat{n}^f_{i\uparrow}\hat{n}^f_{i\downarrow}$$

- Approximate evaluation of observables (exact for $D = \infty$)

$$\langle \Psi_G | \mathcal{O}_i | \Psi_G \rangle \approx \langle \Psi_0 | \hat{P}_i \mathcal{O}_i \hat{P}_i | \Psi_0 \rangle$$

- One can express g as a function of $d^2 = \langle \hat{n}^f_{i\uparrow}\hat{n}^f_{i\downarrow}\rangle$

Statistically-consistent Gutzwiller approximation

- Assume particular $n_f = \langle \hat{n}^f_{i\uparrow} + \hat{n}^f_{i\downarrow} \rangle_0$ and $m_f = \langle \hat{n}^f_{i\uparrow} - \hat{n}^f_{i\downarrow} \rangle_0$ of the Fermi-sea state $|\Psi_0\rangle$
- Introduce Lagrange multipliers to assure $n_f = \langle \hat{n}_f \rangle$ and $m_f = \langle \hat{m}_f \rangle$
- Finding the optimal parameters is equivalent to solving the following free Hamiltonian and minimizing ground state energy with respect to set $\{d, n_f, m_f, \lambda^f_n, \lambda^f_m\}$

$$H_{SGA} = \sum_{\mathbf{k}\sigma} \begin{pmatrix} c^\dagger_{\mathbf{k}\sigma} & f^\dagger_{\mathbf{k}\sigma} \end{pmatrix} \begin{pmatrix} \epsilon^c_{\mathbf{k}} - \mu & \sqrt{q_\sigma} V \\ \sqrt{q_\sigma} V & \epsilon_f - \mu - \lambda^f_n - \sigma \lambda^f_m \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix} + N(Ud^2 + \lambda^f_n n^f + \lambda^f_m m^f)$$

Results

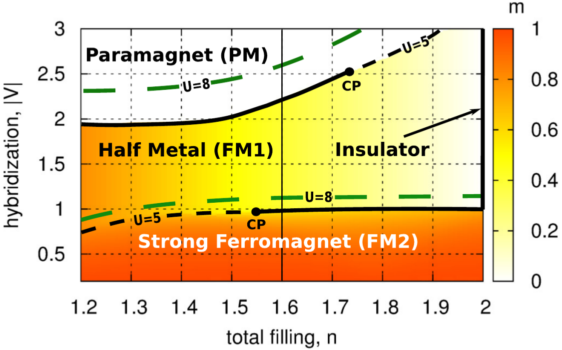

Figure: Magnetization on the filling-hybridization plane (Wysokiński 2014)

- Pressure affects parameters of the model in an unknown way
- It is assumed V is a monotonically increasing function of p

Magnetization and f-filling

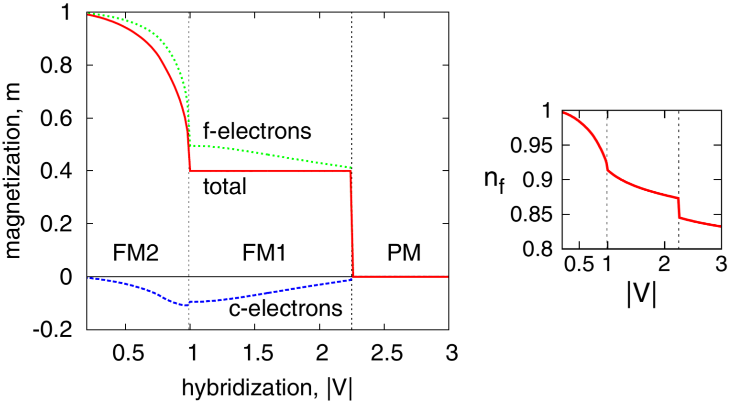

Figure: Magnetization and n_f as a function of hybridization (Wysokiński 2014)

Density of states at Fermi energy

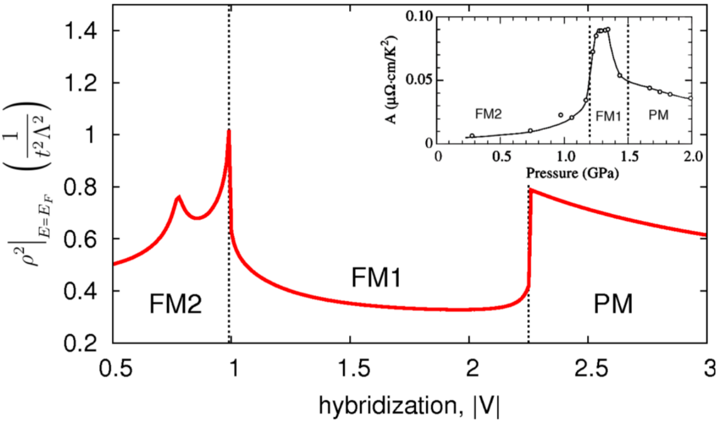

Figure: Square of DOS at E_F vs. V, inset: coefficient A of T^2 term of resistivity vs. pressure (Wysokiński 2014)

Gap function symmetry - general properties

- The gap function must be antisymmetric under the exchange of fermionic indices

$$\langle f_{\mathbf{k}\sigma} f_{-\mathbf{k}\sigma} \rangle \sim \Delta_{\sigma\sigma'}(\mathbf{k}) = -\Delta_{\sigma'\sigma}(-\mathbf{k})$$

- Spin-triplet state is symmetric in spin space so the spatial part needs to be antisymmetric
- However we introduce additional degenerate f-level so the gap function is parametrized by more indices, $l, l' \in \{1, 2\}$

$$\langle f_{\mathbf{k}l\sigma} f_{-\mathbf{k}l'\sigma} \rangle \sim \Delta^{ll'}_{\sigma\sigma'}(\mathbf{k}) = -\Delta^{l'l}_{\sigma'\sigma}(-\mathbf{k})$$

Gap function symmetry assumed in the model

- We consider spin-triplet, orbital-singlet s-wave pairing in the equal-spin channel:

$$\mathbf{\Delta}^{ll'}(\mathbf{k}) = \begin{pmatrix} \Delta_{\uparrow\uparrow}^{ll'} & 0 \\ 0 & \Delta_{\downarrow\downarrow}^{ll'} \end{pmatrix}$$

$$\mathbf{\Delta}^{ll'}(\mathbf{k}) = -\mathbf{\Delta}^{l'l}(\mathbf{k})$$

- This type of spin-triplet pairing is favoured by Hund's rule coupling between the two f-levels (Spałek 2001)

Degenerate Anderson lattice model

- When additional c and f-levels are introduced the inter-orbital Coulomb interactions are included in the Hamiltonian

$$
\begin{aligned}
H = & \sum_{ijl\sigma} t_{ij} c^{\dagger}_{il\sigma} c_{jl\sigma} + \epsilon_f \sum_{il\sigma} \hat{n}^f_{il\sigma} + U \sum_{il} \hat{n}^f_{il\uparrow} \hat{n}^f_{il\downarrow} \\
& + \sum_{il\sigma} \left(V c^{\dagger}_{il\sigma} f_{il\sigma} + V^* f^{\dagger}_{il\sigma} c_{il\sigma} \right) \\
& + \frac{1}{2} U' {\sum_{ill'}}' \hat{n}^f_{il} \hat{n}^f_{il'} - J {\sum_{ill'}}' \left(\mathbf{S}^f_{il} \mathbf{S}^f_{il'} + \frac{1}{4} \hat{n}^f_{il} \hat{n}^f_{il'} \right)
\end{aligned}
$$

Pairing operators

- The inter-orbital part of the Hamiltonian equals

$$\frac{1}{2}(U' + J) \sum_{ill'}' B^\dagger_{ill'} B_{ill'} + \frac{1}{2}(U' - J) \sum_{ill'}' \mathbf{A}^\dagger_{ill'} \mathbf{A}_{ill'}$$

$$B_{ill'} \equiv \frac{1}{\sqrt{2}} \left(f_{il\uparrow} f_{il'\downarrow} - f_{il\downarrow} f_{il'\uparrow} \right)$$

$$\mathbf{A}_{ill'} \equiv \left(f_{il\uparrow} f_{il'\uparrow}, \frac{1}{\sqrt{2}} \left(f_{il\uparrow} f_{il'\downarrow} + f_{il\downarrow} f_{il'\uparrow} \right), f_{il\downarrow} f_{il'\downarrow} \right)$$

- Thus if $U' < J$ spin-triplet condensation will lower the energy
- We assume $U' = U - 2J$

Mean-field approximation

- We analyze the coexisting ferromagnetism and superconductivity by mean-field decoupling

$$\mathcal{O}_\alpha \mathcal{O}_\beta \to \langle \mathcal{O}_\alpha \rangle \mathcal{O}_\beta + \mathcal{O}_\alpha \langle \mathcal{O}_\beta \rangle - \langle \mathcal{O}_\alpha \rangle \langle \mathcal{O}_\beta \rangle$$

- We look for self-consistent solutions for the following parameters

$$\begin{aligned} n_f &= \langle \hat{n}_1^f \rangle = \langle \hat{n}_2^f \rangle \\ m_f &= \langle \hat{m}_1^f \rangle = \langle \hat{m}_2^f \rangle \\ \Delta_\uparrow &= (U' - J) \langle f_{\mathbf{k}1\uparrow} f_{-\mathbf{k}2\uparrow} \rangle \\ \Delta_\downarrow &= (U' - J) \langle f_{\mathbf{k}1\downarrow} f_{-\mathbf{k}2\downarrow} \rangle \end{aligned}$$

Phase diagram

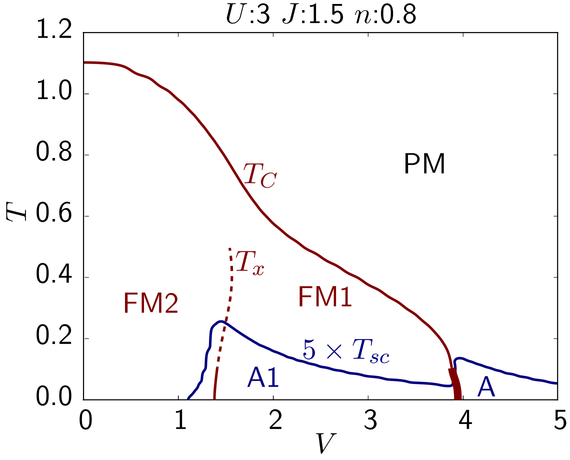

Figure: Phase diagram in MF approximation

A1:
$\Delta_\uparrow = 0, \Delta_\downarrow \neq 0$
A:
$\Delta_\uparrow = \Delta_\downarrow \neq 0$

Magnetization and superconducting gap

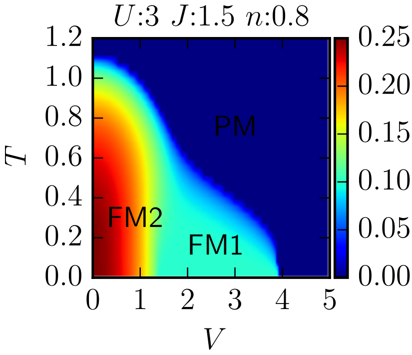

Figure: Magnetization m

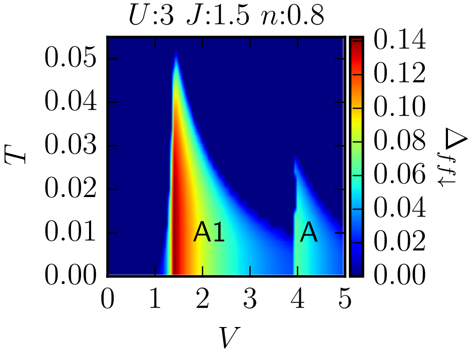

Figure: Superconducting gap $\Delta_\downarrow$

$$m = \frac{1}{2}(m_f + m_c)$$

Magnetization, filling

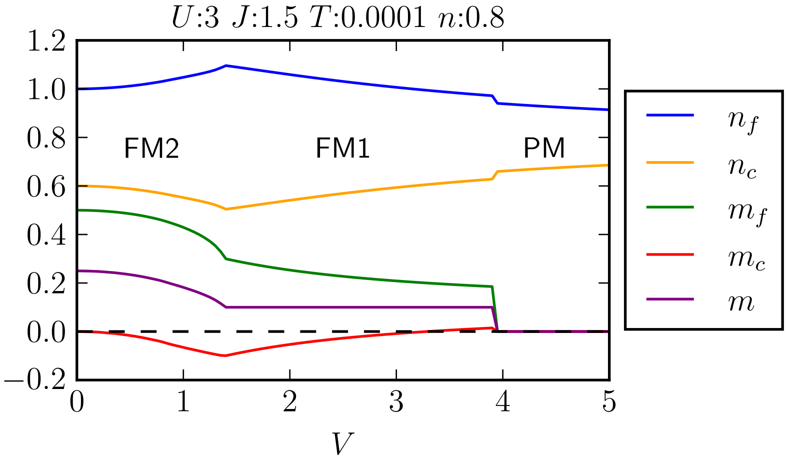

Figure: Magnetization and filling of c and f-levels

Superconductivity

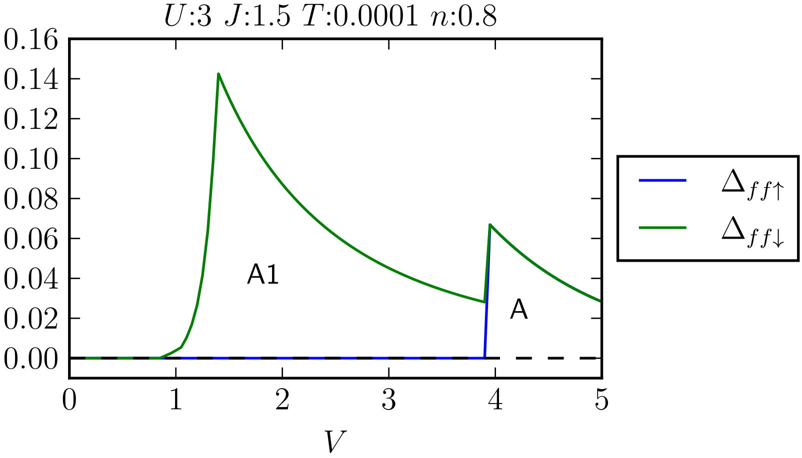

Figure: Superconducting gaps

DOS evolution at the FM2-FM1 transition

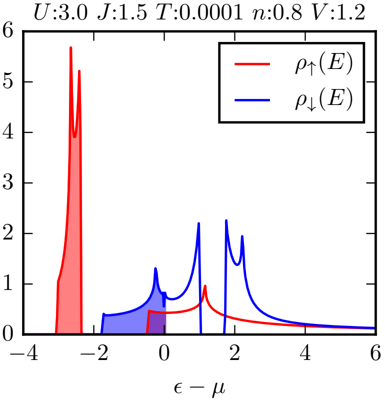

Figure: DOS in FM2 phase

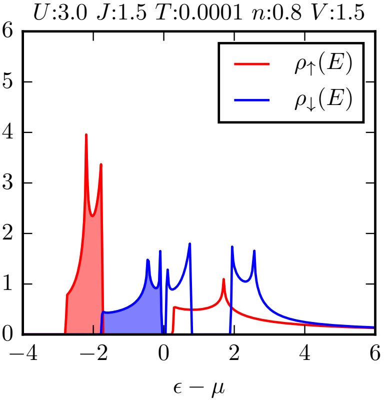

Figure: DOS in FM1 phase

DOS evolution at the FM1-PM transition

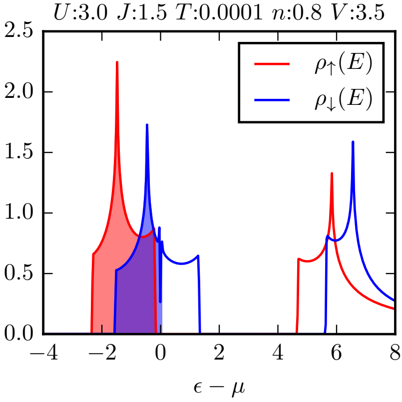

Figure: DOS in FM1 phase

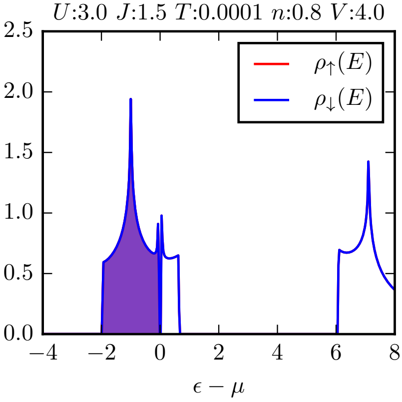

Figure: DOS in PM phase

Summary

- Anderson lattice model away from half-filling can account for the qualititative description of the phases of $\mathrm{UGe_2}$
- The degenerate version of the model predicts interorbital spin-triplet pairing due to Hund's rule at the mean-field level
- Whether such a simplified model is a good microscopic description of $\mathrm{UGe_2}$ remains an open question

Thank you for your attention!

References

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