Technische Universität Braunschweig

Kavli Institute for Theoretical Physics

Magnetism, Bad Metals and Superconductivity: Iron Pnictides and Beyond
September 11, 2014

Superconductivity in Heavy Fermion Systems: Present Understanding and Recent Surprises

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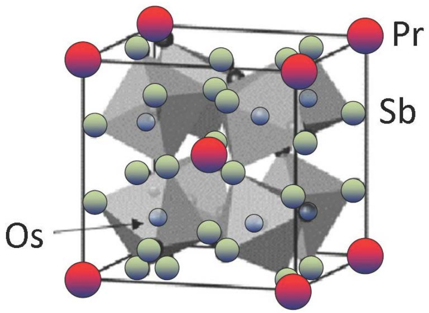
Outline

1. Heavy fermion superconductors
2. $Pr_{1-x}La_xOs_4Sb_{12}$
3. Dual character of 5f electrons: 3=2+1
4. Heavy fermions 4f systems: Kondo scenario
5. Renormalized Band method
6. Kondo lattices: Instabilities
7. $YbRh_2Si_2$
8. Summary and outlook

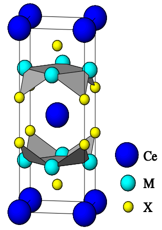
Heavy Fermion Superconductors: Material classes and typical examples

Pr skutterudites

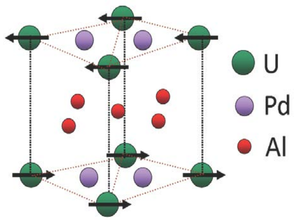


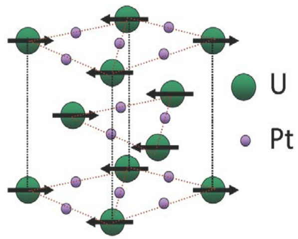
$PrOs_4Sb_{12}$

Actinide compounds

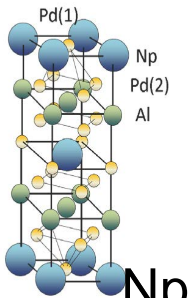


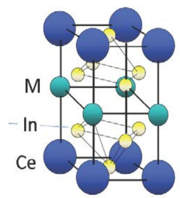
URu_2Si_2





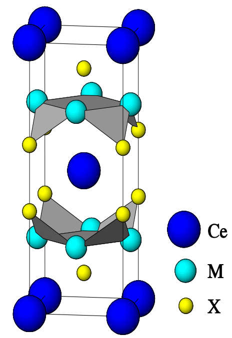
UPd_2Al_3 UPt_3



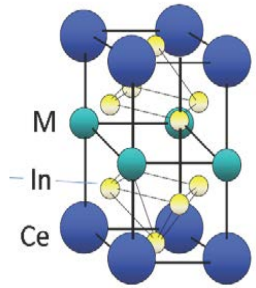


$NpPd_5Al_2$ $PuCoGa_5$

Ce compounds



$CeCu_2Si_2$



$CeCoIn_5$

Heavy fermion superconductors: General properties

- **Normal state**

  Usually not so bad metals

  Effective Fermi temperature 1-10 meV

  However, competing orders => quantum critical points

- **Superconductivity**

  Pairing hypothesis works

  BCS limit, coherence length ξ_0 >> lattice spacing

  Pair states unconventional: Symmetry lower than that of lattice

  Symmetry classification of pair states accounting for SO interaction

  Attractive interaction: Electronic origin

Heavy fermion superconductors

Formation of the Heavy Fermion state

Partially filled f shells

Strong local correlations => local degeneracies

Characteristic low-energy scale from lifting of local degeneracies

We have to distinguish several cases:

- 4f systems: Stable configurations $4f^n$

  Non-Kramers vs Kramers ions
- 5f systems: Intermediate-valent systems

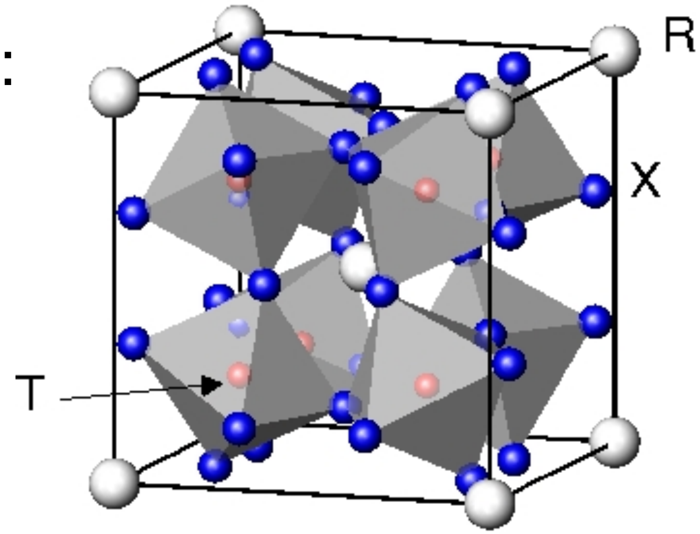
$Pr_{1-x}La_xOs_4Sb_{12}$

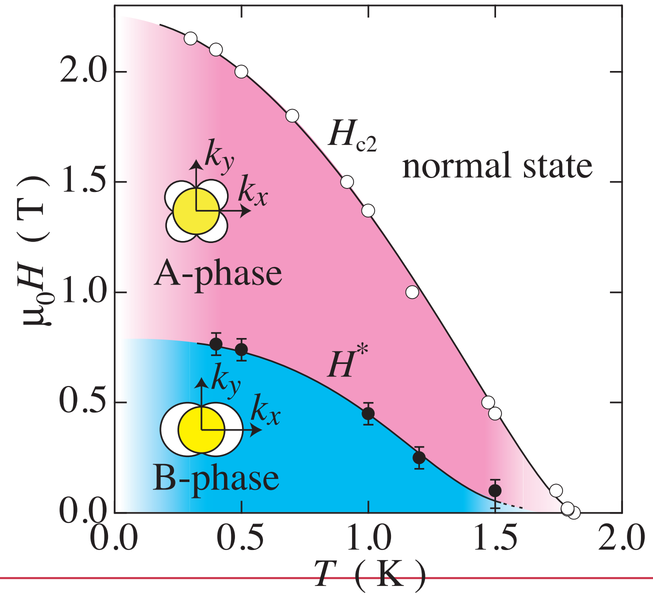
- Stochiometric compounds x=0 and x=1: Fermi liquids

- f-electrons weakly coupled to conduction states

- Mass enhancement due to 4f states
  $PrOs_4Sb_{12}$: γ ~350-500 mJ/mole K^2
  $LaOs_4Sb_{12}$: γ~36 mJ/mole K^2

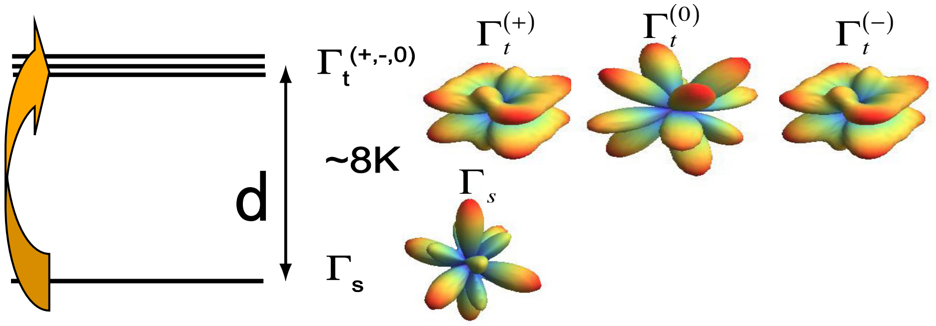
- No Kondo effect:
  Pr J=4 => non- Kramers ion;
  ground state non-degenerate



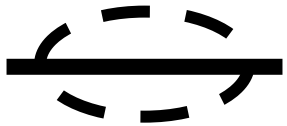


$Pr_{1-x}La_xOs_4Sb_{12}$: Field-dependent mass enhancement

CEF states: T_h symmetry; Singlet ground state and low-lying triplet; CEF transitions: aspherical Coulomb scattering



Mass renormalization:
Itinerant conduction electrons
Scattered off (broadened)
localized f^{2}-excitations



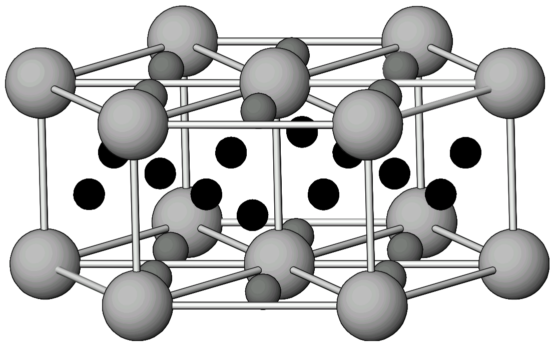
$$\frac{m^*}{m} \sim 1 + \frac{const}{\delta}$$

Question:

Superconductivity due to “intra-atomic“ excitations?
Strong-coupling Eliashberg theory => reasonable Tcs for parameters compatible with mass enhancement
Multi-component order parameter

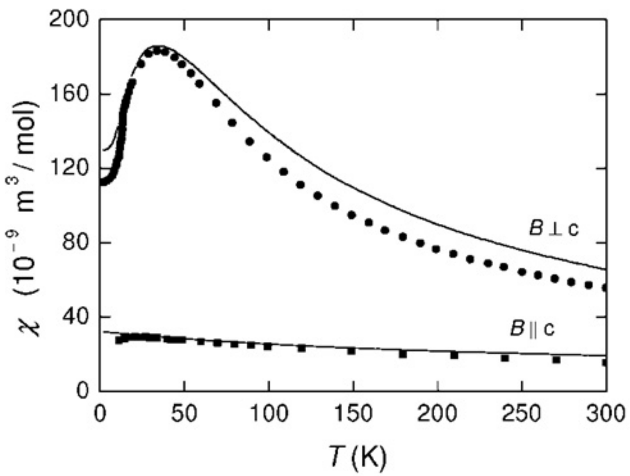
Dual character of 5f-electrons: UPd_2Al_3

Hexagonal structure
$PrNi_2Al_3$



5f moments:
T_N =14.3K; m=0.85 m_B

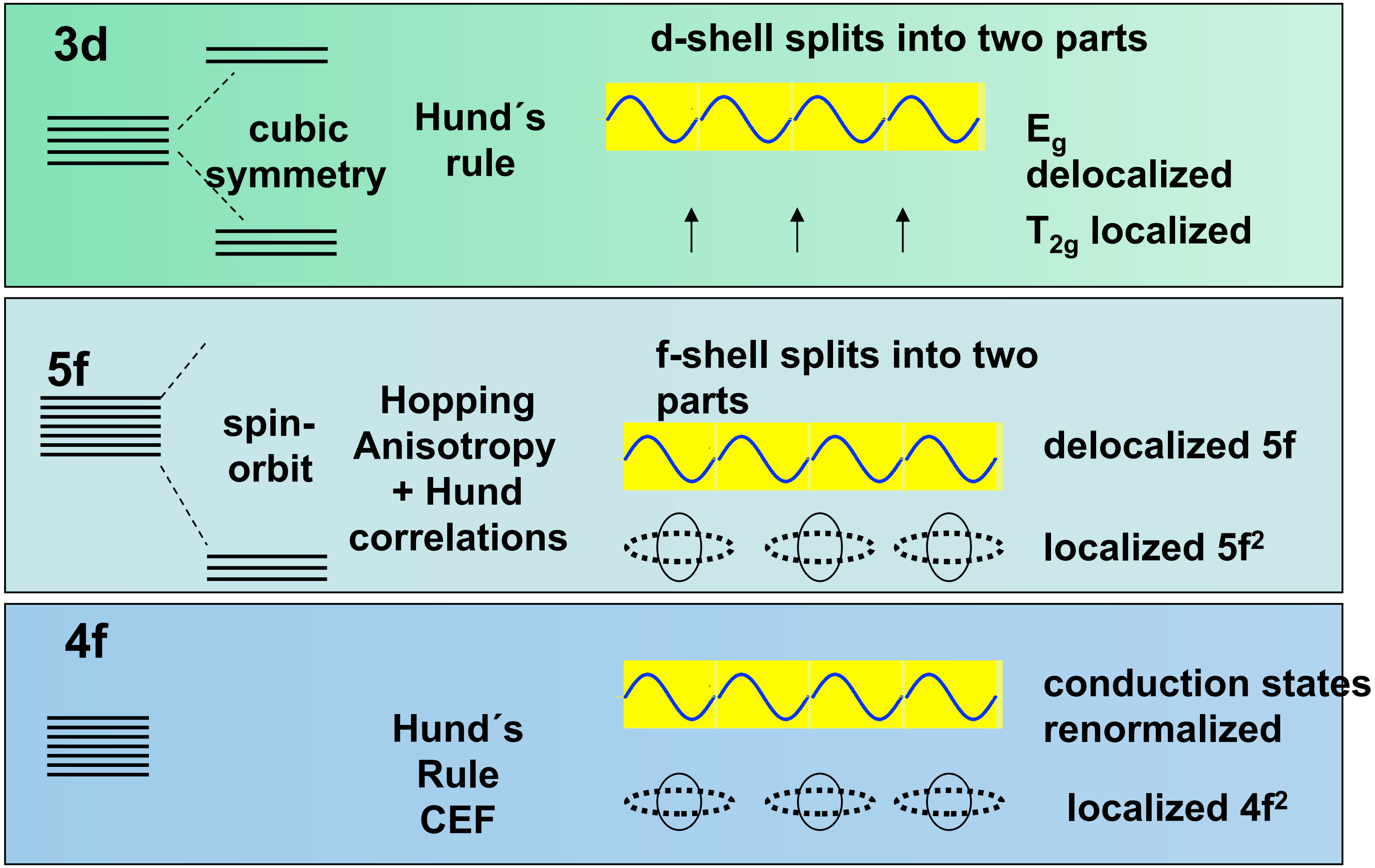
5f bands
γ =140 mJ/mole K^2
T_c=1.8K; $\Delta C=1.2\gamma\, T_c$



Anisotropic static magnetic susceptibility
(Grauel et al., 1992)

Analysis:
CEF-states of f^2-configuration
(Shiina, 2001)

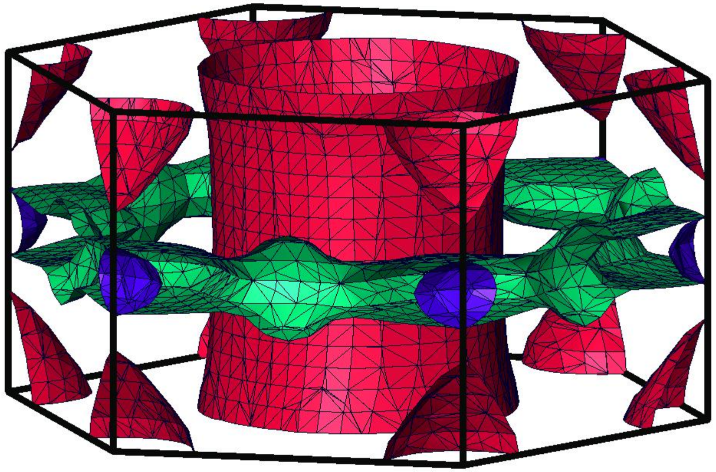
Dual character of 5f-electrons

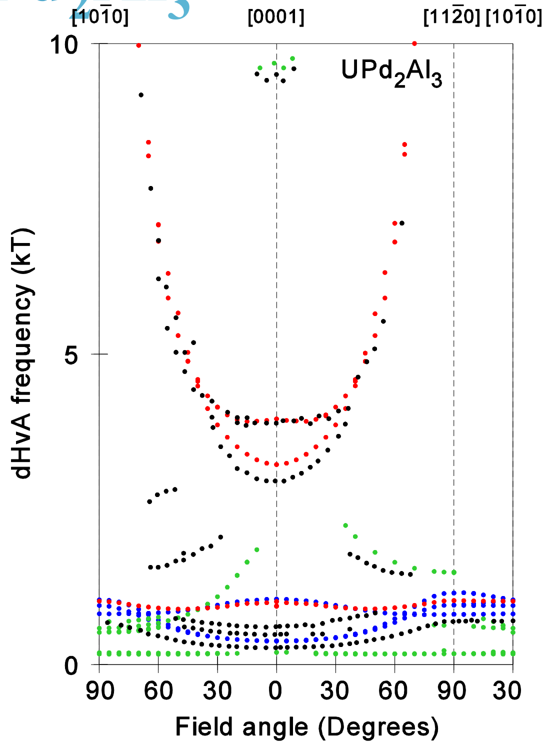


Dual character of 5f electrons: UPd_2Al_3

Co-existence of delocalized and localized 5f electrons

UPd_2Al_3: Fermi surface and effective masses reproduced by dual model



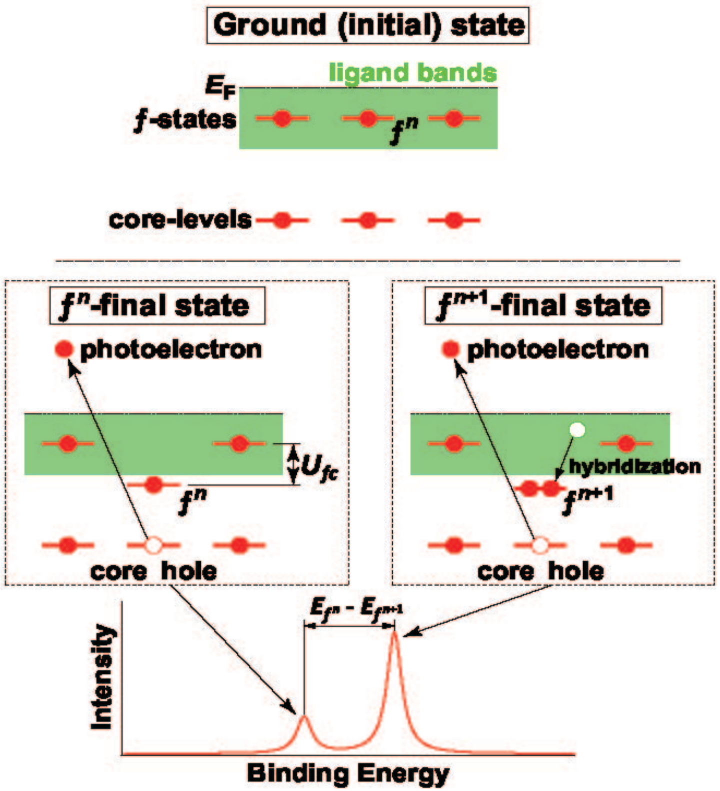


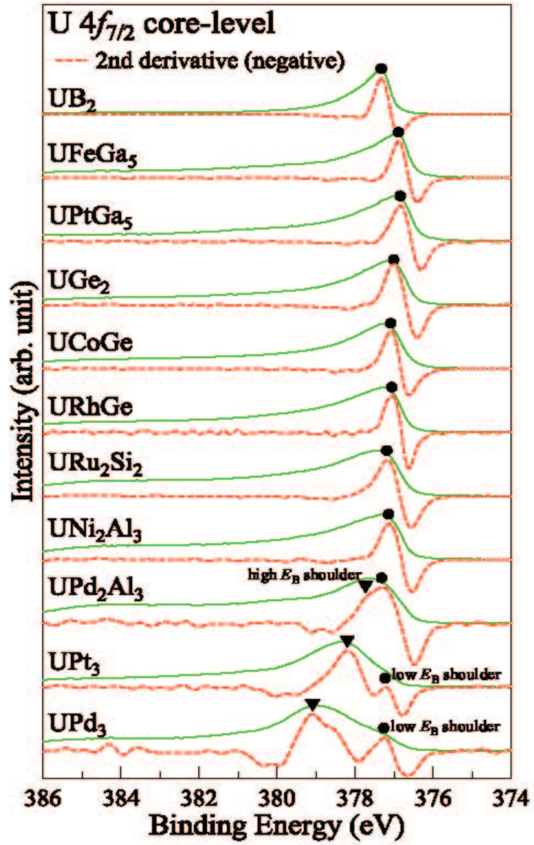
Branch	Exp	Theory
γ	33	31.9
β	19	25.1
ε_2	18	17.4
ε_3	12	13.4
α	5.7	9.6
ζ	65	59.6

Exp: Inada et al (1999)
Th : GZ et al (2003)

Dual character of 5f electrons: Core-Level PES Experiment

Localization vs delocalization reflected in screening properties





From S.-i. Fujimori et al, JPSJ (2011)

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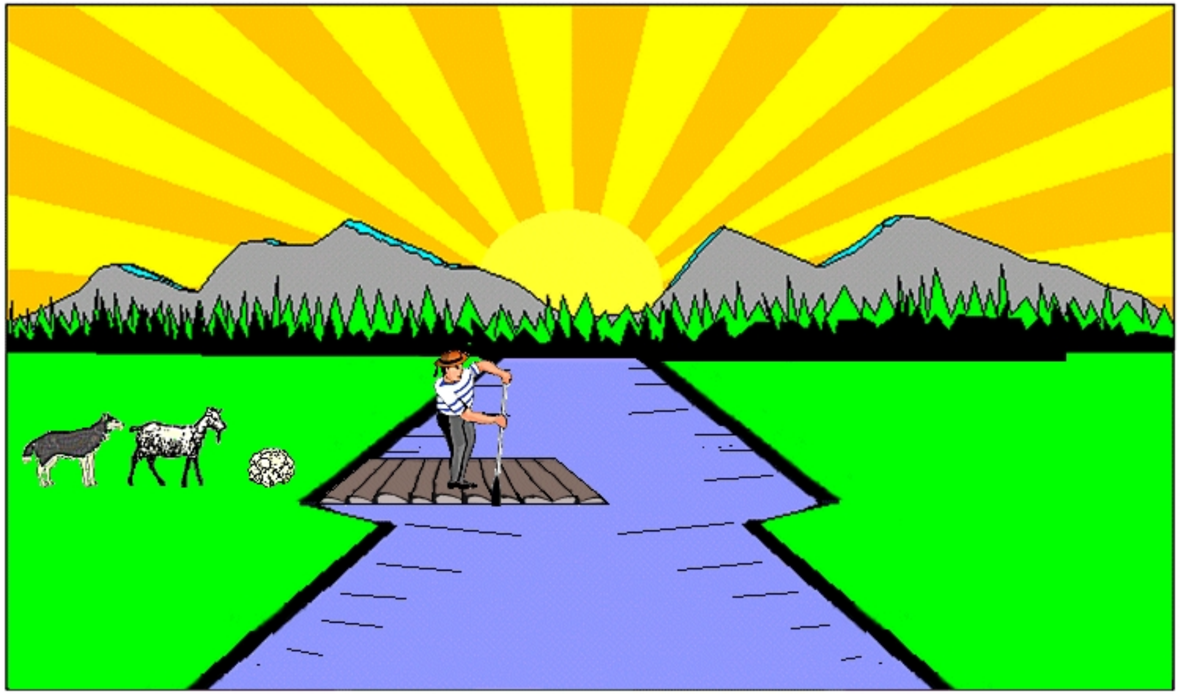
Dual character of 5f electrons – a correlation effect



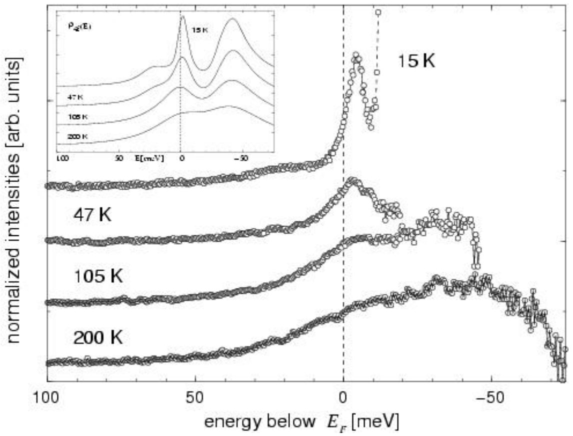
Orbital-selective Mott transition due to competition between anisotropic hybridization and Hund's rule correlations

Dual character of 5f electrons

Unusual properties of actinide-based SC

- Co-existence of SC and ferromagnetism
- Hidden order in URu_2Si_2
- High T_cs in Pu-compounds
- …

Heavy Fermions in 4f-systems: Kondo scenario

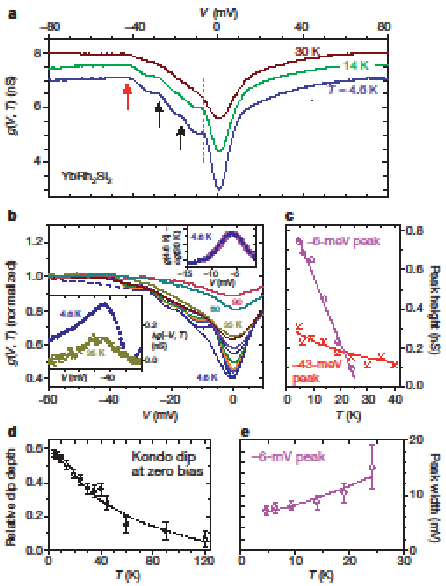


PES

Kondo resonance in $CeCu_2Si_2$

(Reinert et al (2001)

Detailled studies in Yb-systems



STM

Formation of the local Kondo singlet

Coherence effects from the periodic lattice

LETTER

doi:10.1038/natu

Emerging local Kondo screening and spatial coherence in the heavy-fermion metal $YbRh_2Si_2$

S. Ernst[1], S. Kirchner[1,2], C. Krellner[1], C. Geibel[1], G. Zwicknagl[3], F. Steglich[1] & S. Wirth[1]

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Heavy fermions in 4f-systems

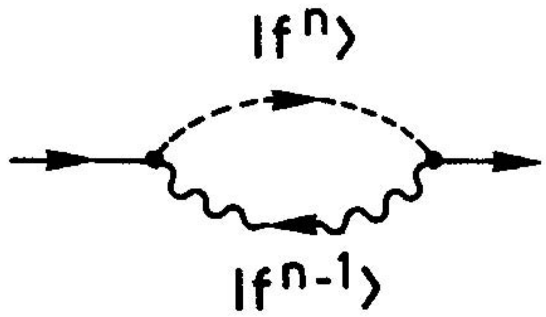
Construction of realistic models:

Electrons scatter off (effective non-local) potentials at atomic sites

Material-specific information: single-site t-matrix

Kondo lattice:
Use many-body single-site t-matrix for 4f-channels

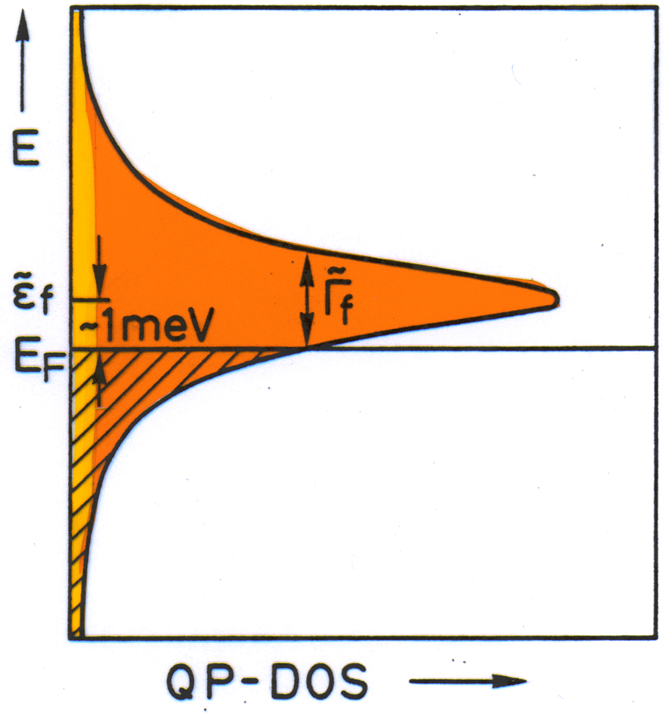
4f spectral function
Resonant structure at low temperatures
parametrization



Non-4f states: t-matrix from standard band structure (DFT)

Renormalized Band method

Quasiparticle bands



Phase shift: $\tilde{\eta}_f = \arctan \dfrac{\tilde{\Gamma}_f}{\tilde{\varepsilon}_f - E}$

Condition: No re-distribution of charge $\Rightarrow \tilde{\varepsilon}_f$

Single parameter $\tilde{\Gamma}_f$ adjusted to specific heat

Magnetic field: H-dependent parameters

$$\tilde{\varepsilon}_f(H)\ ,\ \tilde{\Gamma}_f(H)$$

Renormalized Band method

Calculational scheme:

Selfconsistent LDA band structure calculation starting from atomic potentials and lattice structure

↓

Selfconsistent potentials

↓

Dispersion of conduction states

Heavy Masses

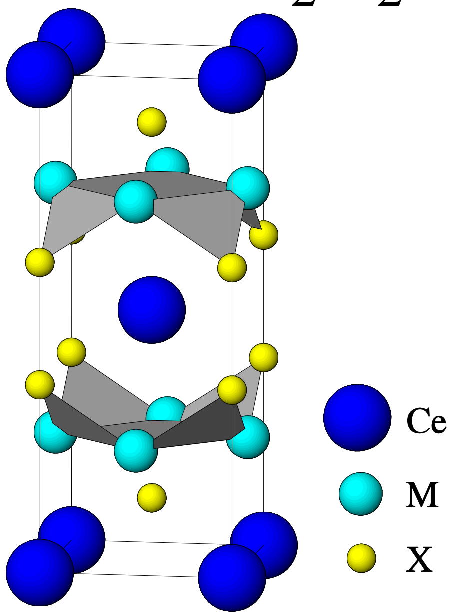
↓

Renormalized Bands

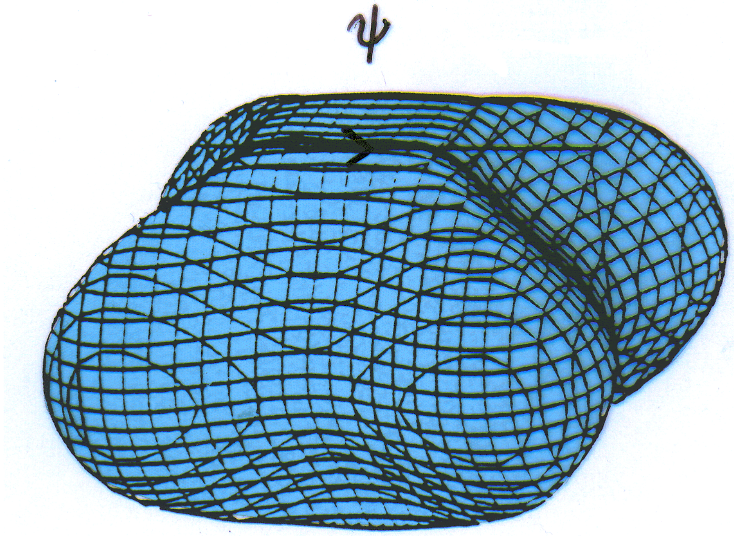
Renormalized Band method

Confirmation of the quasiparticle model

$CeRu_2Si_2$ $\gamma \sim 350 mJ/(mole\, K^2)$



Fermi surface for Heavy Fermions in (GZ, E. Runge, N. E. Christensen, Physica B 163, 97 (1990))



Experimentally confirmed
Aoki et al., PRL 72,797 (1992)

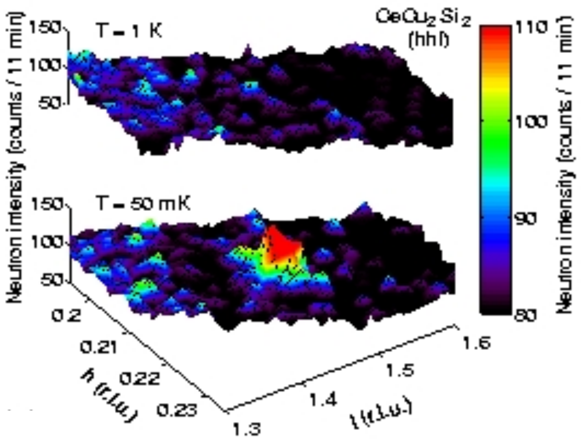
Effective mass consistent with specific heat

Kondo lattices: Instabilities of the heavy Fermi liquid

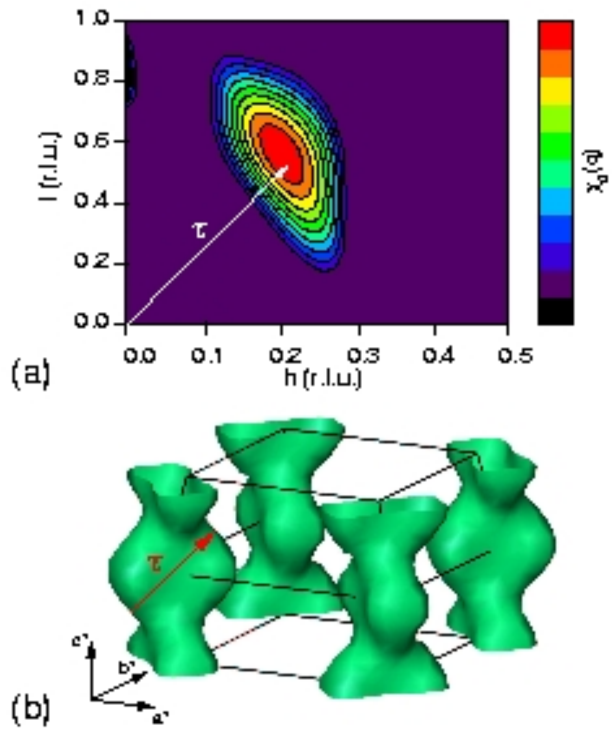
Spin density wave of heavy fermions in $CeCu_2Si_2$

(E. Faulhaber et al PRL **92**, 136401(2004))

Inelastic neutron scattering



Calculated susceptibility of the heavy quasiparticles

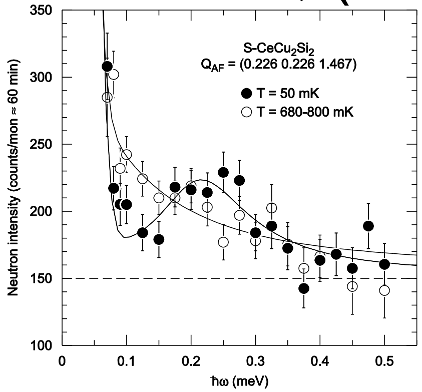


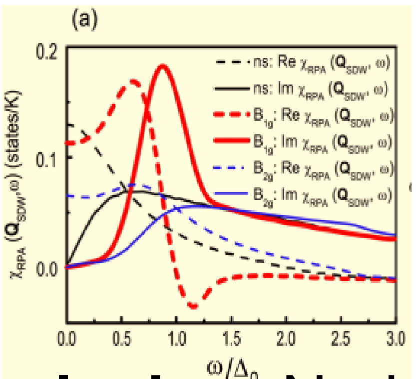
Kondo lattices: Instabilities of the heavy Fermi liquid

Resonance peak in superconducting $CeCu_2Si_2$

O. Stockert et al (2008)

I. Eremin et al, (2008)

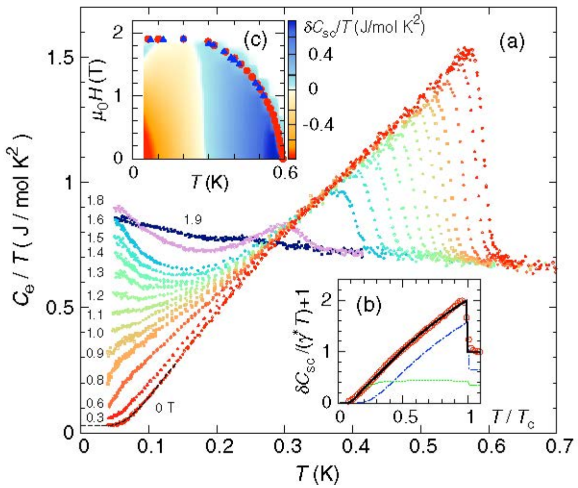




Surprise and open question:

Exponential specific heat at low T

Shunichiro Kittaka et al., 2013



Conclusion: Nodal superconducting order parameter $\Delta(\boldsymbol{k})$: $\cos k_x - \cos k_y$

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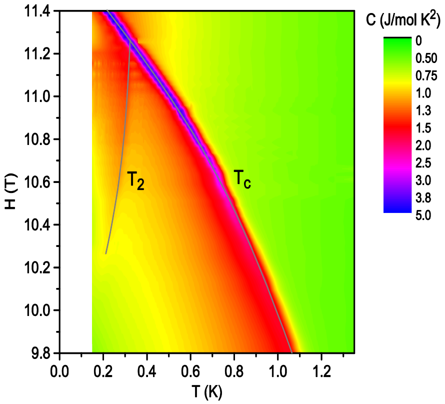
Kondo lattices: Instabilities of the heavy Fermi liquid

Inhomogeneous superconducting state in $CeCoIn_5$

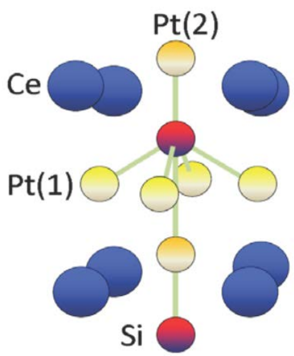


A. Bianchi et al. (2003)

Modulation vector $q \sim a \gg \xi_0$ weak B dependence => not FFLO

Complicated interplay with af order

Unusual properties in non-centrosymmetric SC: $CePt_3Si$



Strong SO interaction

Order parameter superposition of singlet and triplet

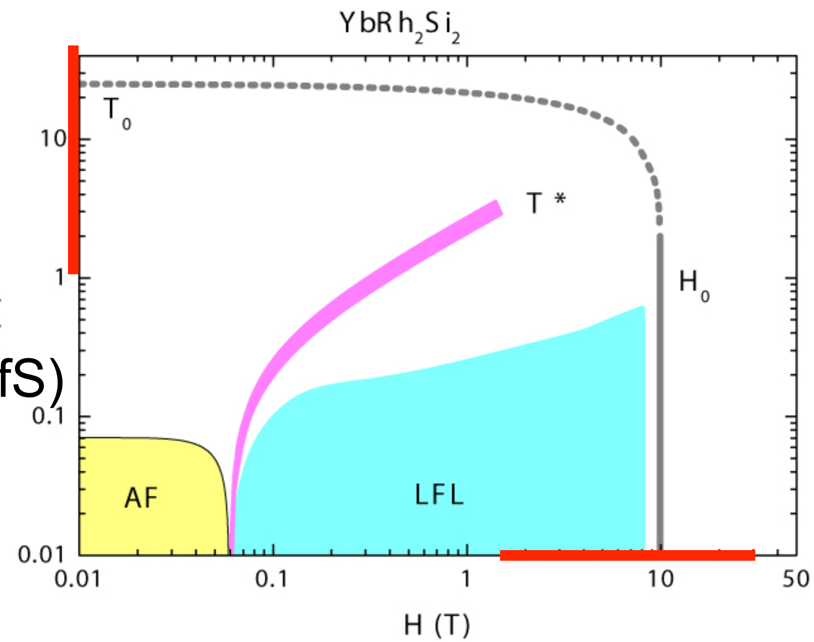
$YbRh_2Si_2$: Nature of the Quantum Critical Point?

Material-specific treatment of
highly correlated metals
Periodic lattice

Experimental properties

Identification of unusual phases
Characterization of reference states
Nature of quantum phase transitions
....

ARPES
(TUD)
RXES
(ESFR)
STM (CPfS)
:::



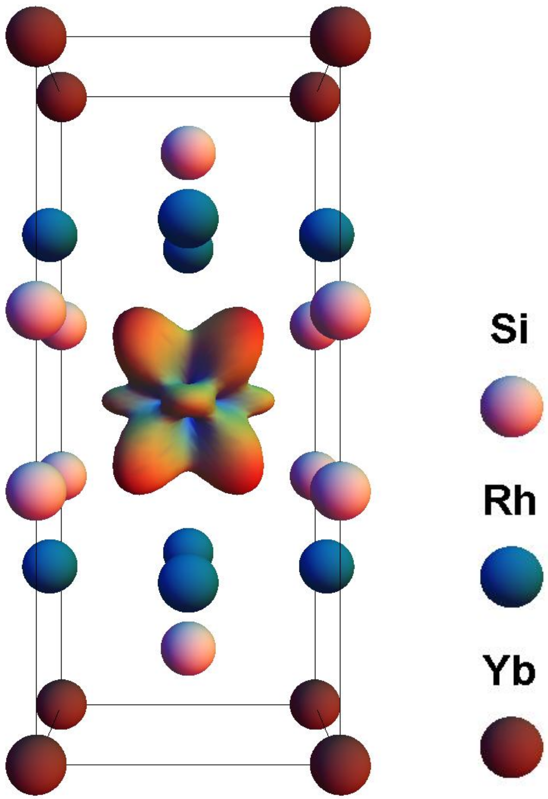
Transport
CPfS, Grenoble

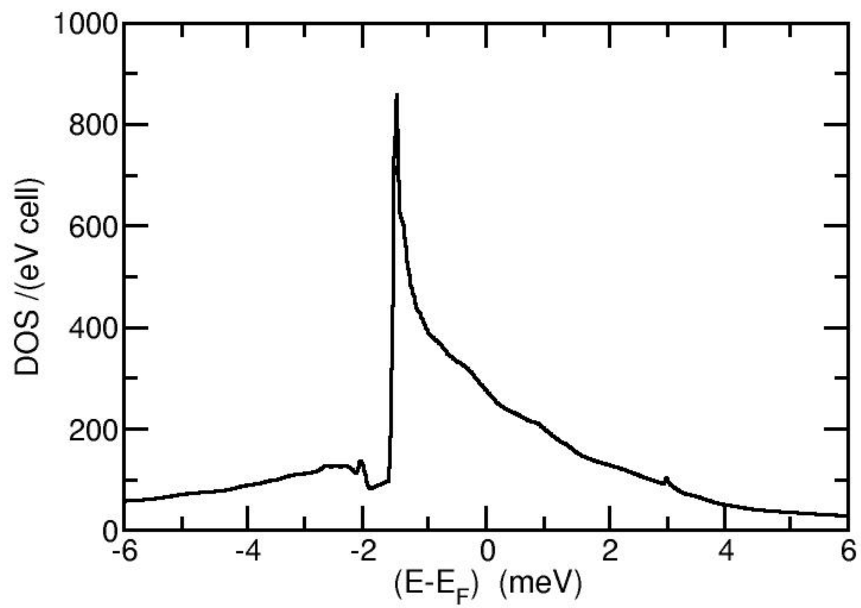
$YbRh_2Si_2$: Heavy quasiparticles in high magnetic fields

CEF ground state: Weak hybridization with conduction states

Anisotropic effective masses, flat dispersion in large parts of BZ

=> van Hove-type singularity in DOS



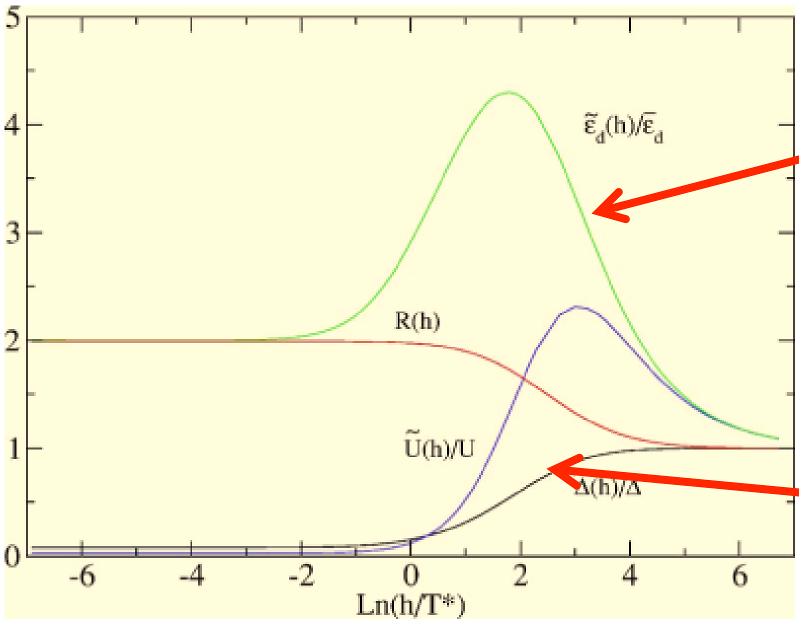


$YbRh_2Si_2$: Heavy quasiparticles in high magnetic fields

QP parameters:

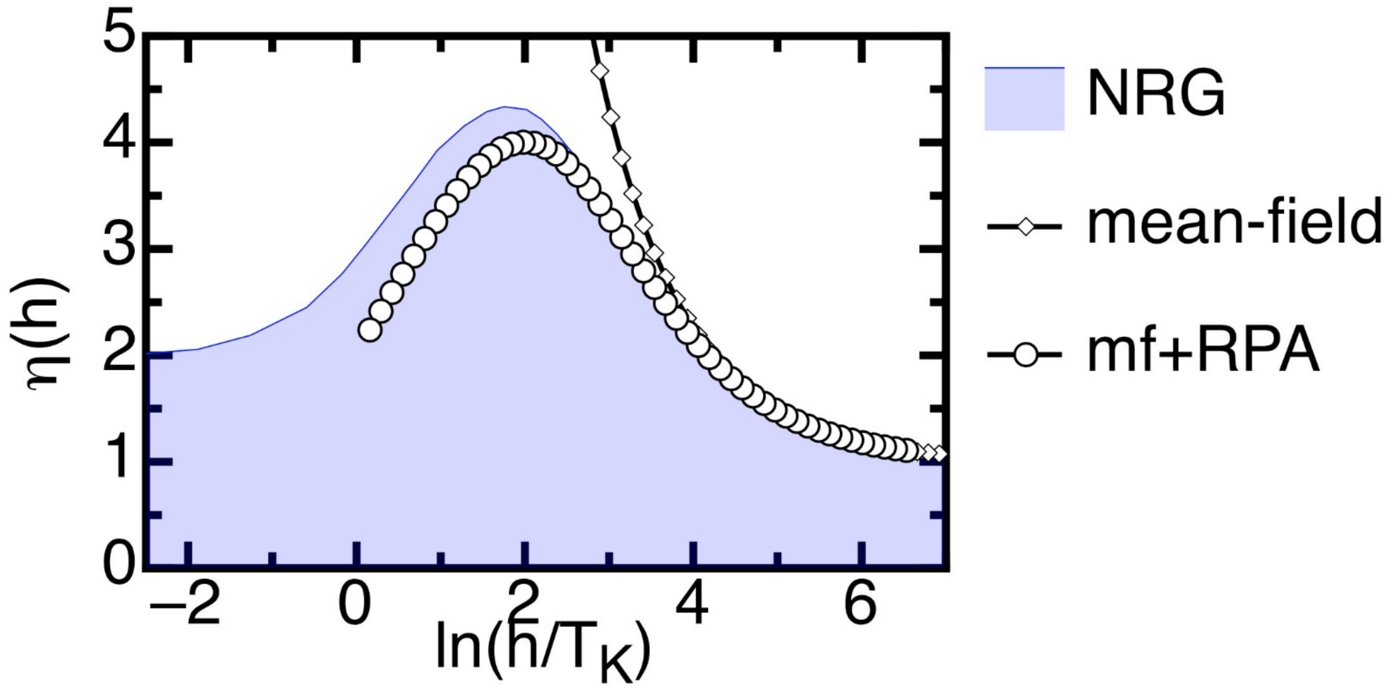
Fit to DOS from Numerical Renormalization Group: Highly non-trivial variation with H (Hewson, Bauer (2007), Peters et al (2006)), Anders)

Example: Particle-hole symmetric case



$YbRh_2Si_2$: Field-dependent qp parameters

Origin of non-monotonic variation with field of enhanced Zeeman splitting



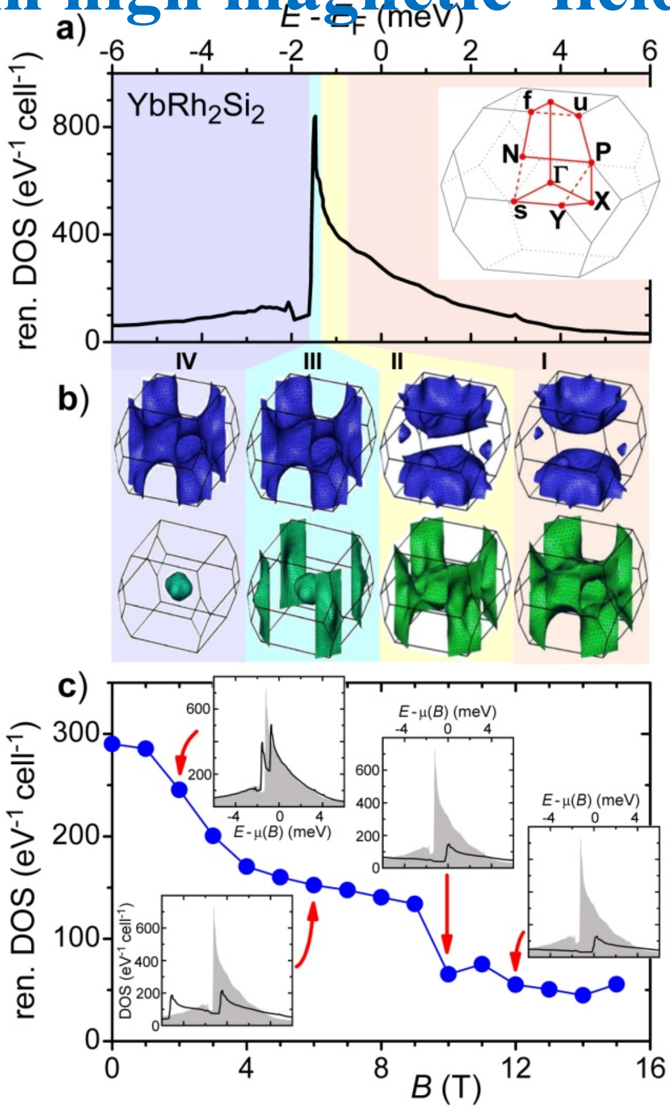
$YbRh_2Si_2$: Heavy quasiparticles in high magnetic fields

Minority Fermi surface undergoes a series of Lifshitz-transitions

Observed anomalies in thermodynamic and transport properties

Topology of high-field FS differs from H=0 result

GZ, J. Phys.: Condens. Matter (2011)



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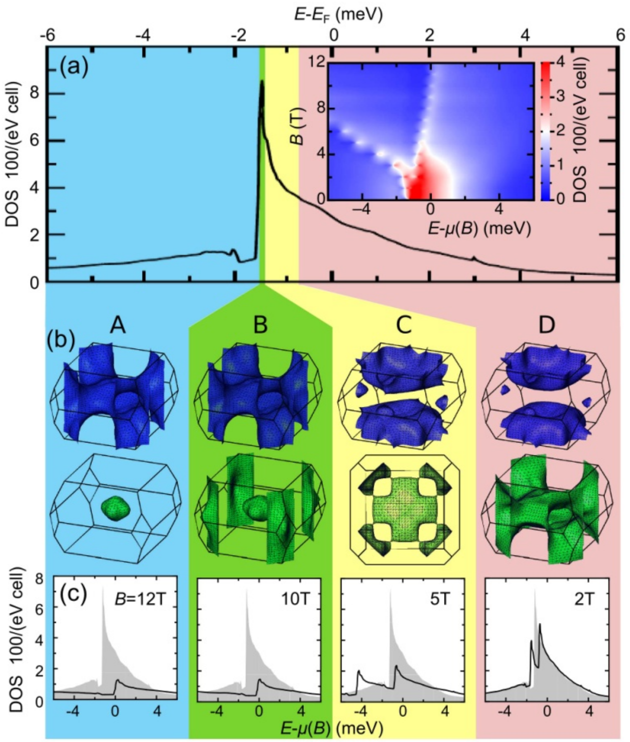
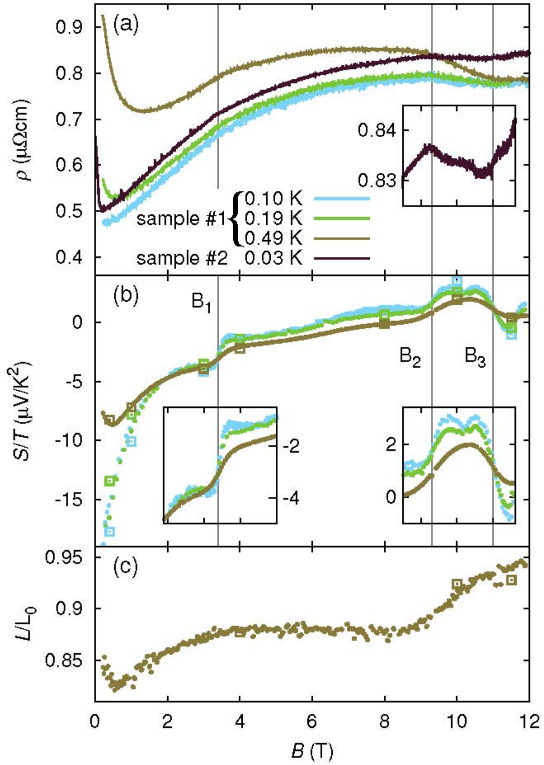
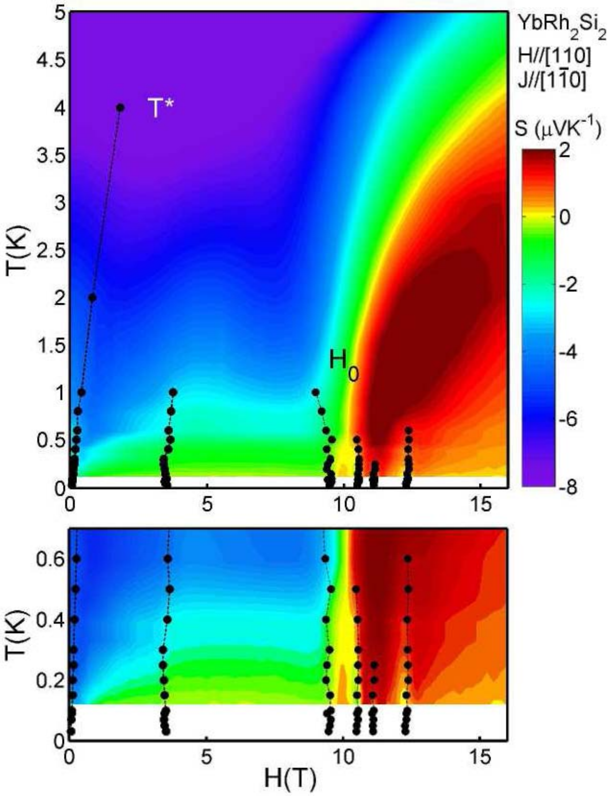
$YbRh_2Si_2$: Heavy quasiparticles in high magnetic fields







Four major +several small regimes around B=11 T (not displayed here)

H. Pfau et al PRL **110**, 256403 (2013)

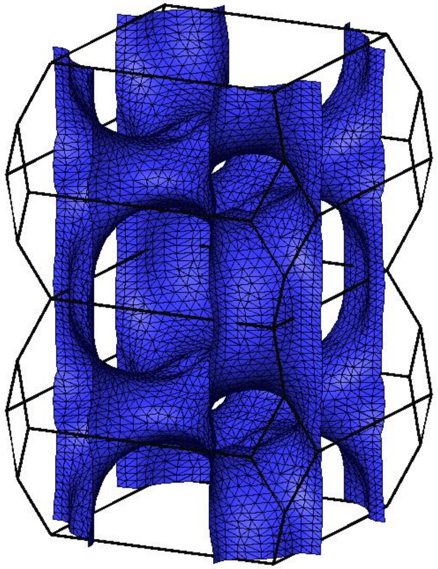
A. Pourret et al., JPSJ **82** (2013) 053704

Quasiparticle de-renormalization+Sommerfeld-Wilson ratio+ CEF states =>Structures at characteristic fields: Lifshitz transitions ,...

$YbRh_2Si_2$: Heavy quasiparticles in high magnetic fields

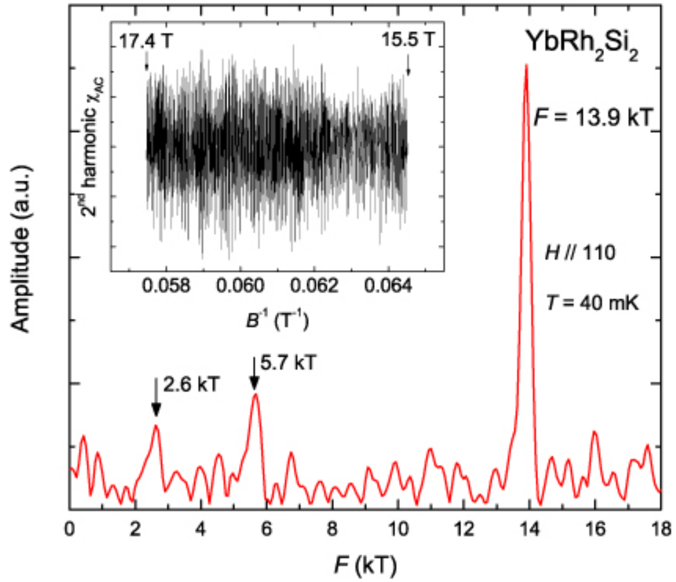
$YbRh_2Si_2$

Quantum oscillations show closed orbit in narrow angle range



B || 110

F~13 kT



T. Westerkamp (2008)

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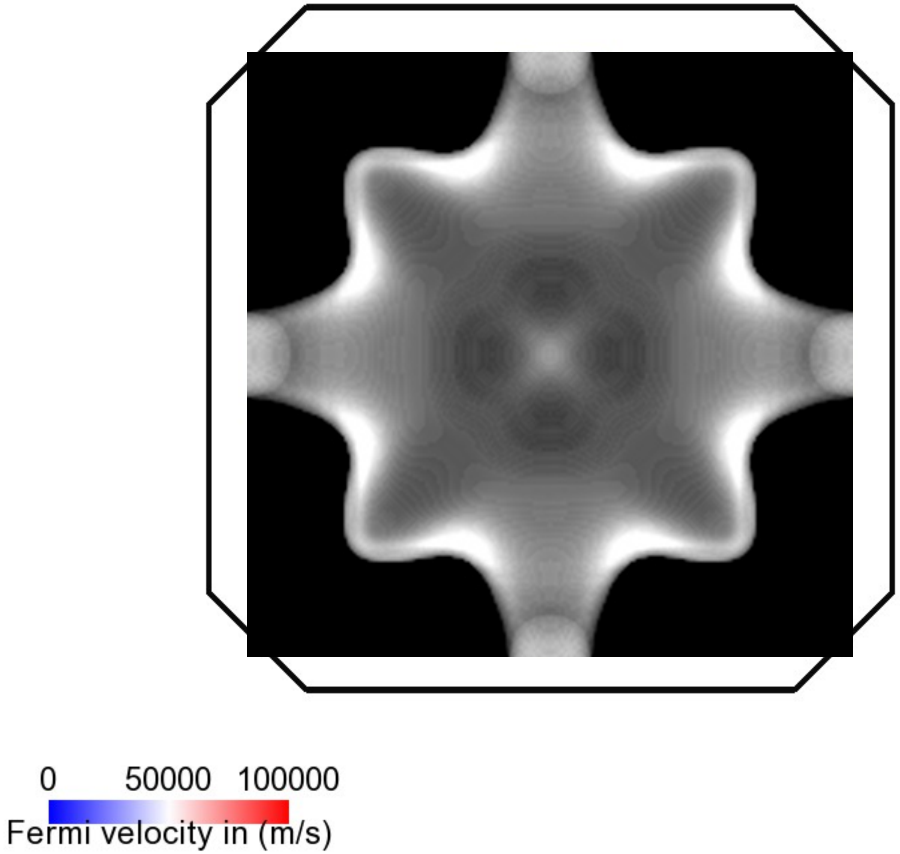
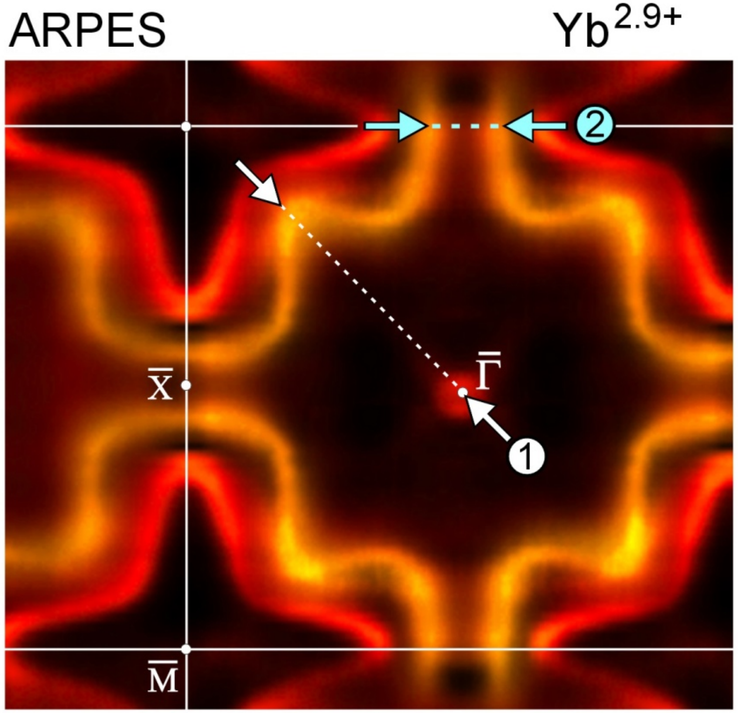
$YbRh_2Si_2$: Fermi surface

ARPES : B=0, paramagnetic





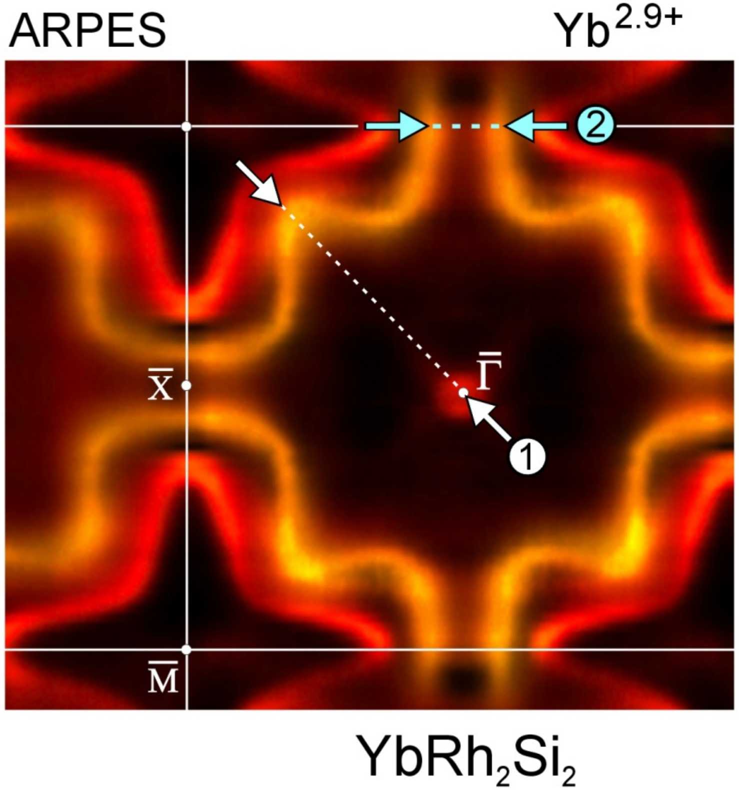
$YbRh_2Si_2$

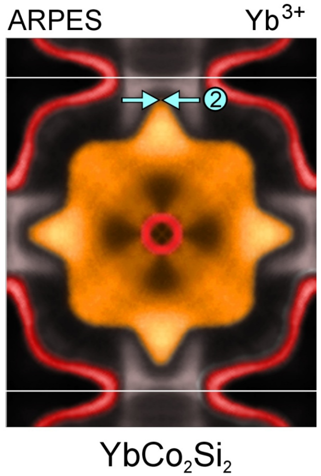
K. Kummer et al (2014)

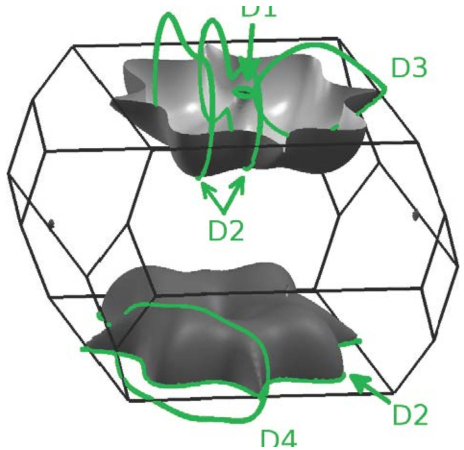
Low T, low B FS confirmed

Work in progress: Photoemission from $YbRh_2Si_2$ at elevated T

ARPES: f delocalized vs 4f localized







$LuRh_2S_{i2}$ FS from SdH

K. Kummer et al (2013)

Relevant temperature scale?

$YbRh_2Si_2$: 4f spectral function at elevated T

Theory:

Calculate 4f-spectral function for lattice from 4f propagator

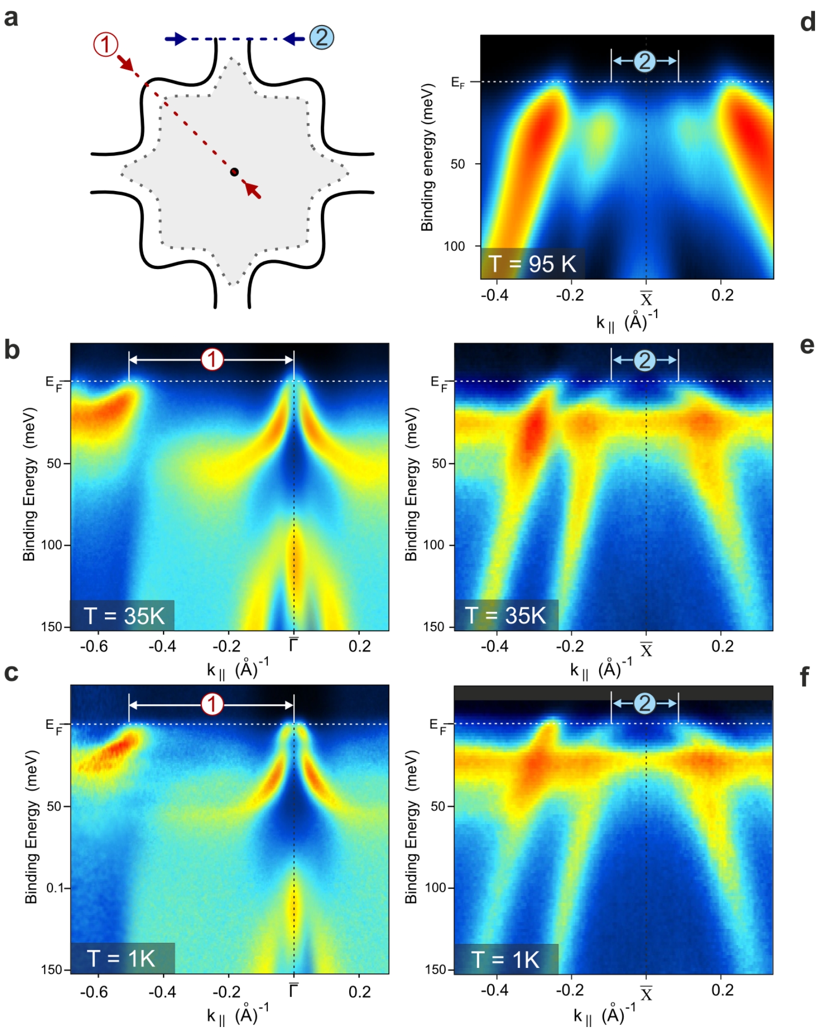
$$\mathbf{G}_{4f}^{-1}(\mathbf{k}\omega;T) = \underbrace{\mathbf{g}_{4f}^{-1}(\omega;T)}_{\substack{\text{local 4f-propagator} \\ \text{T-dependence}}} - \underbrace{\sum_n \left(\mathbf{W}_{n,n}(\mathbf{k}\omega;T) - \sum_{\mathbf{k}} \mathbf{W}_{n,n}(\mathbf{k}\omega;T) \right)}_{\substack{\text{hybridization with conduction states} \\ \text{weak T-, } \omega\text{-dependence}}}$$

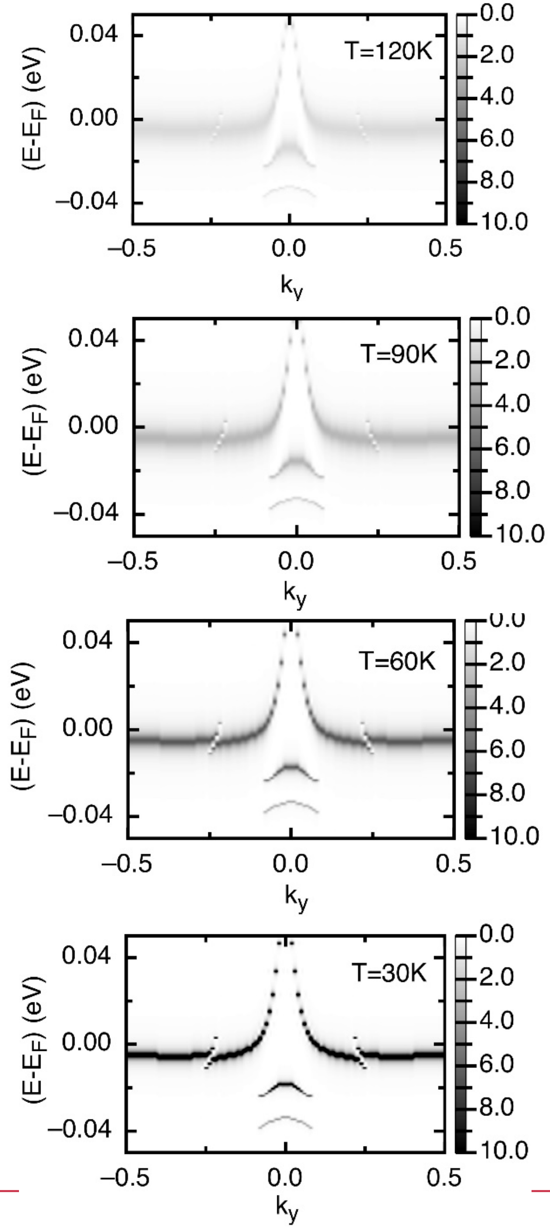
Use single-impurity propagator

Close-to-integer limit => small transfer of spectral weight between Kondo resonance and charge fluctuation peak
=> Keep conduction bands fixed

Rather smooth cross-over expected

$YbRh_2Si_2$: 4f spectral function at elevated T





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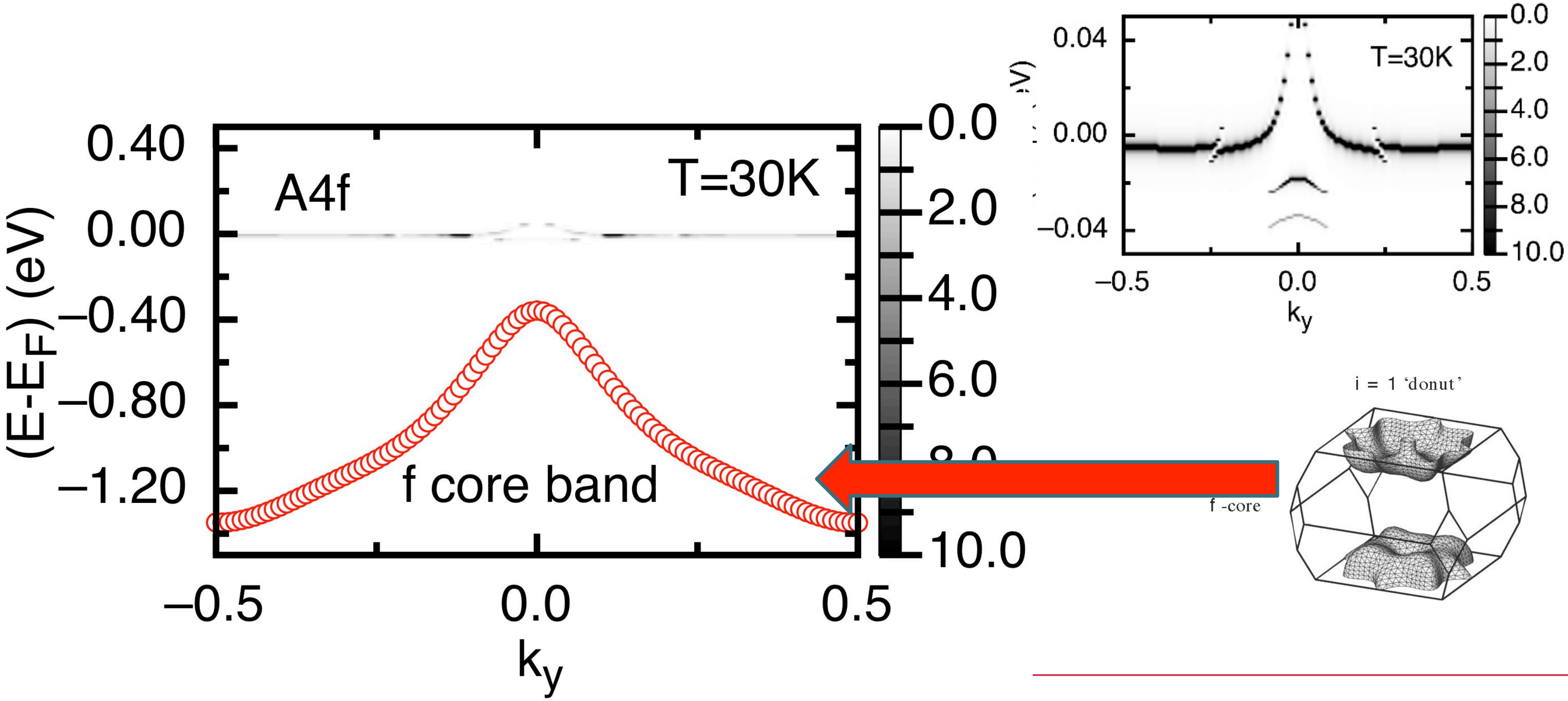
$YbRh_2Si_2$: 4f spectral function at elevated T

Comparison: 4f spectral function and f core band



$YbRh_2Si_2$: Critical quasiparticles (?)

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Strong-coupling theory of heavy-fermion criticality

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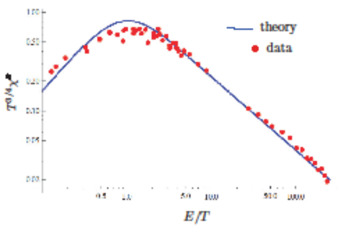

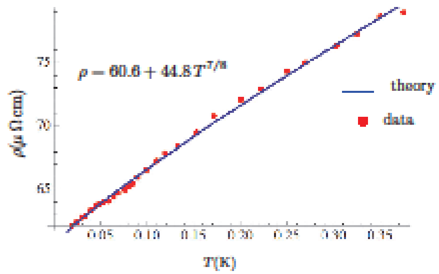

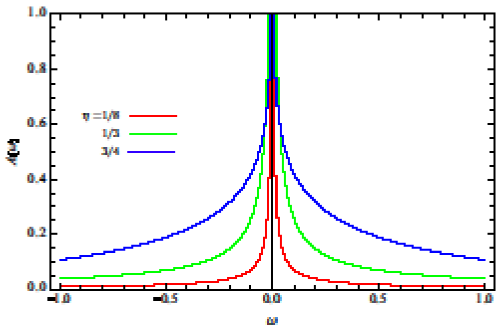

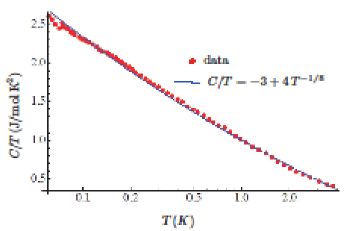

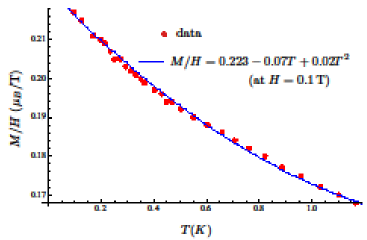

Finally, we emphasize that we assumed the heavy quasiparticles to be robust, though modified by scattering from critical spin fluctuations. There is no breakdown of the Kondo effect nor an associated collapse of part of the Fermi surface in our scenario. Experimental features, such as the crossover behavior observed in transport properties (and, to a lesser extent, in the thermodynamic quantities) across the "T^* line" in the T-H phase diagram of YRS, may be accounted for by a change in quasiparticle scattering strength associated with thermal activation of the (ESR) spin resonance as well as by single-quasiparticle spin-flip scattering [29,30].

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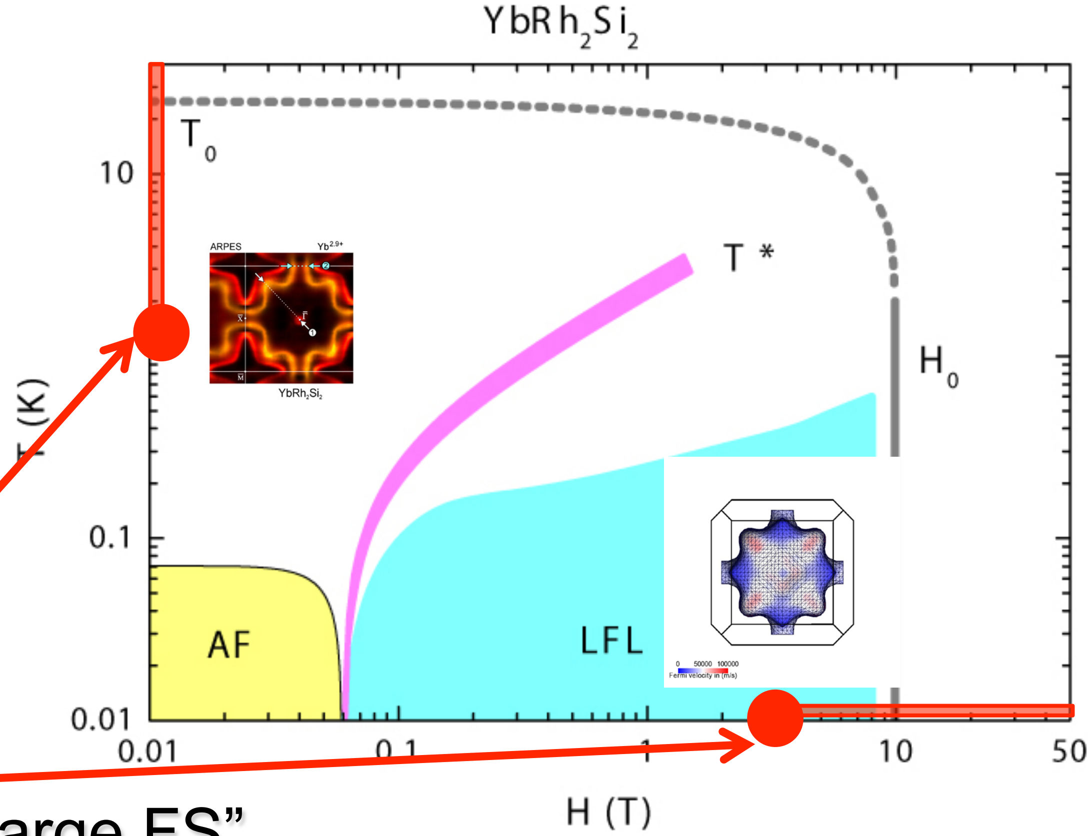
Work in progress: Photoemission from $YbRh_2Si_2$ at elevated T



Spectral function: "Large FS"
Variation with B and T from de-renormalization of heavy quasiparticles due to local break-up of Kondo singlets
"Small" FS related to magnetic order? Meaning of the T*-line?

Instead of summary and outlook ...

Questions in HF superconductivity

1. Actinides: 5f valence => Hidden order
2. $CeCu_2Si_2$: order parameter nodes
3. $CeCoIn_5$: Modulated sc state
4. Ce- Yb asymmetry
5. Nature of QCPs
6. 4f spectral functions at elevated T
7. ....