Fermi surface instabilities in $YbRh_2Si_2$ at high field

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thanks to H. Harima, Kobe University

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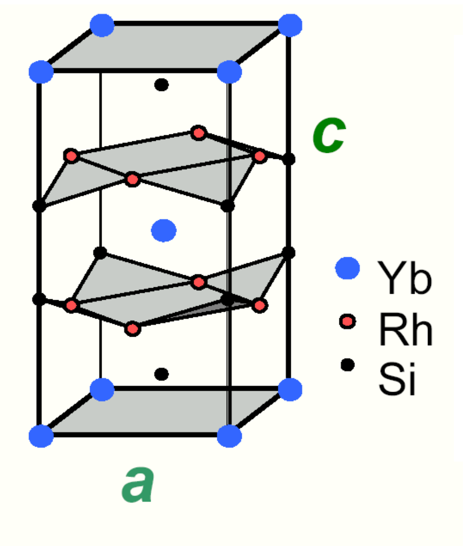
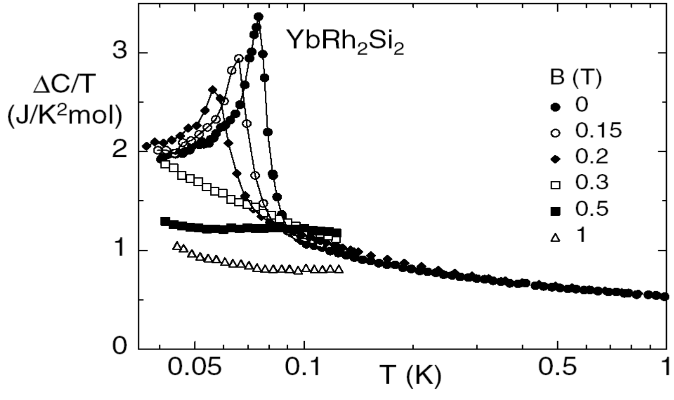
see : A. Pourret et al. J.Phys. Soc. Jpn. **82** (2013) 053704

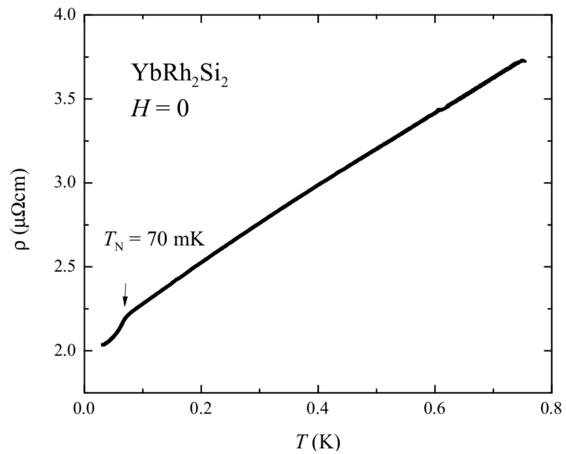
outlook

- Introduction
- Some experimental details
- Magnetoresistance of $YbRh_2Si_2$
- Thermoelectric power through H_0
- Quantum oscillation experiments
- Comparison to band structure calculations

Unconventional metallic state in $YbRh_2Si_2$





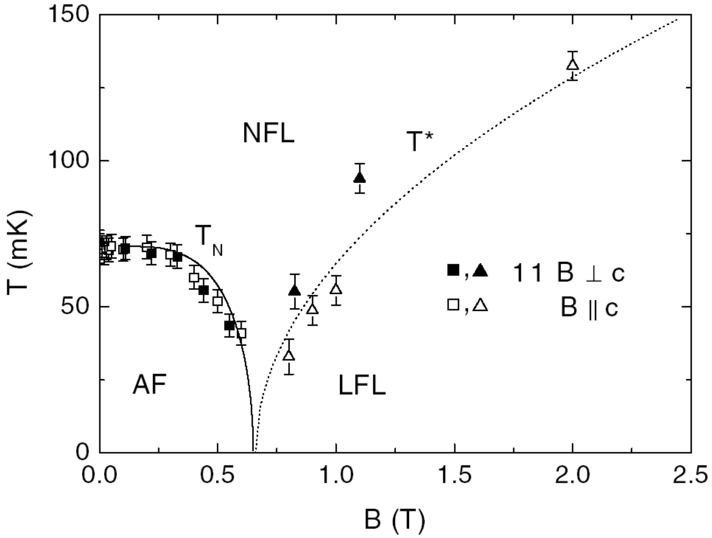


- Yb based heavy fermion system with very low magnetic order
  - T_K = 25 K, T_N ~ 70mK
  - Δ_{CF}= 200, 290, 500 K
  - m~ 0.02 μ_B , but magnetic structure not known

- field induced QCP, H_c = 0.066 T, *H // a*
- above H_c, strong FM fluctuations

Ishida et al, PRL 89, 107202 (2002)

Gegenwart et al. PRL 94, 076402 (2005)



Trovarelli et al. PRL 85, 626 (2000)

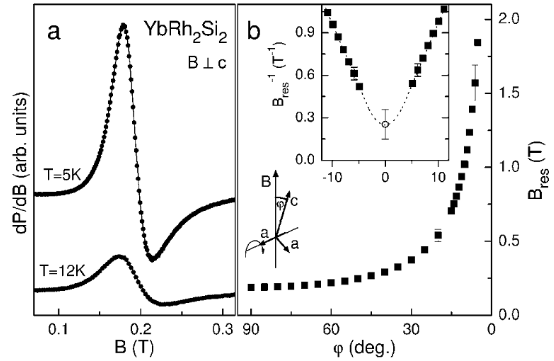
Gegenwart et al. PRL 89, 056402 (2002)

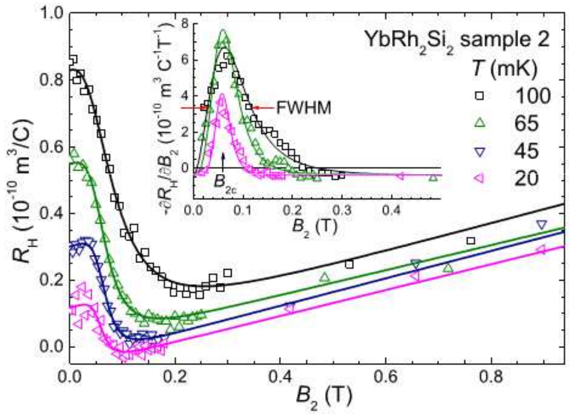
Custers et al. nature 2003

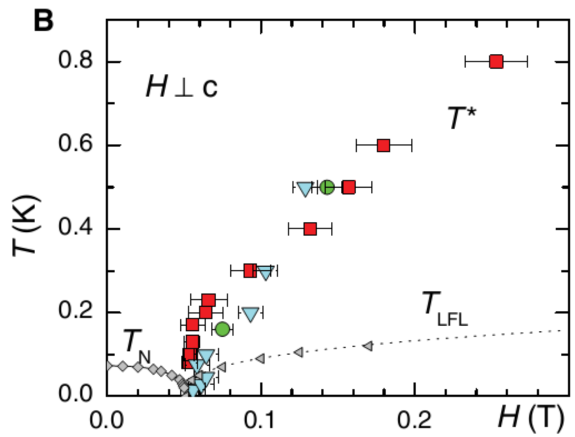
Quantum criticality in $YbRh_2Si_2$: localized versus itinerant

Kondo breakdown :

- Discrepances with “standard” spin-fluctuation model:
  - *J. Custers et al, Nature **424**, 524 (2003)*
  - decomposition of heavy fermions ?
  - Divergence of Grüneisen ratio R. Küchler, PRL **91**, 066405 (2003)
- ESR signal of dense Kondo lattice from Yb^{3+} ion :
  - *J. Sichelschmidt et al. PRL, **91**, 156401 (2003)*
  - strong anisotropic g factor (more than factor 10)
- Hall effect : small → large Fermi surface
  - *S. Paschen et al. Nature **432**, 881 (2004)*
  - *Friedemann et al. PNAS 107 (2010) 14547*
  - Destruction of renormalized Fermi surface ?
- Thermodynamic evidence for multiple energy scales at the QCP
  - *P. Gegenwart, Science 315, 969 (2007)*
- Violation of Wiedemann-Franz *(Pfau, Nature 484 (2012) 493)*
  - *Strongly debated recently (Sherbrooke, Tokyo, Grenoble)*





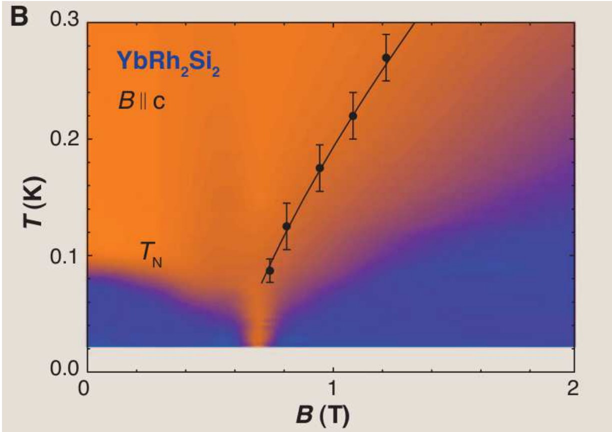


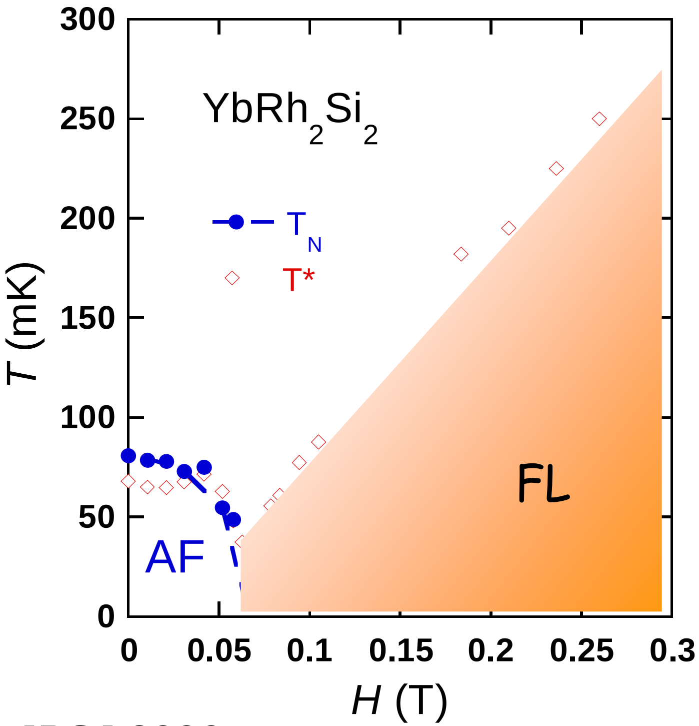
- **role of valence fluctuations** *(Watanabe, Miyake)*
- **Zeeman driven Lifshitz transition ?**

Hackl, Vojta PRL 106 (2011) 137002

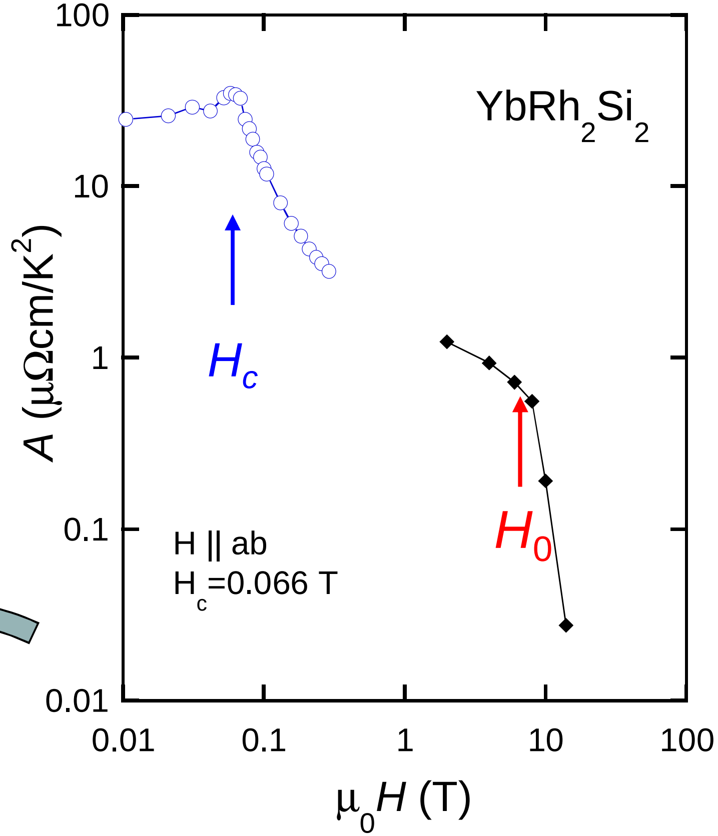
$^{174}YbRh_2Si_2$: ($H - T$) phase diagram ($H||a$)

Custers nature 2003





GK et al. JPSJ 2006

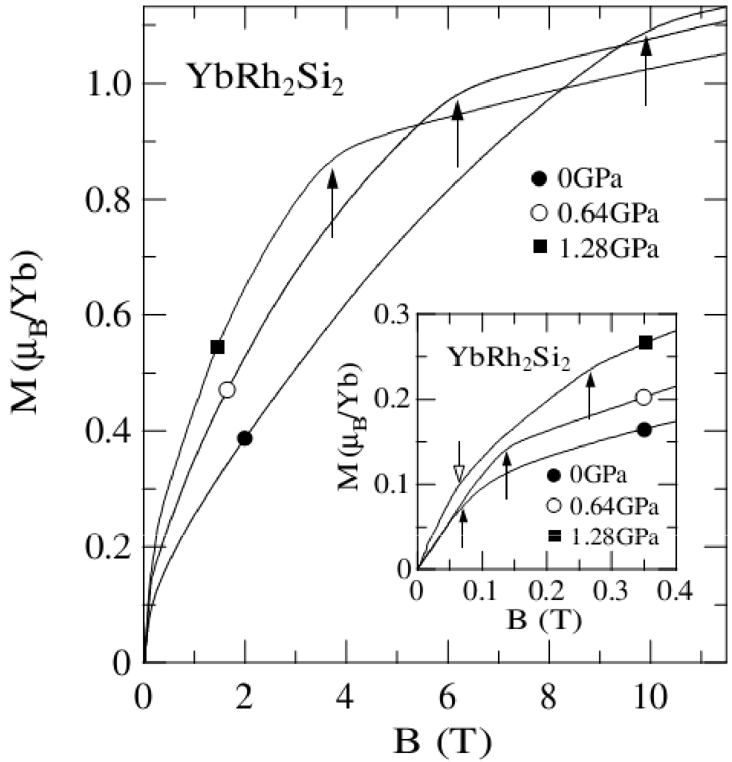


2 characteristic fields !

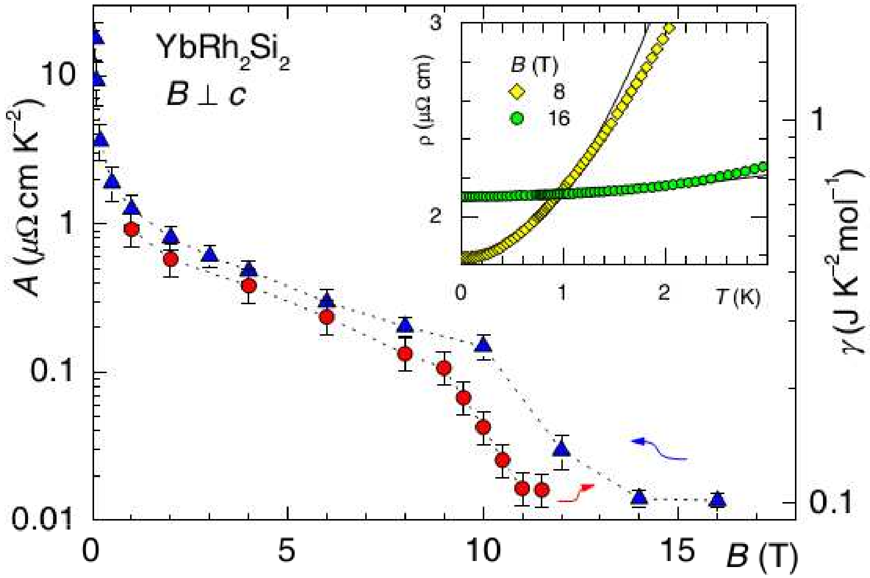
H_c=0.066 T: suppression of AF order

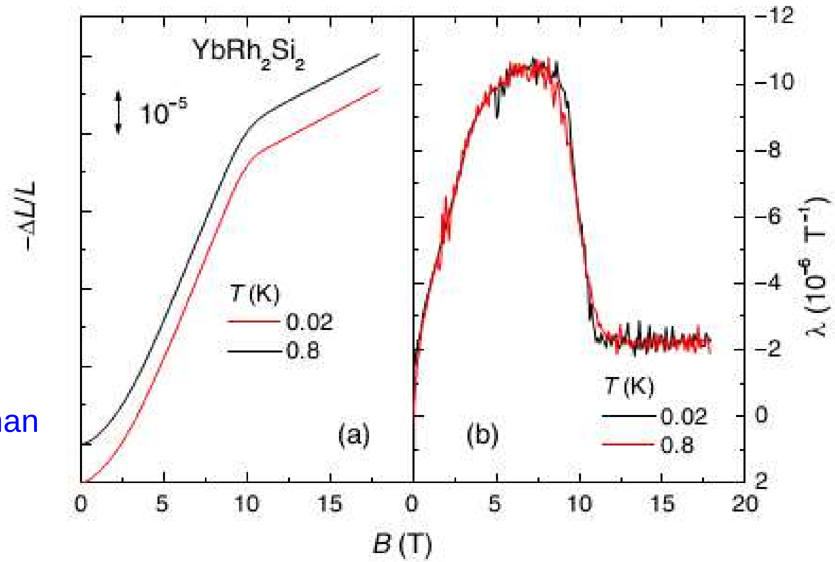
H_0=9.5 T : suppression of heavy mass

High field properties : $T_K \sim T_{zeeman}$



Tokiwa PRL 2005





Gegenwart NJP 2006

Interpretation 2006:

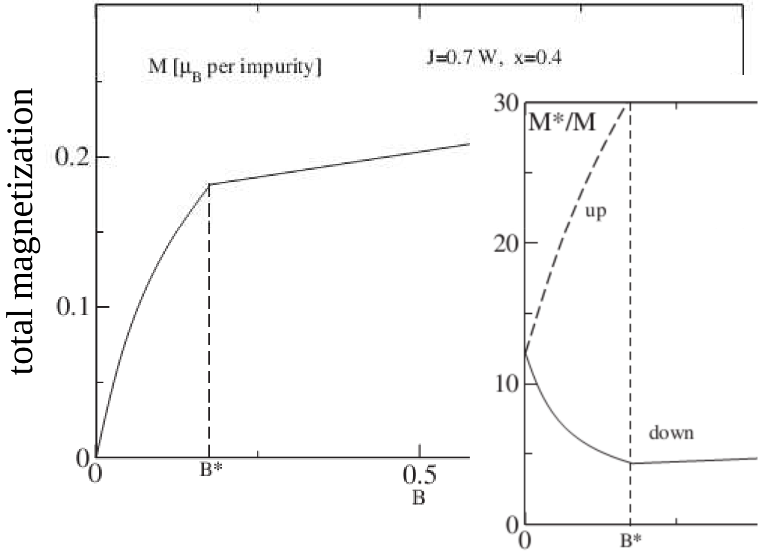
- no signature of metamagnetism
- destruction of the Kondo effect, $T_K \sim T_{Zeeman}$
- possible localization of *f* electron

Lifshitz-type transition through H_0

Kusminskiy et al. PRB 77 (2008) 094419:
static mean field theory, Kondo lattice coherence of same order than Zeeman splitting , one band model, parameter exchange J, band filling x

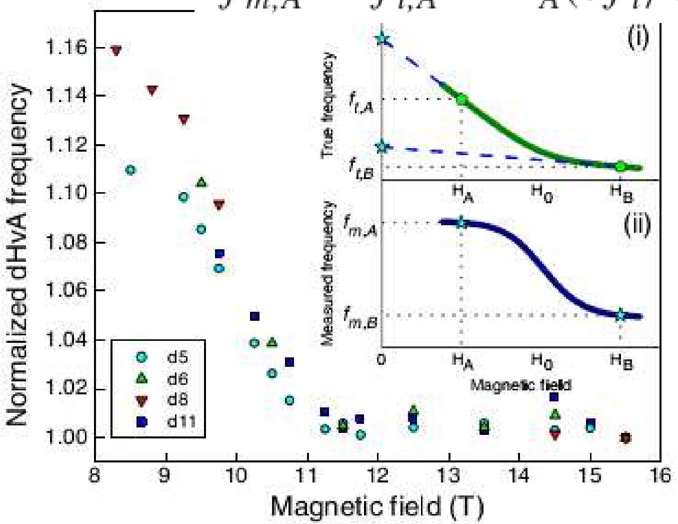
Spin-split FS undergoes a Lifshitz transition:

- spin split branch drops below the chemical potential at *B**
- Fermi surface of heavy quasi-particles vanished at *B**, leaving only moderately heavy particle above *B**
- no localization of f electron, but continuous evolution of the Fermi surface.



dHvA :
Toronto University

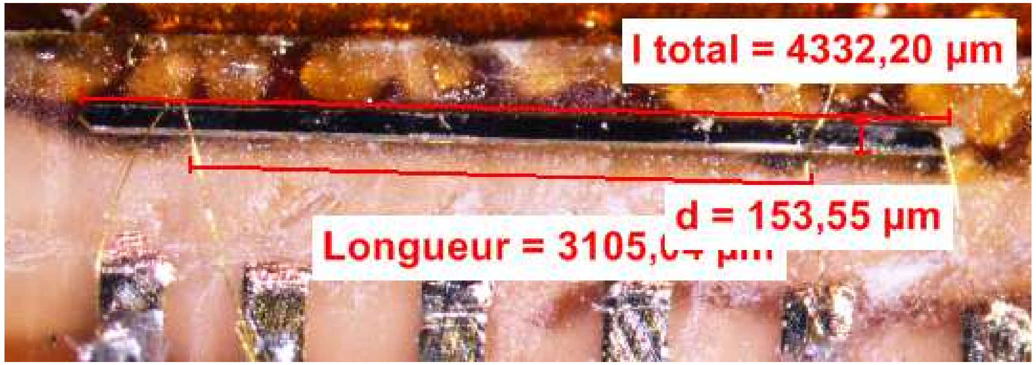
$$f_{m,A} = f_{t,A} - H_A(\partial f_t/\partial H)_A$$

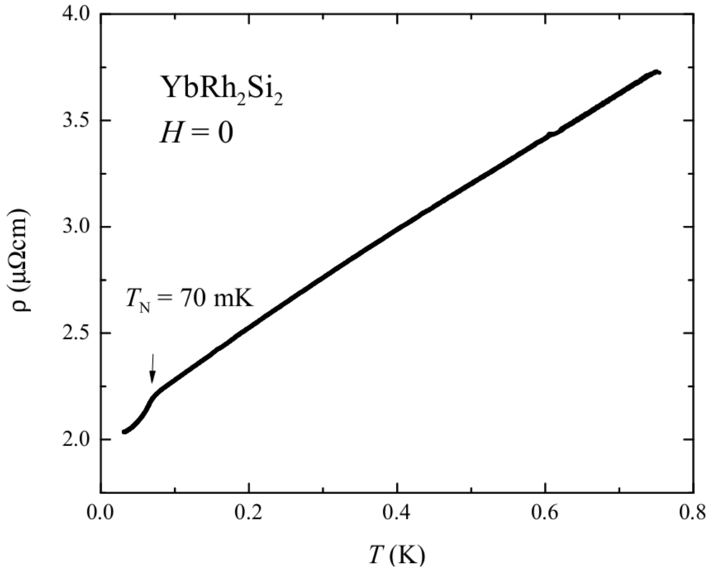


Rourke et al. PRL 2008
Sutton et al. PSS 2010

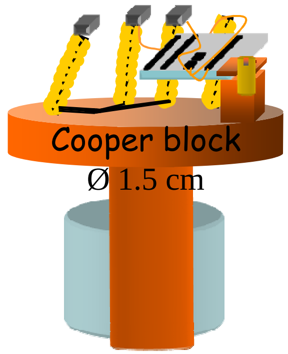
Experimental details

In flux grown single crystal
RRR ~ 65 , not the highest but .....





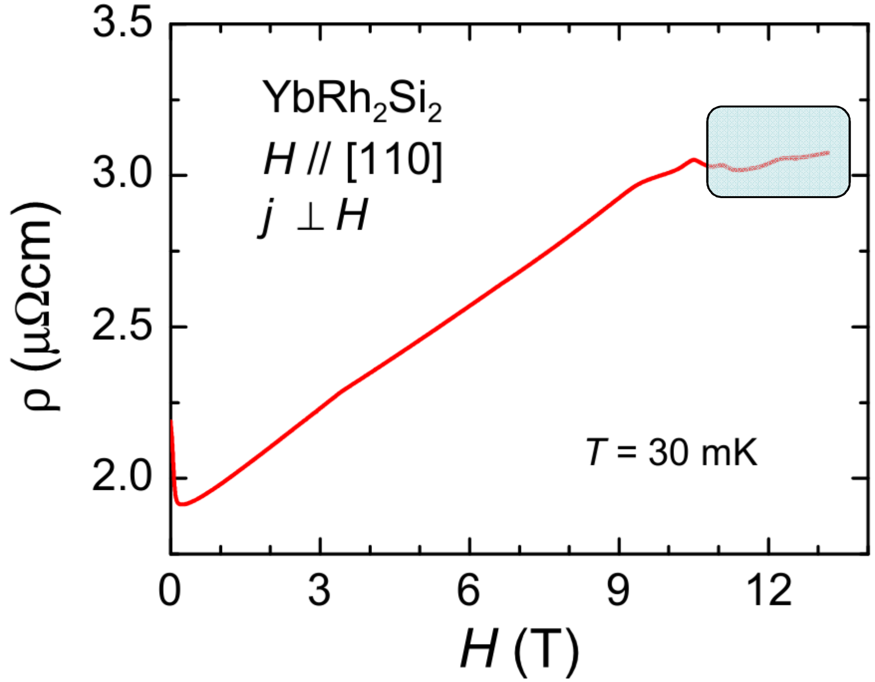
resistivity : 30 mK, 13.5 T
thermoelectric power : 150 mK, 16 T
dHvA : 15 mK top loading dilution, 15 T

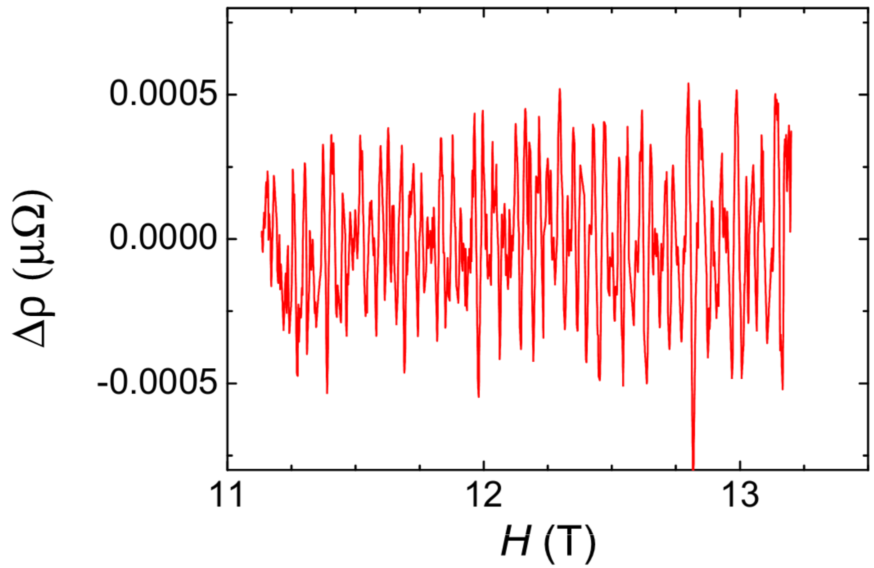


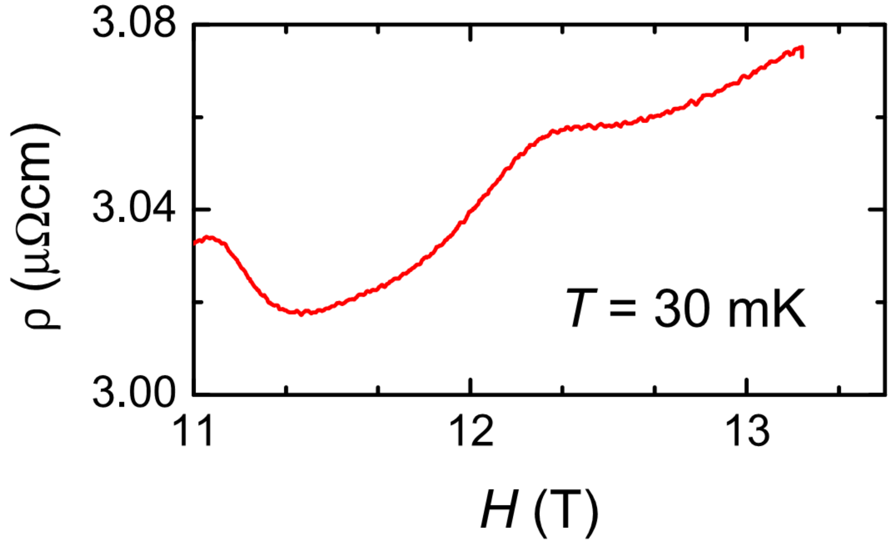
$$F = \frac{1}{\Delta\left[\frac{1}{B}\right]} = \frac{\hbar}{2\pi e} S_F \quad \text{and } S_F = \left|\overrightarrow{k_F}\right|^2$$

$$S = \frac{-E_x}{\nabla_x T}$$

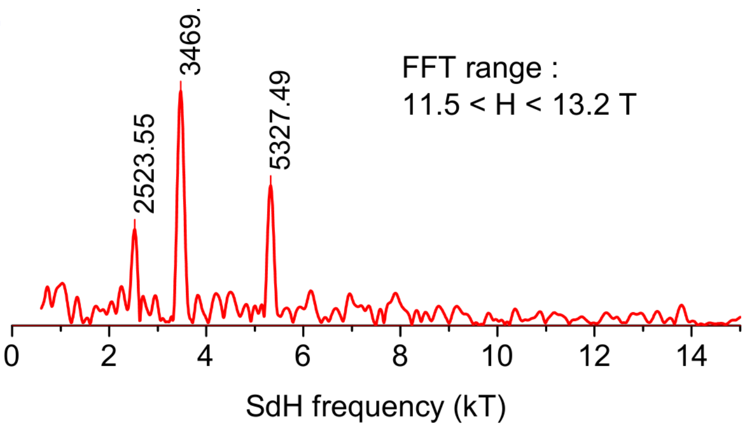
Magnetoresistance H | | [110]





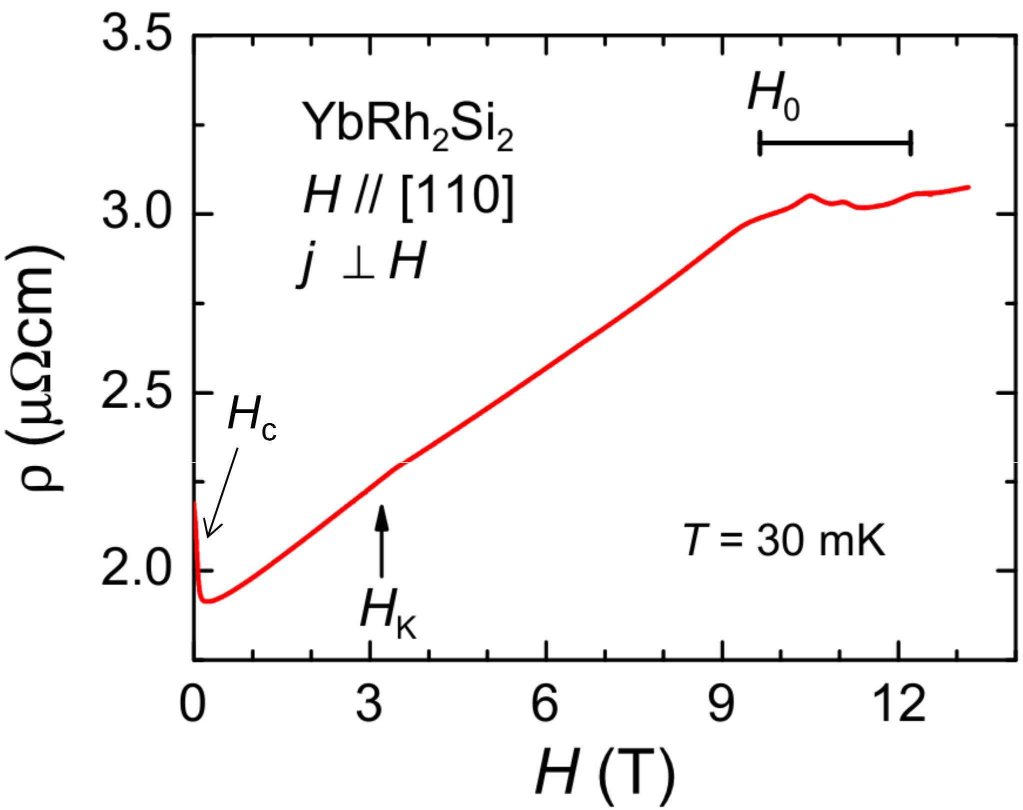


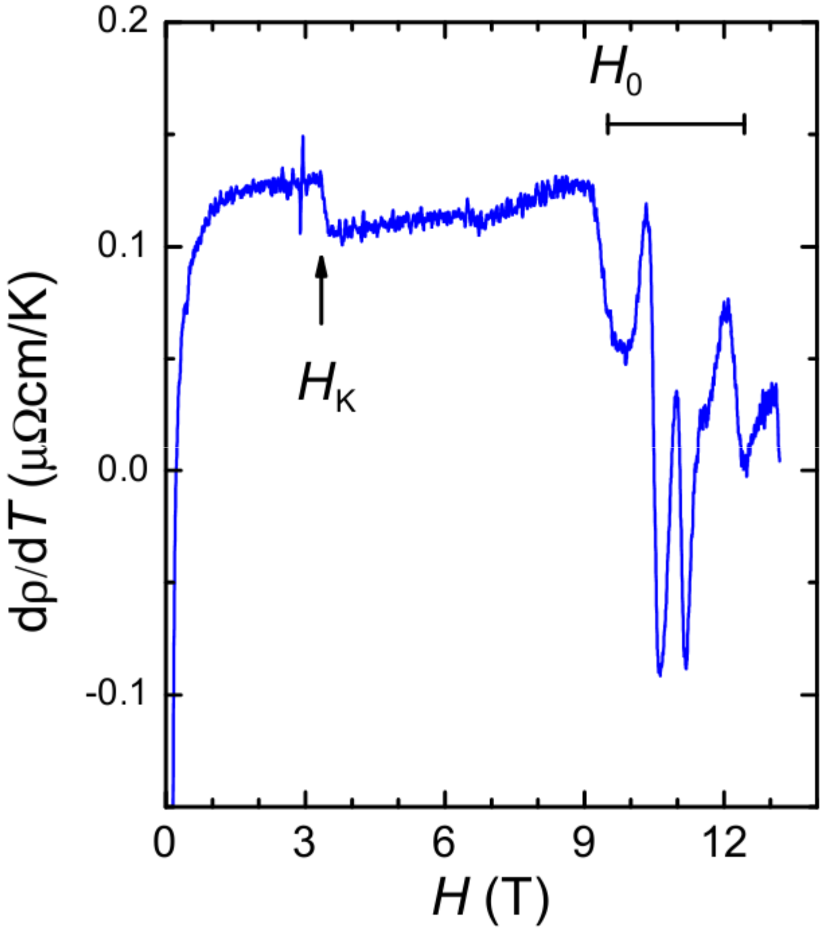
FFT



first observation of SdH in YbRh$_2$Si$_2$

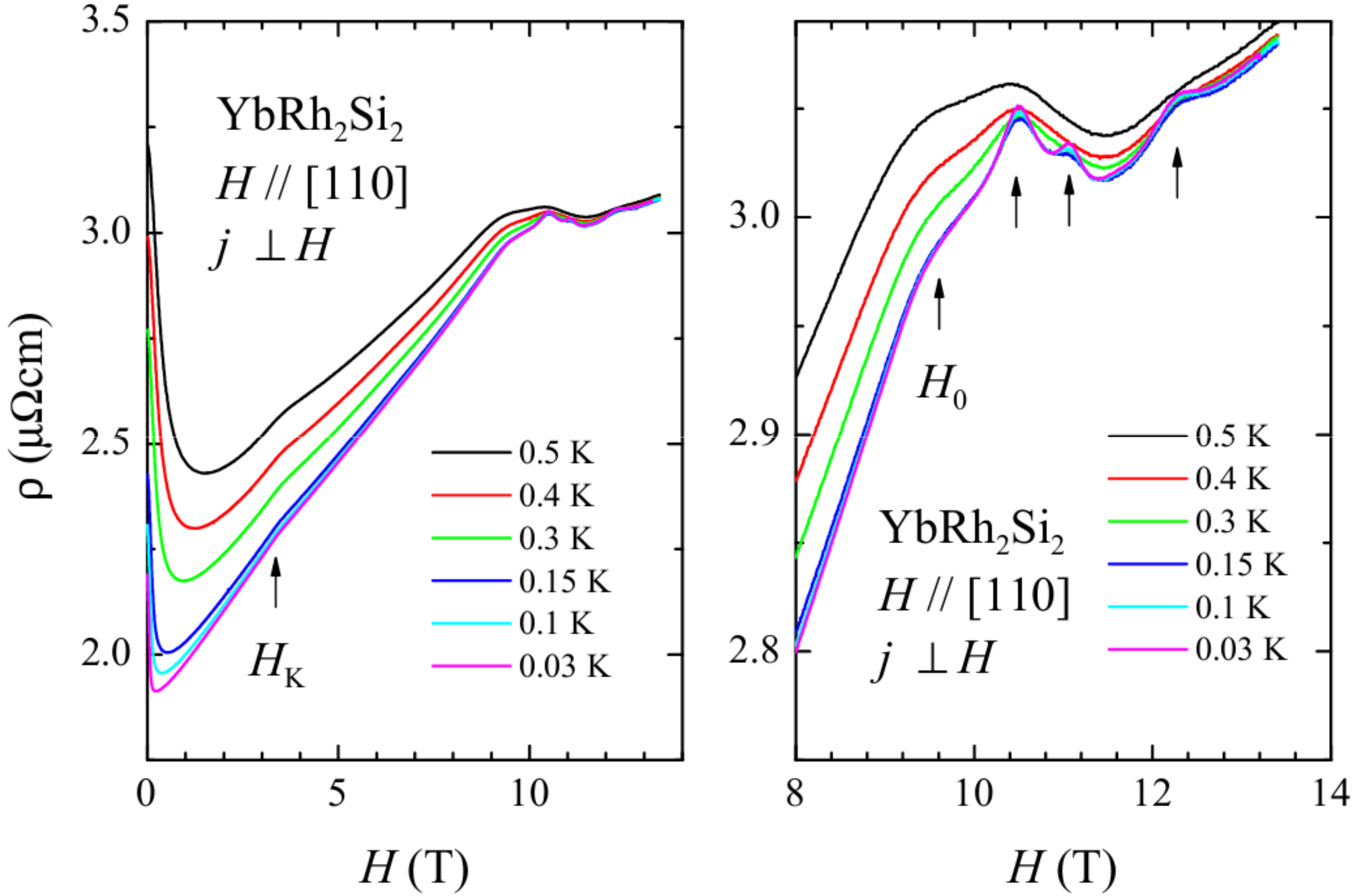
Magnetoresistance H // [110]





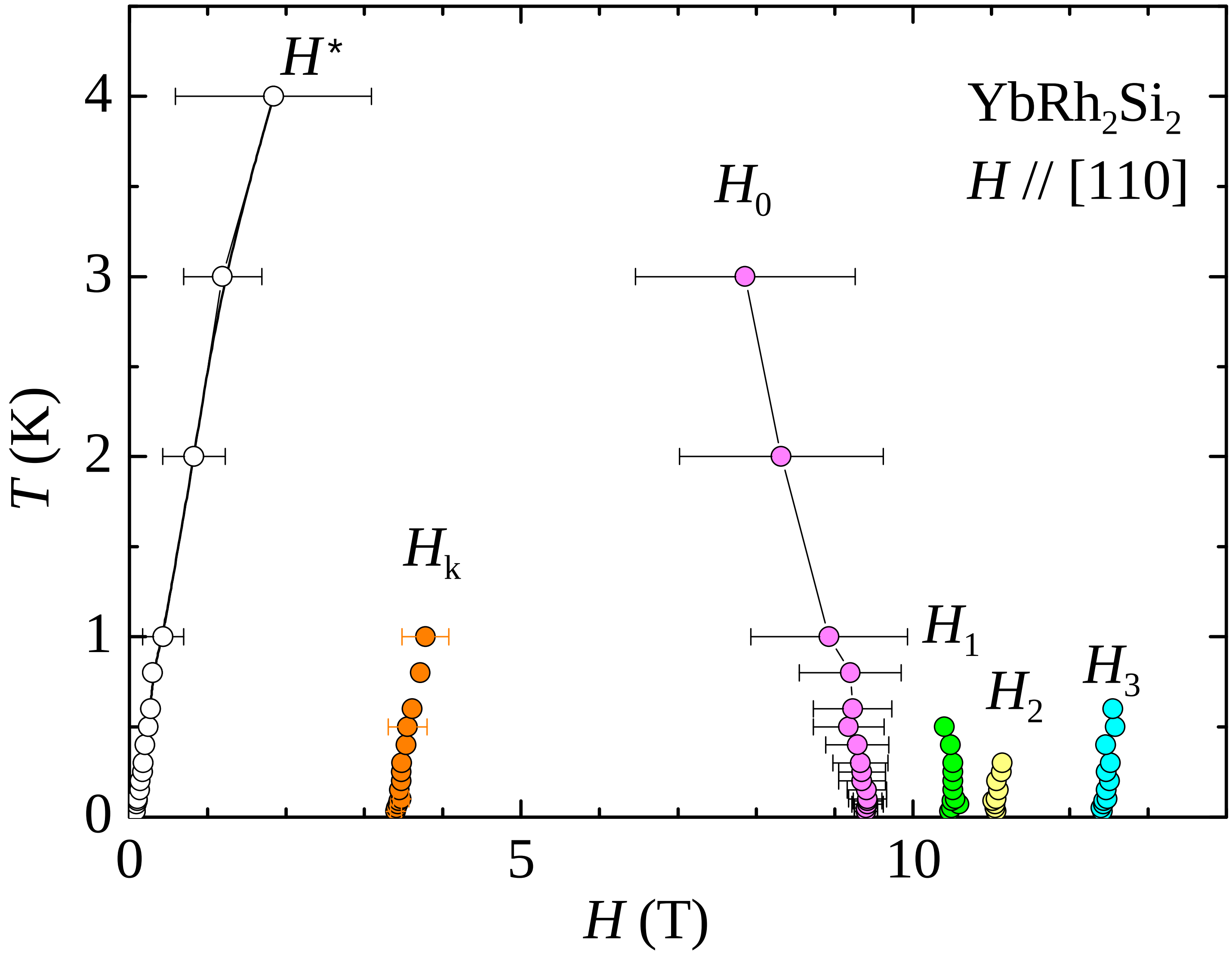
- kink at 3.4 T
- cascade of transitions above H_0 ~ 9.5 T

Temperature dependence of ρ(H)



Anomalies smeared out with increasing temperature !

Magnetic Phase Diagram from Magnetoresistance



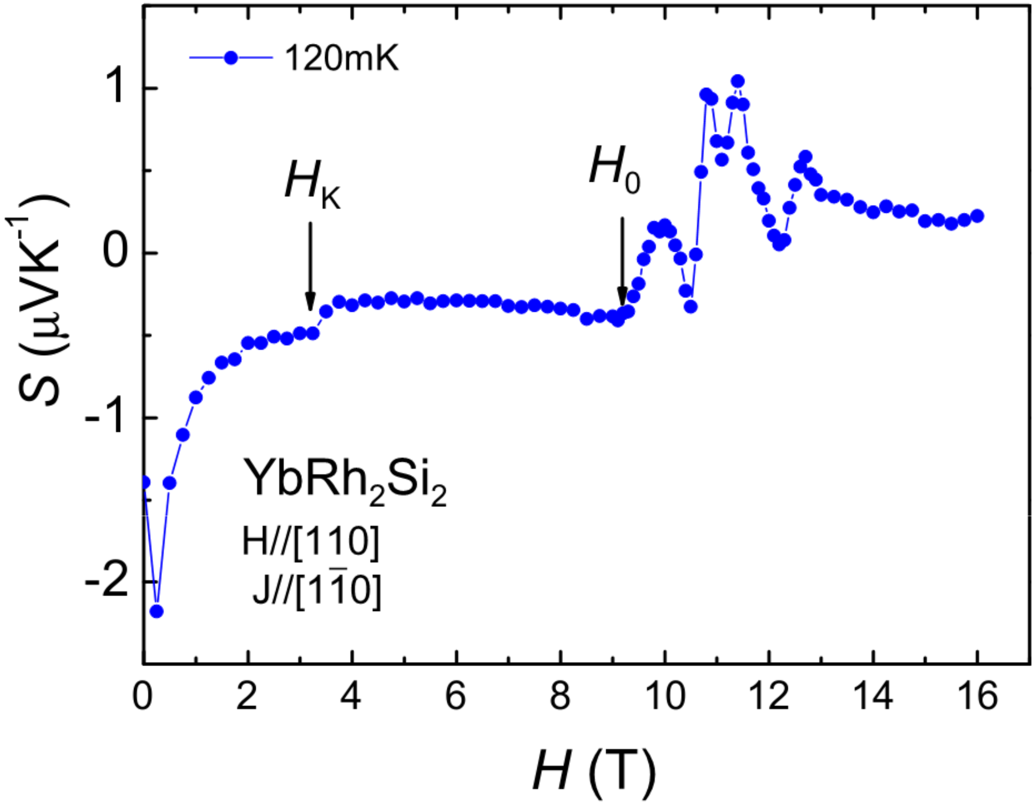
Thermoelectric power

Mott formula

$$S = -\frac{\pi^2 k_B^2 T}{3e}\left(\frac{\partial \ln \sigma(\epsilon)}{\partial \epsilon}\right)_{\varepsilon=\epsilon_F}$$

$$S = -\frac{\pi^2 k_B^2 T}{3e}\left(\frac{\partial \ln \tau(\epsilon)}{\partial \epsilon} + \frac{\partial \ln N(\epsilon)}{\partial \epsilon}\right)$$

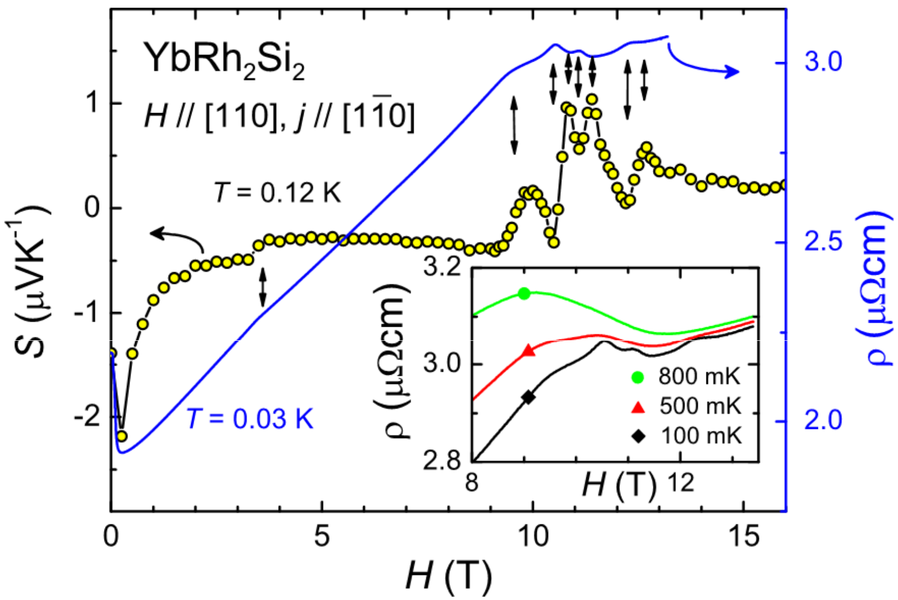
TEP sensitive to changes:
- **carrier type** (hole, electron)
- **scattering rate**
- **density of state** (measures the derivative of N)
- **Fermi surface topology**

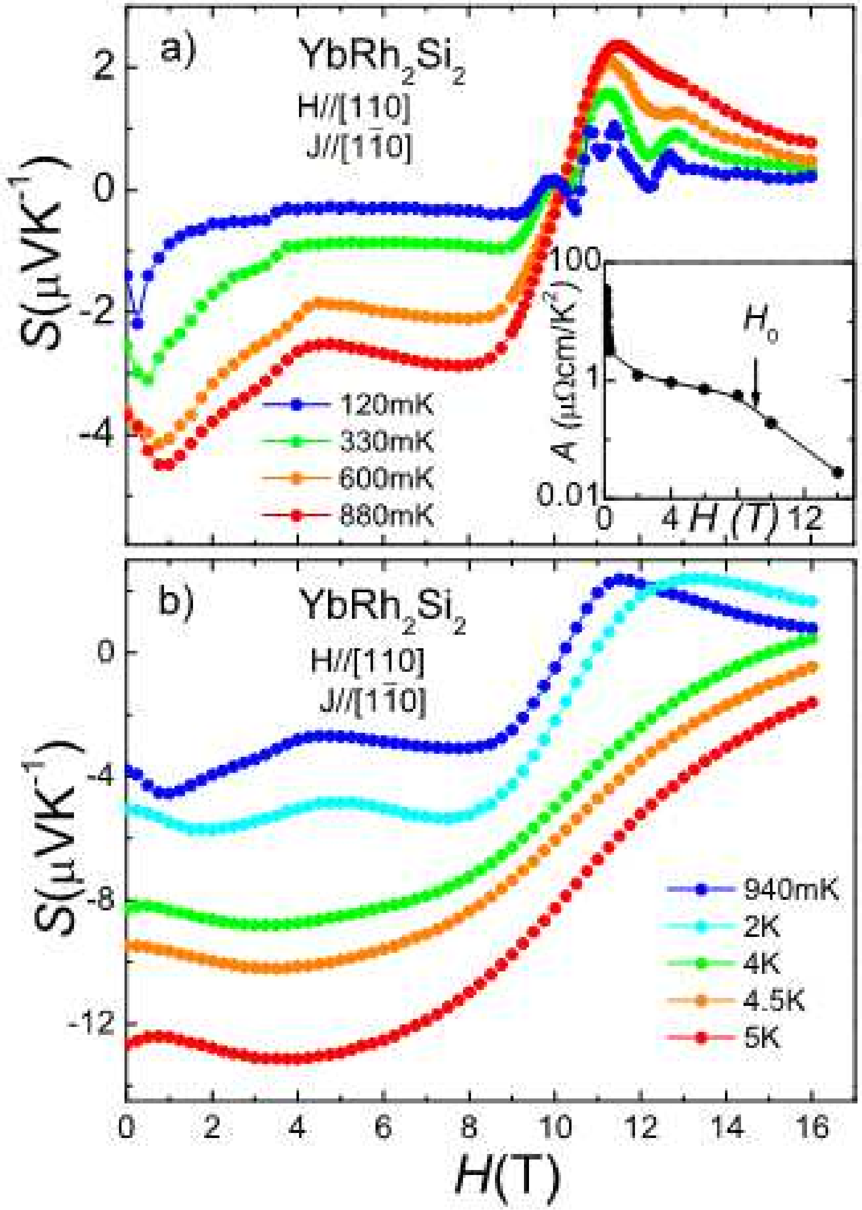


- Successive anomalies close to H_0
- Change of sign of $S(H)$ close to H_0

TEP : thermoelectric power

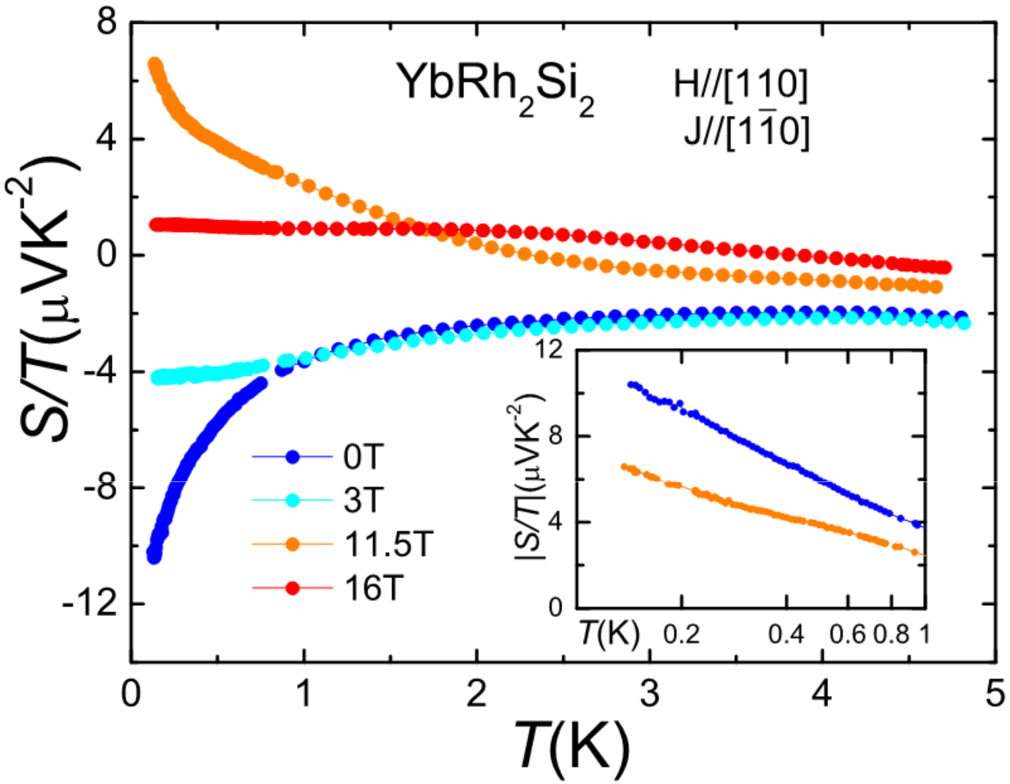
- excellent agreement with magnetoresistivity



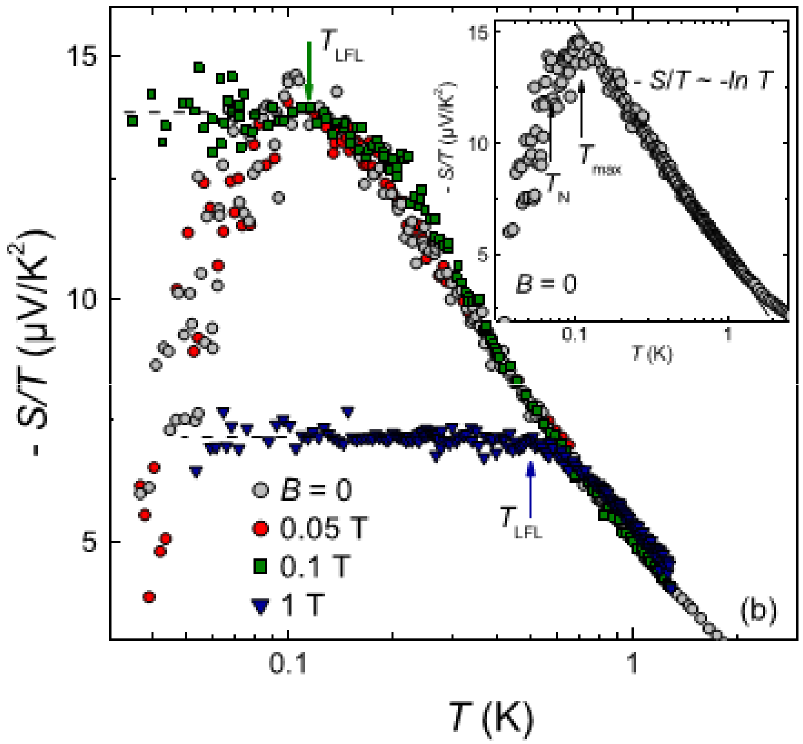


similar results:
H. Pfau et al. PRL 110, 256403 (2013)

Temperature dependence of S/T



compare to low field data:



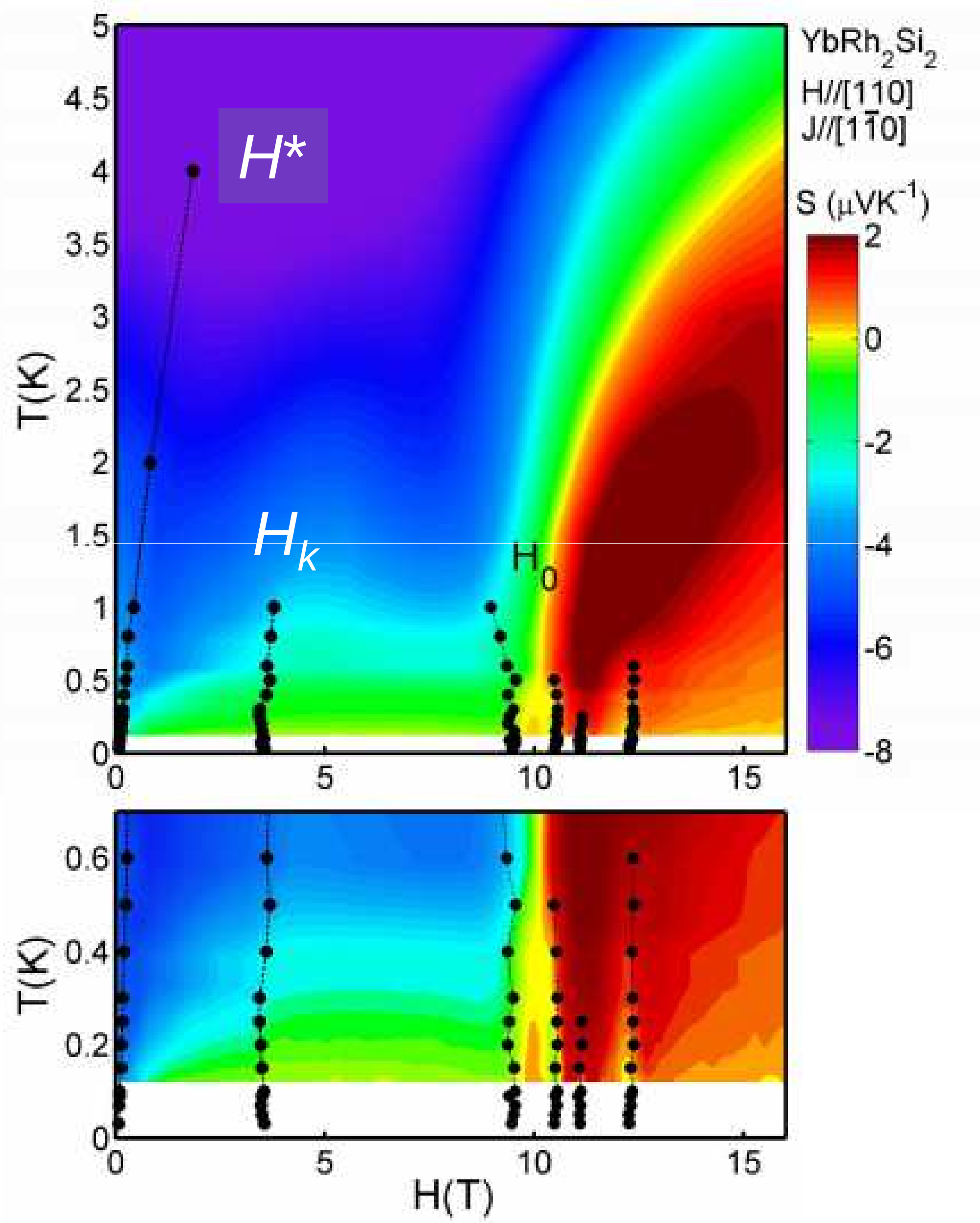
Hartmann et al, PRL 104 (2010) 096401

For 120 mK < T < 1.5 K:

- - ln *T* dependence for *H* = 0
- - ln *T* for *H* = 11.5 T (close to H_0)

see also: Buhmann and Sigrist, arXiv 1307.8235

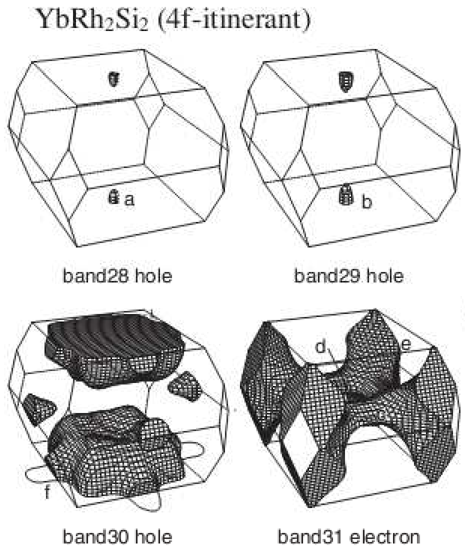
Phase diagram

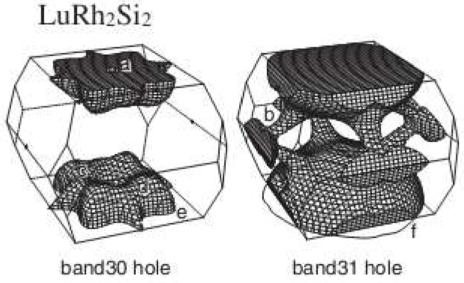


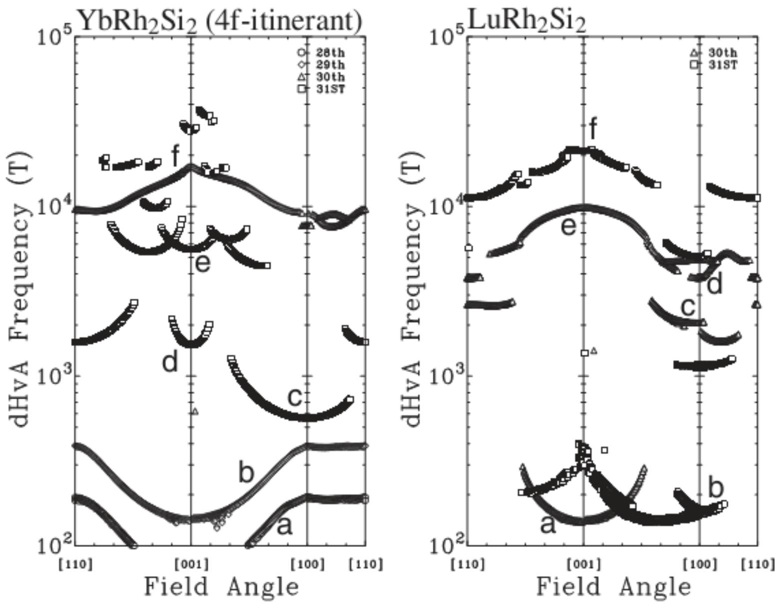
- Magnetoresistivity and thermoelectric power indicate field induced transitions.
- **Strong indications of topological transitions of the Fermi surface**.
- **Field scale of Lifshitz transitions given by $k_B T_K \sim g\mu_B H_0$**
- TEP is an extremely sensitive probe to detect topological transitions as it is directly determined by $d \ln N(E)/dE$

Band structure: “small”↔”large” Fermi surface

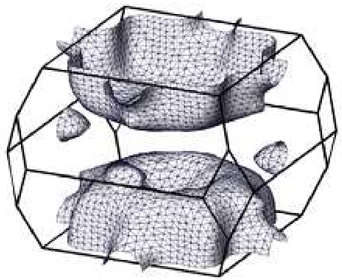
H. Harima, 2006
LDA



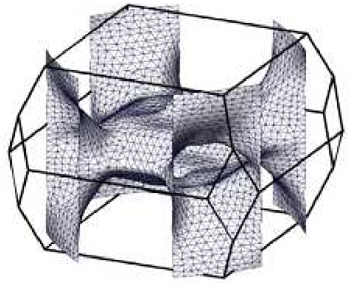




- *Zwicknagl JPCM **23** (2011) 094215 renormalized band structure*



f character
hole-like



- hybridized states
- electron-like
- multilple connected Fermi-surface

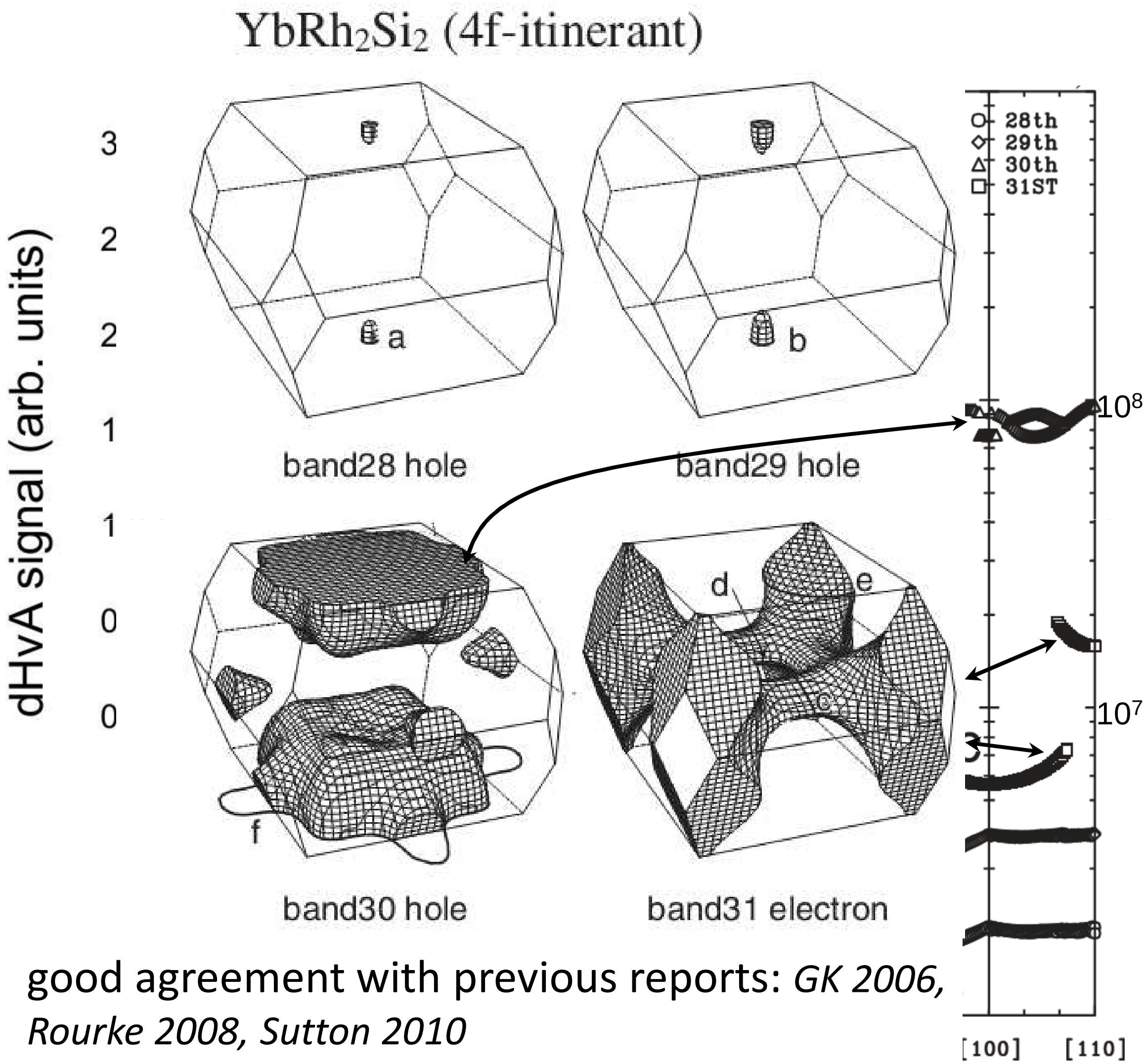
two main Fermi surfaces :

- hole like donut
- electron-like jungle-gym

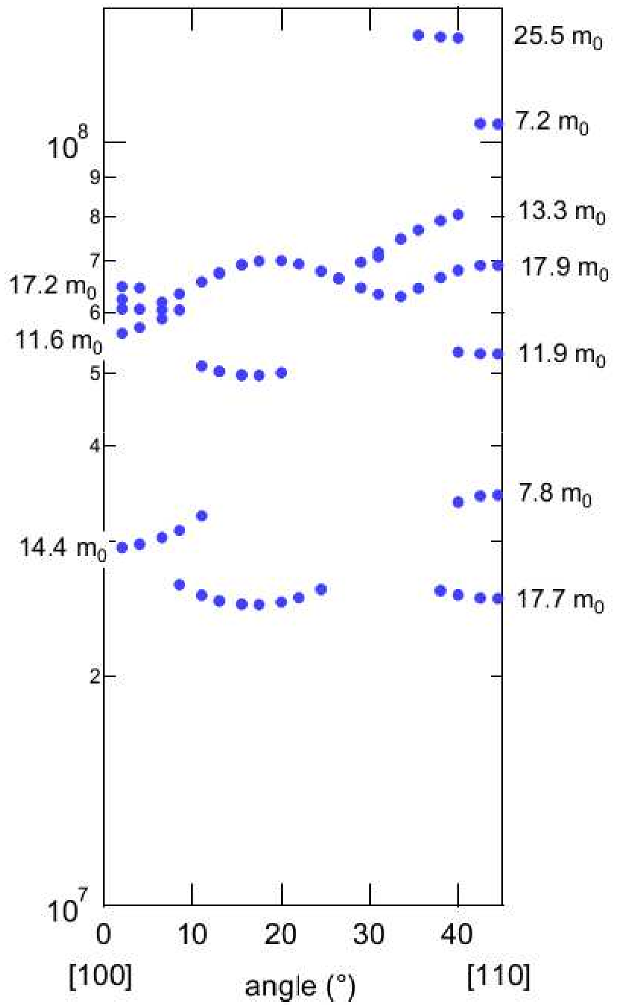
See also

- Rourke PRL **101** (2008) 237205, Sutton PSS B**247** (2010) 549
- Wigger PRB **76** (2007) 035106
- Yasui PRB **87** (2013) 075131

Angular dependence in plane

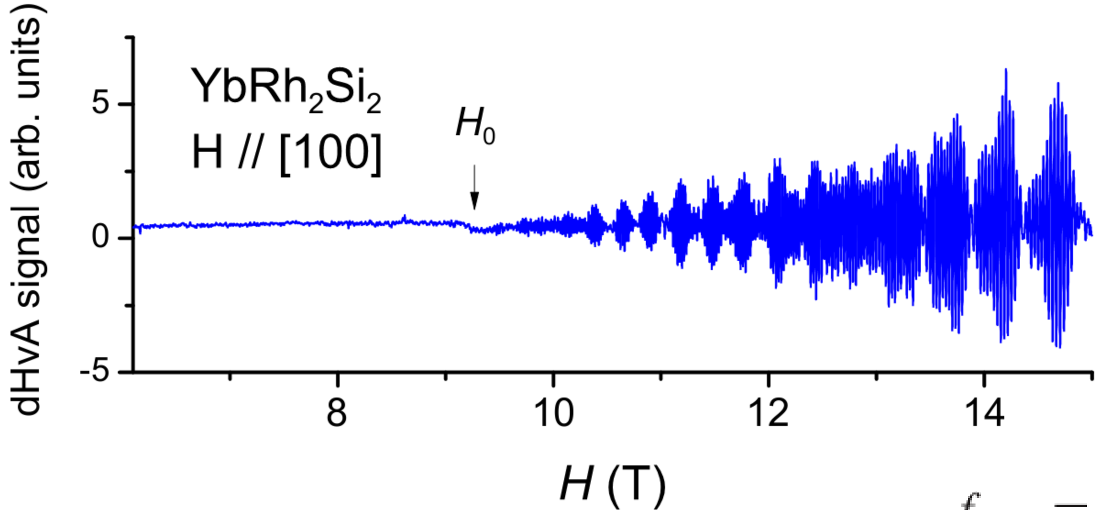


$H > H_0$



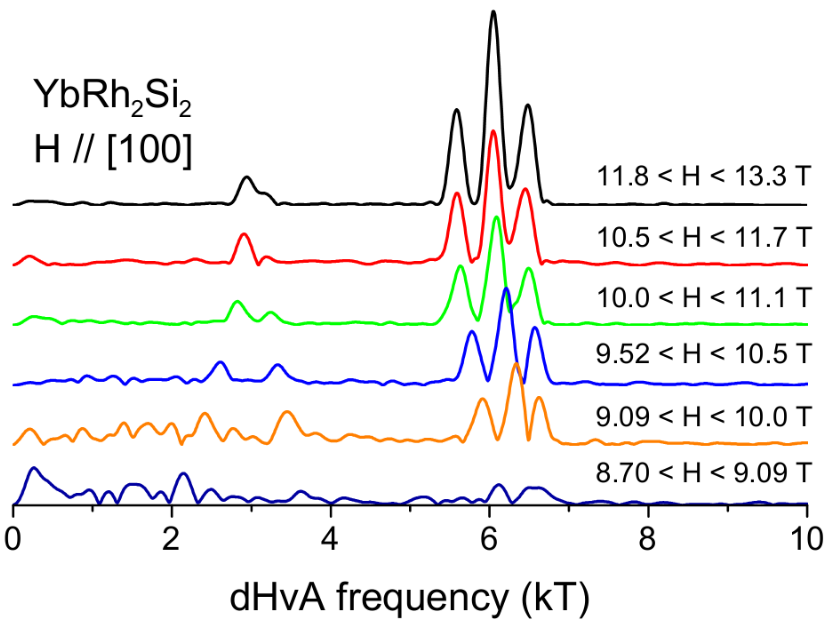
- good agreement with previous reports: *GK 2006, Rourke 2008, Sutton 2010*
- Comparison to band structure calculation 4f itinerant (Harima)
- observed large FS along [110] not reproduced

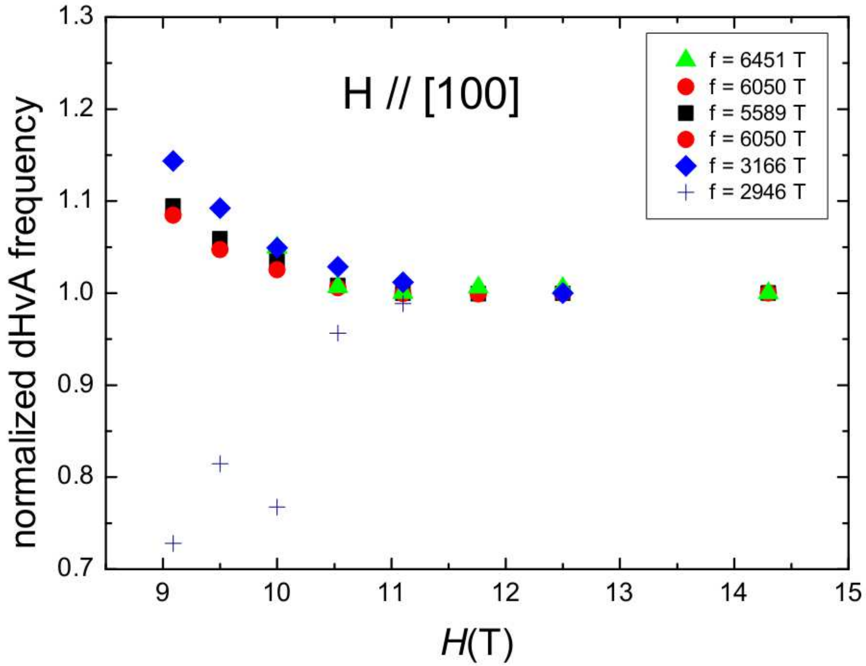
Quantum oscillation experiments H // [100] through H_0



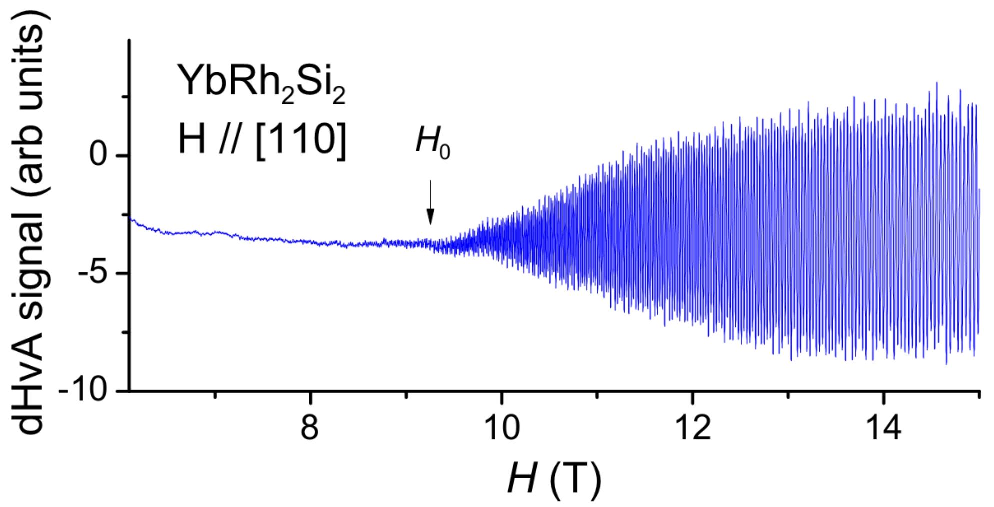
$$f_{m,A} = f_{t,A} - H_A(\partial f_t/\partial H)_A$$

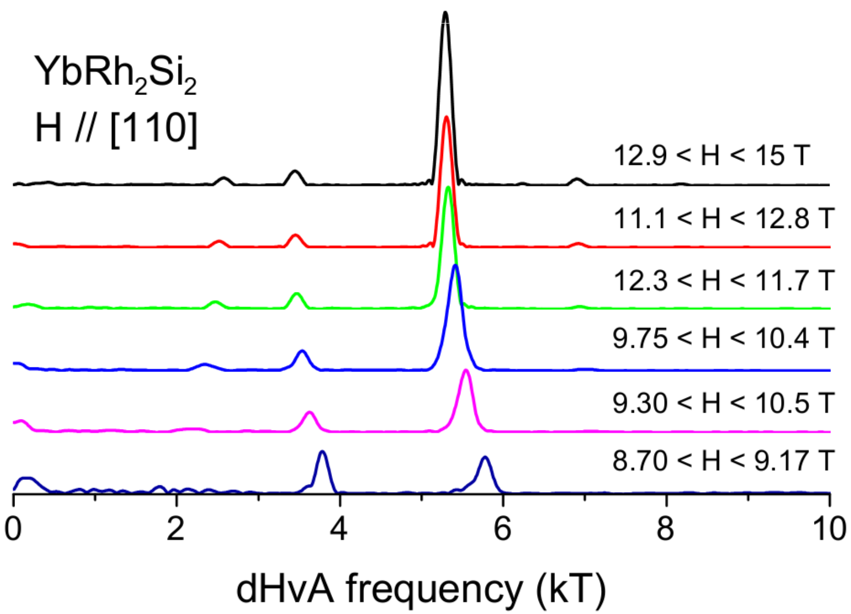
Field dependence of oscillations :

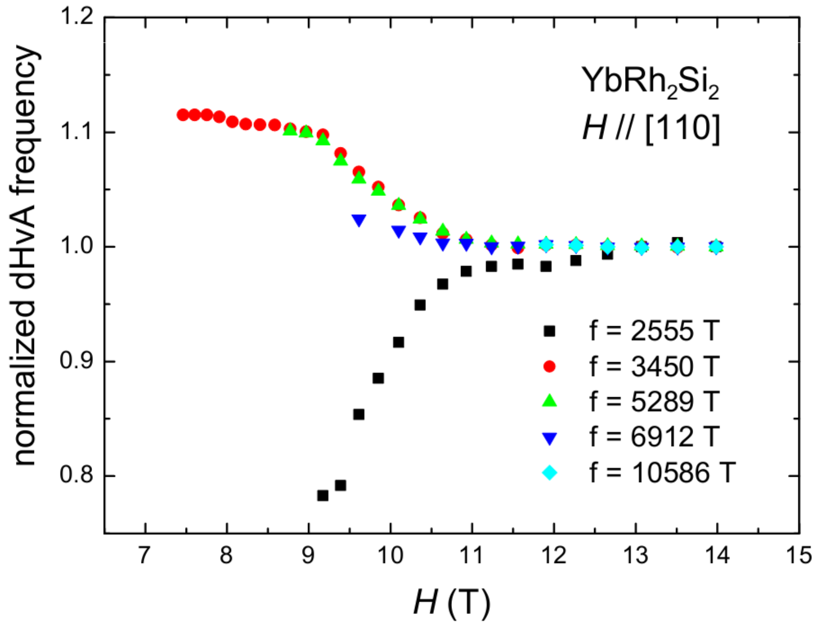




Quantum oscillation experiments H // [110] through H_0







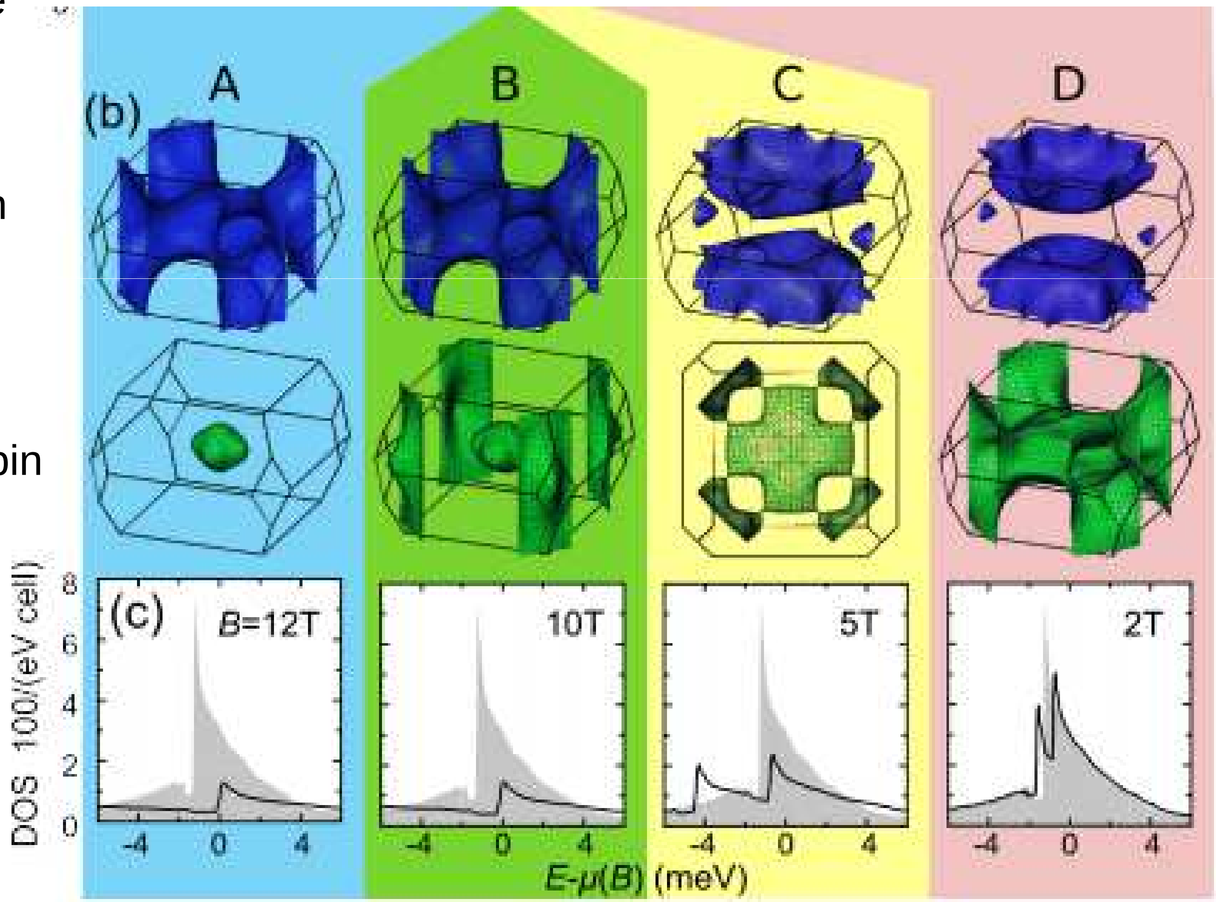
gradual field dependence of dHvA frequencies in (a,b) plane through H_0

Renormalized band structure calculation

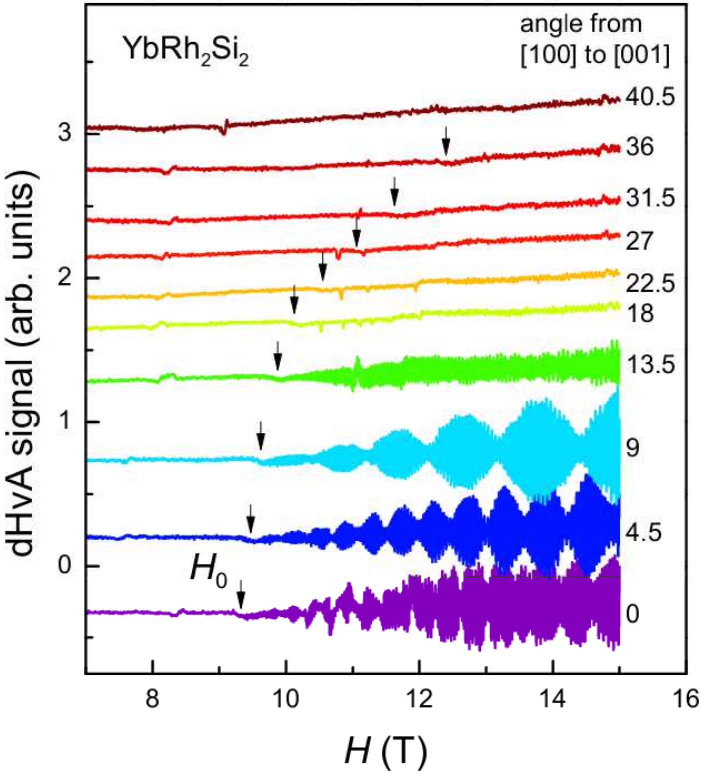
G. Zwicknagl
in Pfau et al. PRL 110, 256403 (2013)

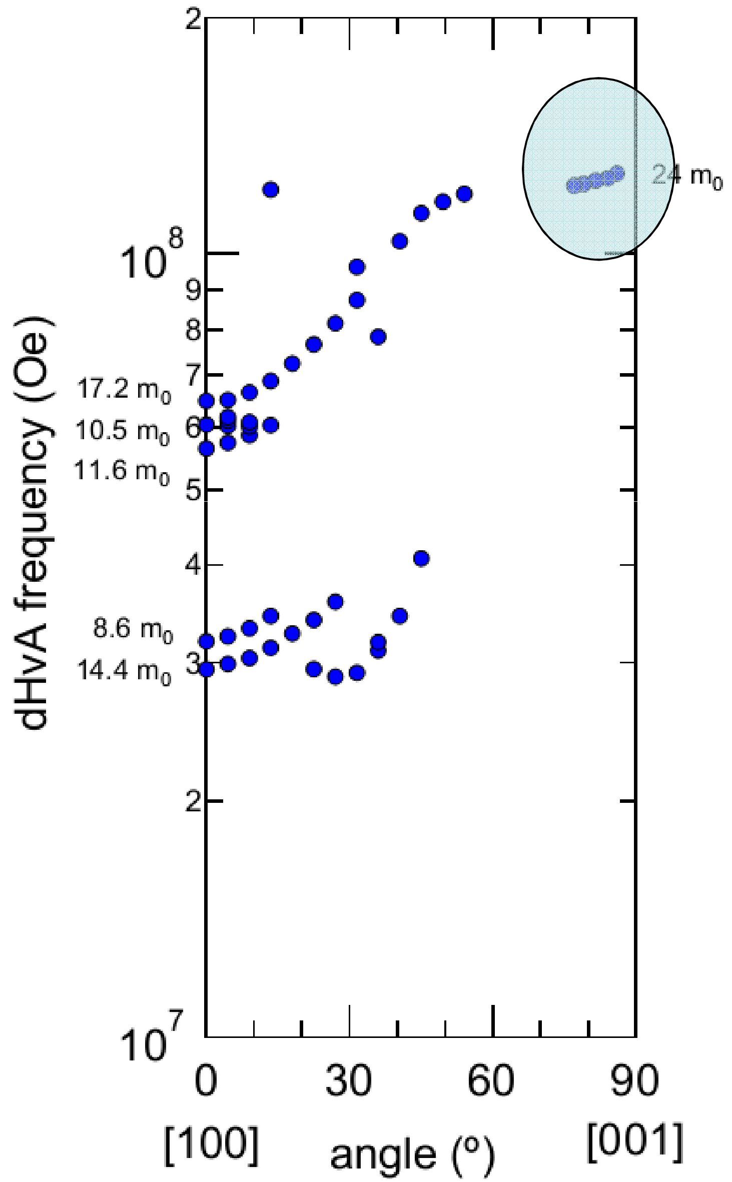
- Anisotropic hybridization of the *4f* states with the conduction bands, caused by the highly anisotropic crystalline electric field ground state, leads to van Hove–type singularities in the quasiparticle DOS.

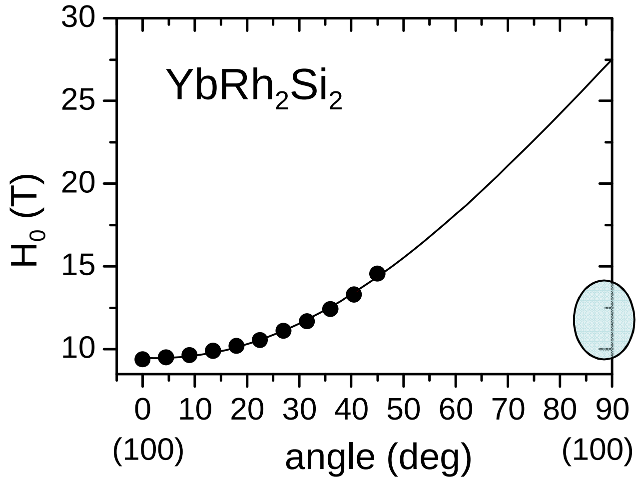
- Lifshitz transition of minority spin band



Angular dependence dHvA [100] to [001]

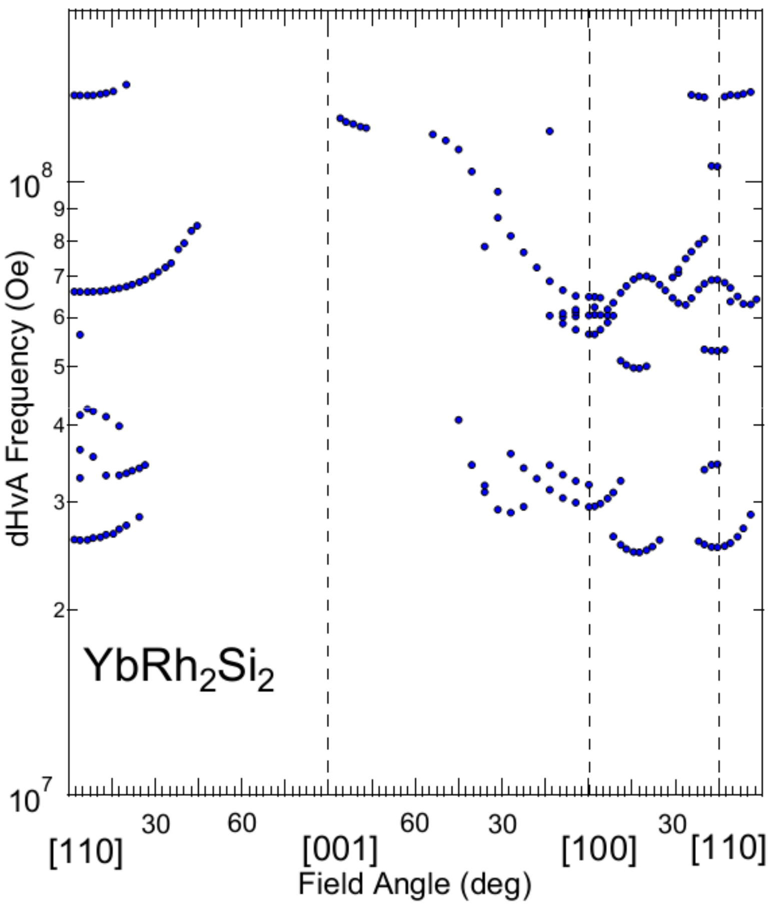




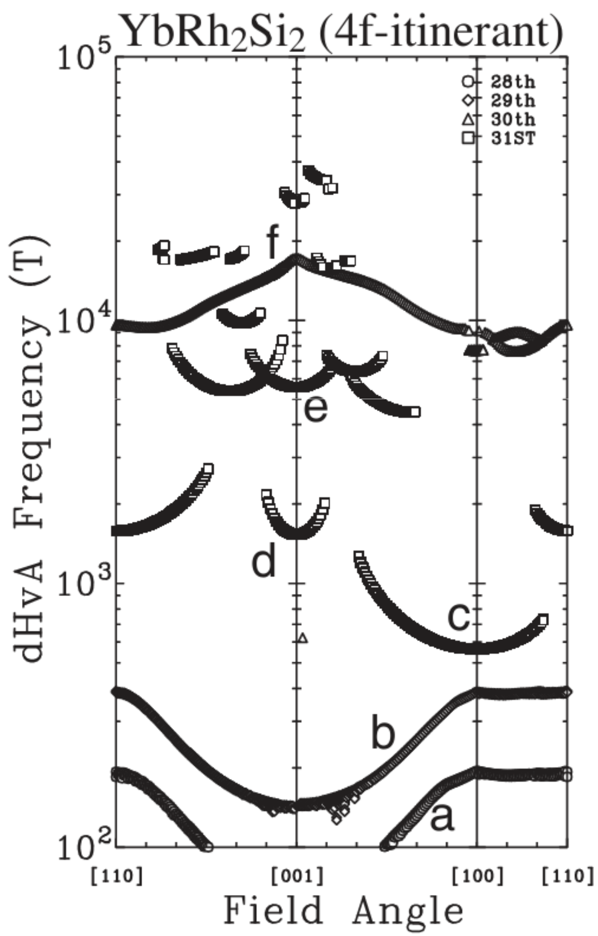


$H_0 \sim \cos\theta$

Experiment ($H > H_0$)



LDA bandstructure calculation (Harima)



about 75 % of the heavy mass is still missing !

summary

- topological changes of the Fermi surface as function of magnetic field observed in TEP and resistivity
- observed orbits from the “donut” hole and “jungle-gym” electron Fermi surfaces
- continuous change of dHvA frequencies through H_0
- Lifshitz-transition of spin-splitted bands :“hole” Fermi surface decreases, electron Fermi surface increase through H_0
- up to now Fermi surface determination only in the polarized state, H // [001] incomplete
- determination of Fermi surface in “heavy fermion” state below H_0 still missing

The End

of correlated electrons in Inac ?