Electronic Structure investigations in Yb-based heavy fermion materials

Sven Friedemann

UNIVERSITY OF CAMBRIDGE
Cavendish Laboratory

Heavy Fermions and Quantum Phase Transitions
Beijing 2012

Outline

Composite Quasiparticles

Ingredients

- local moments (f-electrons) periodic lattice
- conduction electrons (s,p,d)

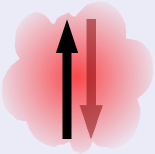
Composite Quasiparticles

Ingredients

- ↑ local moments (f-electrons) periodic lattice
- conduction electrons (s,p,d)

Kondo effect

- $H_K \propto -J\vec{S}\vec{s}$
- Heavy quasiparticles
- paramagnetic
- Landau Fermi Liquid



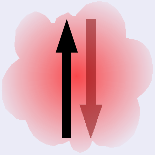
Composite Quasiparticles

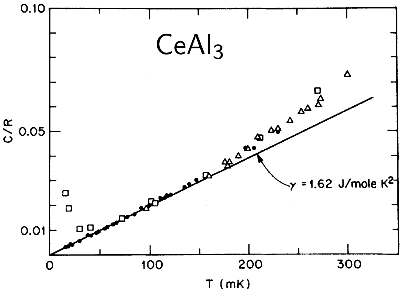
Ingredients

- local moments (f-electrons) periodic lattice
- conduction electrons (s,p,d)

Kondo effect

- $H_K \propto -J\vec{S}\vec{s}$
- Heavy quasiparticles
- paramagnetic
- Landau Fermi Liquid





Andres, K, et al., PRL **35** 1779 (1975).

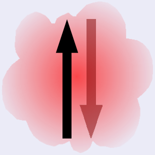
Composite Quasiparticles

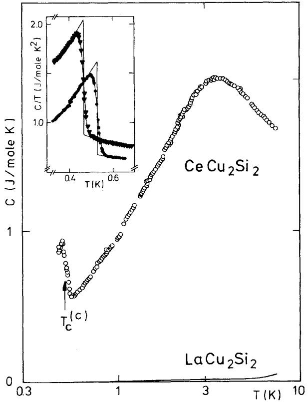
Ingredients

- local moments (f-electrons) periodic lattice
- conduction electrons (s,p,d)

Kondo effect

- $H_K \propto -J\vec{S}\vec{s}$
- Heavy quasiparticles
- paramagnetic
- Landau Fermi Liquid





Steglich, F et al., PRL **43** 1892 (1979).

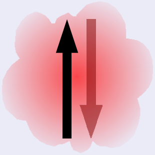
Composite Quasiparticles

Ingredients

- local moments (f-electrons) periodic lattice
- conduction electrons (s,p,d)

Kondo effect

- $H_K \propto -J\vec{S}\vec{s}$
- Heavy quasiparticles
- paramagnetic
- Landau Fermi Liquid



UPt$_3$

Branch:FS orbit	F (MG) Expt.	F (MG) Calc.	m^*/m_e Expt.	m^*/m_e Calc.
		a axis (ΓK)		
α:$ML4$	5.4(3)	10.4	25(3)	2.2
β:$L4$	6.0(4)	5.2	⋯	1.0
γ:$\Gamma1$	7.3(3)	8.2	40(7)	2.0
δ:$A5$	14.0(3)	9.1	50(8)	1.9
ϵ:$\Gamma2$	21.0(3)	24.0	60(8)	4.6
ω:$\Gamma3$	58.5(5)	52.8	90(15)	5.3

Taillefer, L et al., PRL **60** 1570 (1988).

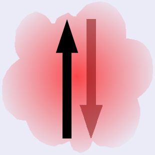
Composite Quasiparticles

Ingredients

- local moments (f-electrons) periodic lattice
- conduction electrons (s,p,d)

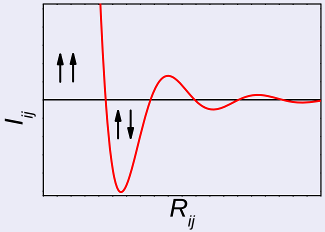
Kondo effect

- $H_\text{K} \propto -J\vec{S}\vec{s}$
- Heavy quasiparticles
- paramagnetic
- Landau Fermi Liquid

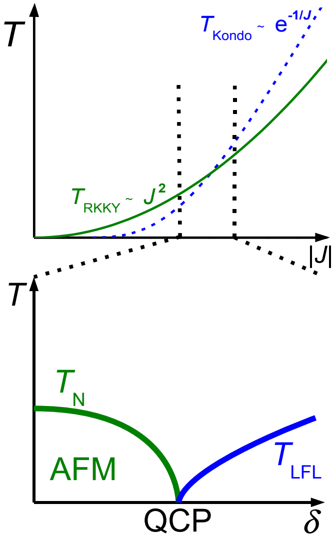


RKKY Interaction

- $H_\text{RKKY} \propto -I_{ij}\vec{S}_i\vec{S}_j$
- magnetically ordered



Quantum Critical Point



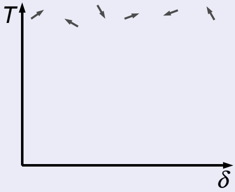
Doniach, Physica B+C **91**, 231-234 (1977)

Exchange interaction J between conduction and f-electrons

- weak J: RKKY dominates: **AFM** ground state
- crit. J_c: continuous phase transition at $T = 0$: **QCP**
- strong J: Kondo effect dominates: paramagnetic **Heavy Fermi Liquid**

Quantum Critical Point

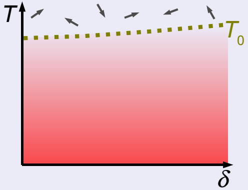
Spin-Density-Wave



Hertz, Millis, Moriya

Quantum Critical Point

Spin-Density-Wave

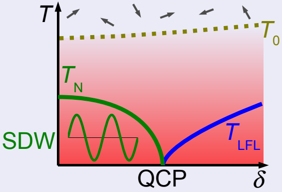


Hertz, Millis, Moriya

Quantum Critical Point

Spin-Density-Wave

Quasiparticles stay intact

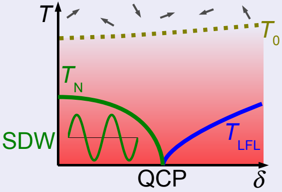


Hertz, Millis, Moriya

Quantum Critical Point

Spin-Density-Wave

Quasiparticles stay intact



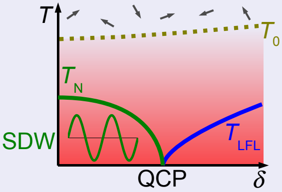
- no dynamical E/T-scaling

Hertz, Millis, Moriya

Quantum Critical Point

Spin-Density-Wave

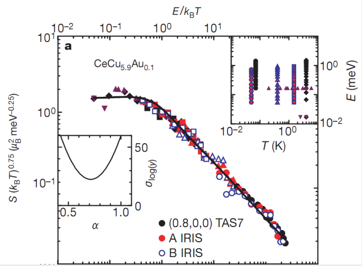
Quasiparticles stay intact



- no dynamical E/T-scaling

Hertz, Millis, Moriya

$CeCu_{5.9}Au_{0.1}$



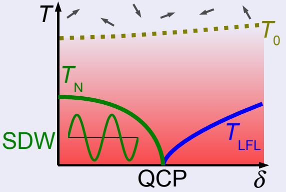
- E/T-scaling
- incompatible with SDW

Schröder et al., Nature **407** 351 (2000)

Quantum Critical Point

Spin-Density-Wave

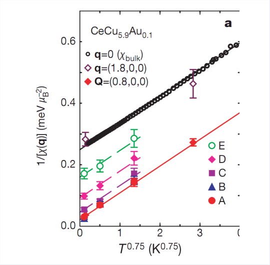
Quasiparticles stay intact



- no dynamical E/T-scaling

Hertz, Millis, Moriya

$CeCu_{5.9}Au_{0.1}$



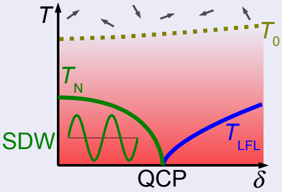
- E/T-scaling
- incompatible with SDW
- no q-dependence
- local effect

Schröder et al., Nature **407** 351 (2000)

Quantum Critical Point

Spin-Density-Wave

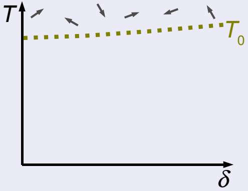
Quasiparticles stay intact



- no dynamical E/T-scaling

Hertz, Millis, Moriya

Kondo breakdown

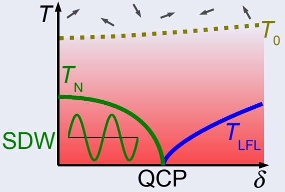


Coleman, Pépin, Senthil, Si, Vojta, Kirchner

Quantum Critical Point

Spin-Density-Wave

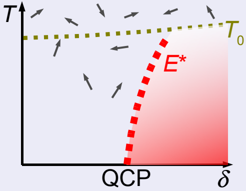
Quasiparticles stay intact



- no dynamical E/T-scaling

Kondo breakdown

Mott transition of $4f$ electrons



- dynamical E/T-scaling

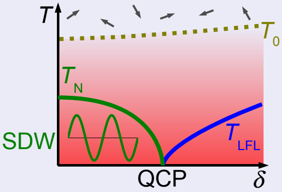
Hertz, Millis, Moriya

Coleman, Pépin, Senthil, Si, Vojta, Kirchner

Quantum Critical Point

Spin-Density-Wave

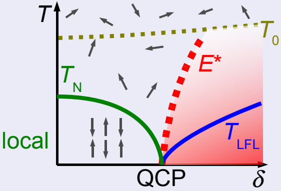
Quasiparticles stay intact



- no dynamical E/T-scaling

Kondo breakdown

Mott transition of $4f$ electrons



- dynamical E/T-scaling

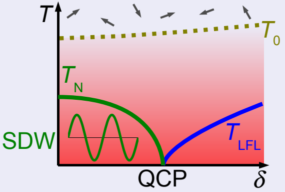
Hertz, Millis, Moriya

Coleman, Pépin, Senthil, Si, Vojta, Kirchner

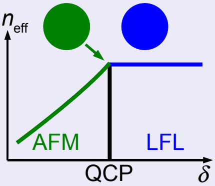
Quantum Critical Point

Spin-Density-Wave

Quasiparticles stay intact



- no dynamical E/T-scaling

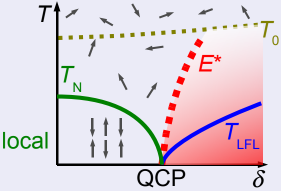


- Fermi Surface: continuous

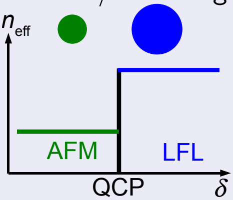
Hertz, Millis, Moriya

Kondo breakdown

Mott transition of $4f$ electrons



- dynamical E/T-scaling



- reconstruction of Fermi surface

Coleman, Pépin, Senthil, Si, Vojta, Kirchner

Fermi Surface and dynamical scaling

Fermi Surface

- **P**hoto**E**lectron **S**pectroscopy
- **d**e **H**aas-**v**an **A**lphen effect
- Hall effect

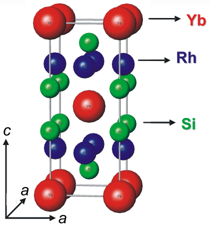
Dynamical Scaling

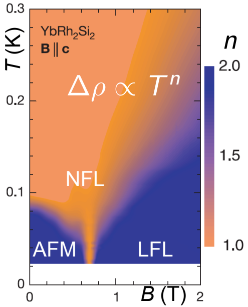
- **I**nelastic **N**eutron **S**cattering
- optical spectroscopy
- PES
- ...

$YbRh_2Si_2$

$YbRh_2Si_2$

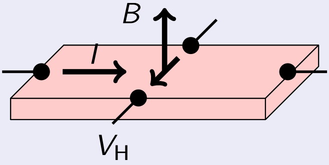
structure	tetragonal
CEF	effective $S = 1/2$ ground state
	$T_0 \approx 25\,\mathrm{K}$
AFM	$T_N = 70\,\mathrm{mK}$
QCP	field induced at
	$B_{c2} = 60\,\mathrm{mT}$ for $B \perp c$
	$B_{c1} = 0.66\,\mathrm{T}$ for $B \parallel c$
NFL	non-Fermi liquid above the QCP
	e.g. $\rho \propto T$





Custers et al., Nature **424**, 524 (2003).

Hall Effect at the QCP

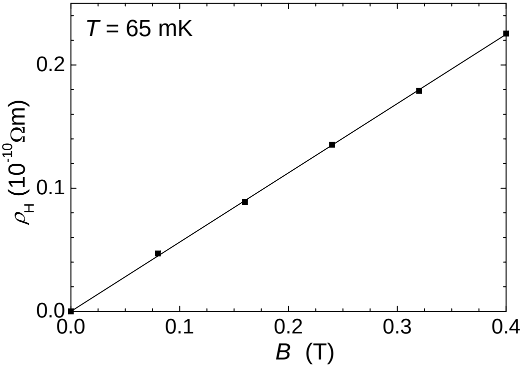


Hall coefficient

$$R_H = \frac{\rho_H}{B} = \frac{V_H d}{I}$$

carrier density

$$R_H \propto \frac{1}{n_{eff}}$$

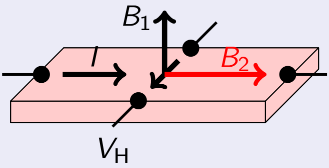


Hall Effect at the QCP

Crossed-Field Experiment

B_1 Hall Field

B_2 Tuning Field

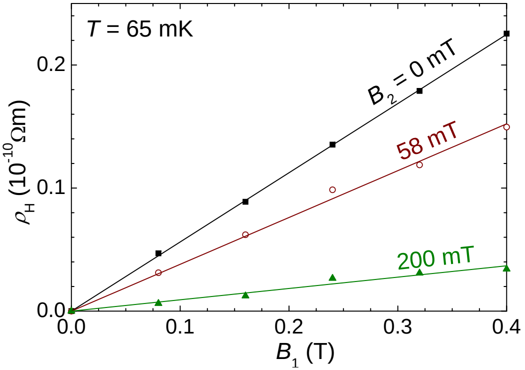


Hall coefficient

$$R_H = \frac{\rho_H}{B_1} = \frac{V_H d}{I}$$

carrier density

$$R_H(B_2) \propto \frac{1}{n_{eff}(B_2)}$$

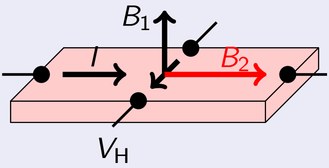


Hall Effect at the QCP

Crossed-Field Experiment

B_1 Hall Field (Solenoid)

B_2 Tuning Field (Split Pair)

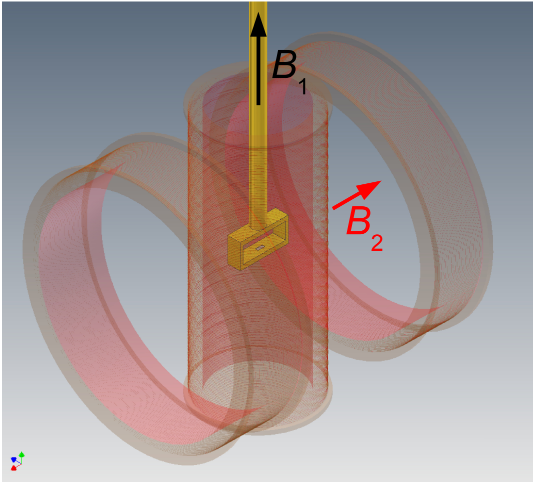


Hall coefficient

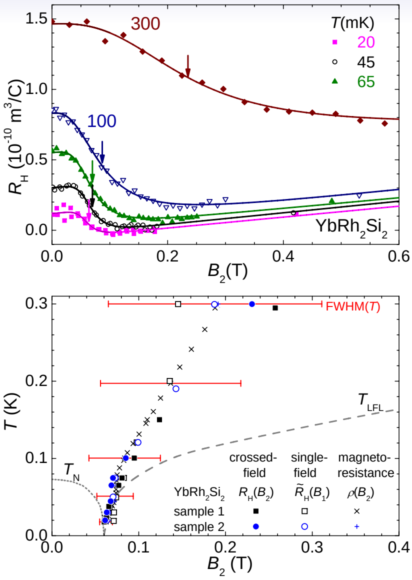
$$R_H = \frac{\rho_H}{B_1} = \frac{V_H d}{I}$$

carrier density

$$R_H(B_2) \propto \frac{1}{n_{eff}(B_2)}$$



Hall effect in $YbRh_2Si_2$

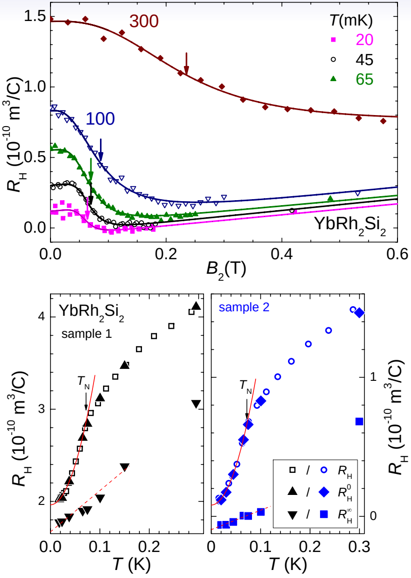


SF *et al.*, 2010. PNAS 107: 14547

Critical Crossover in $R_H(B_2)$

- converges to QCP

Hall effect in $YbRh_2Si_2$

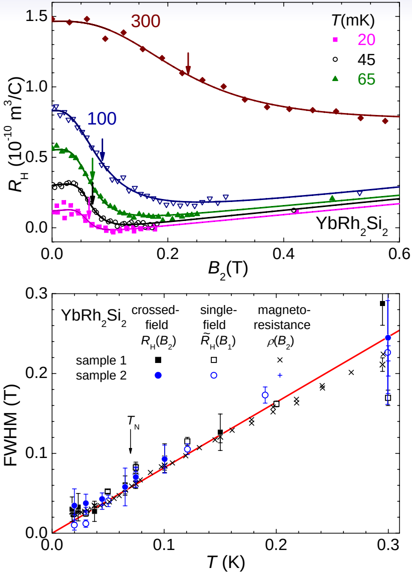


SF *et al.*, 2010. PNAS 107: 14547

Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences

Hall effect in $YbRh_2Si_2$

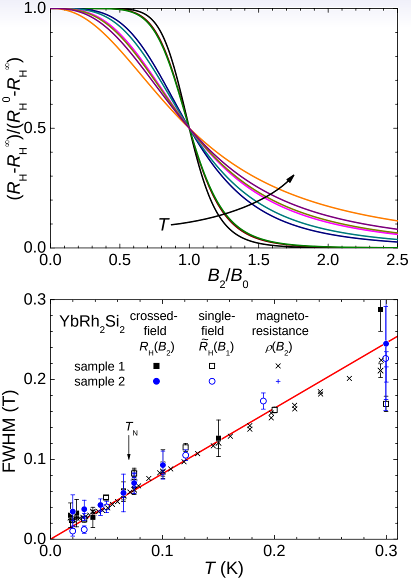


SF *et al.*, 2010. PNAS 107: 14547

Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences
- FWHM $\to 0$ at $T = 0$

Hall effect in $YbRh_2Si_2$

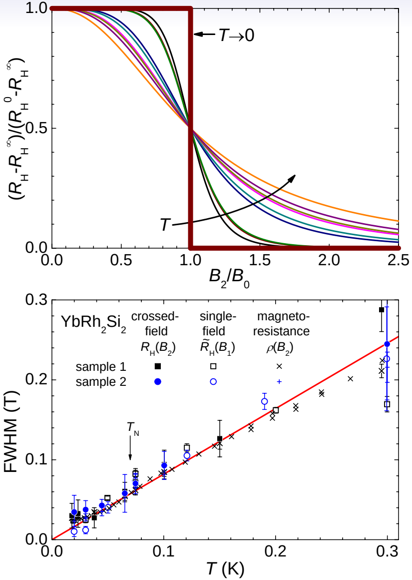


SF *et al.*, 2010. PNAS 107: 14547

Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences
- FWHM $\rightarrow 0$ at $T = 0$

Hall effect in $YbRh_2Si_2$

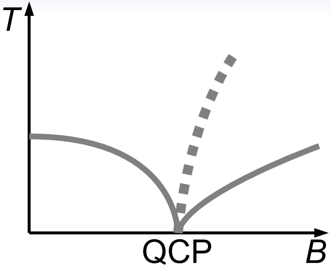


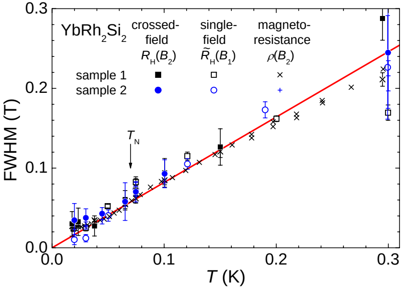
SF *et al.*, 2010. PNAS 107: 14547

Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences
- FWHM $\to 0$ at $T = 0$
- Jump in R_H for $T \to 0$
- Fermi surface reconstruction

Hall effect in $YbRh_2Si_2$



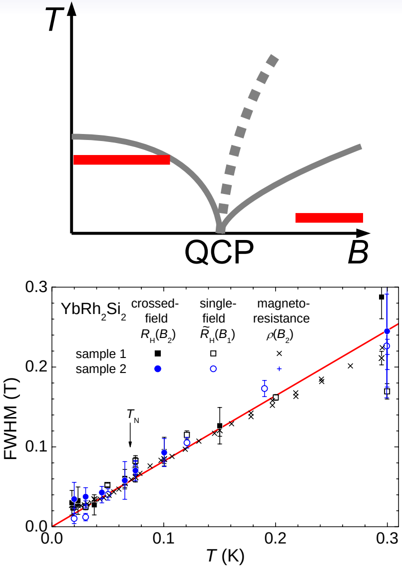


SF *et al.*, 2010. PNAS 107: 14547

Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences
- FWHM $\to 0$ at $T = 0$
- Jump in R_H for $T \to 0$
- Fermi surface reconstruction

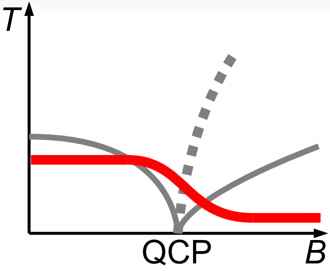
Hall effect in $YbRh_2Si_2$

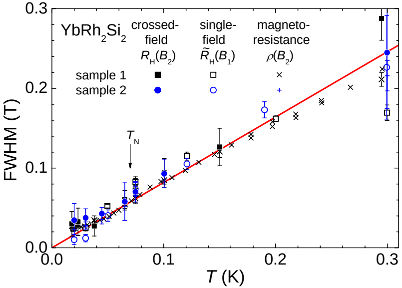


SF *et al.*, 2010. PNAS 107: 14547

Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences
- FWHM $\rightarrow 0$ at $T = 0$
- Jump in R_H for $T \rightarrow 0$
- Fermi surface reconstruction



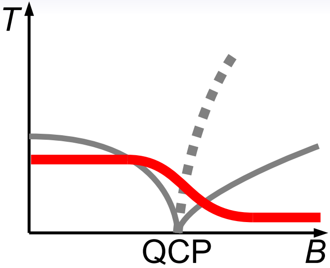


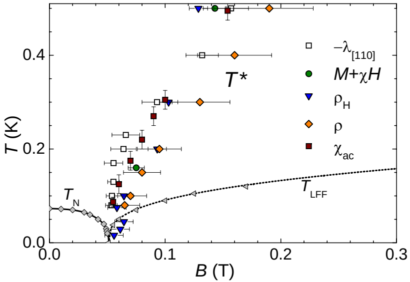
Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences
- FWHM $\rightarrow 0$ at $T = 0$
- Jump in R_H for $T \rightarrow 0$
- Fermi surface reconstruction
- dynamical E/T-scaling

SF *et al.*, 2010. PNAS 107: 14547

Hall effect in $YbRh_2Si_2$



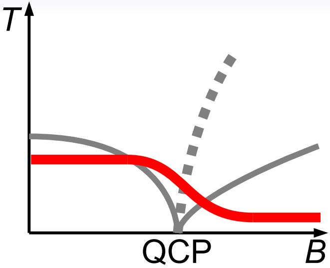


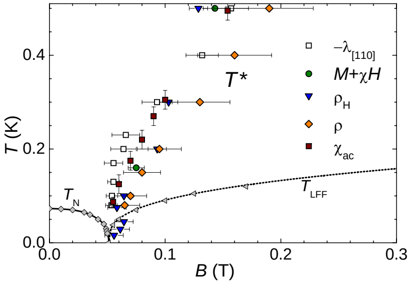
Gegenwart *et al.*, Science **315** 969 (2007).

Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences
- FWHM $\rightarrow 0$ at $T = 0$
- Jump in R_H for $T \rightarrow 0$
- Fermi surface reconstruction
- dynamical E/T-scaling
- energy scale $T^\star$
- incompatible with SDW
- Kondo breakdown

Hall effect in $YbRh_2Si_2$



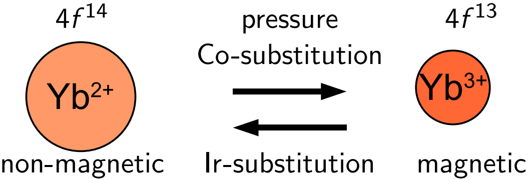


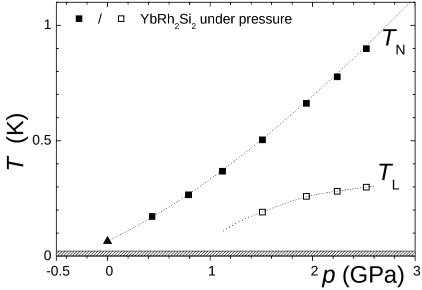
Gegenwart *et al.*, Science **315** 969 (2007).

Critical Crossover in $R_H(B_2)$

- converges to QCP
- finite height
- robust against sample dependences
- FWHM $\rightarrow 0$ at $T = 0$
- Jump in R_H for $T \rightarrow 0$
- Fermi surface reconstruction
- dynamical E/T-scaling
- energy scale $T^\star$
- incompatible with SDW
- Kondo breakdown
- coincidence of all energy scales

Pressure and Substitution Effects

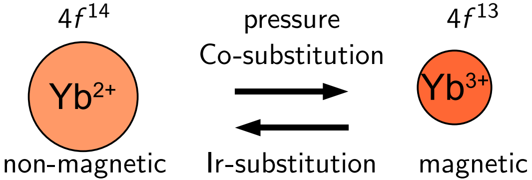


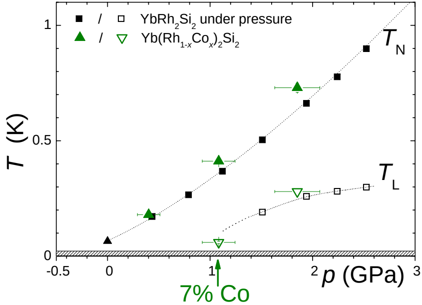


Mederle et al., JPCM **14**, 10731 (2002)
M. Macovei et al., JPCM **20**, 505205 (2008)

$Yb(Rh_{1-x}M_x)_2Si_2$

Pressure and Substitution Effects



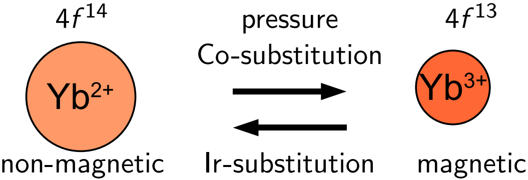


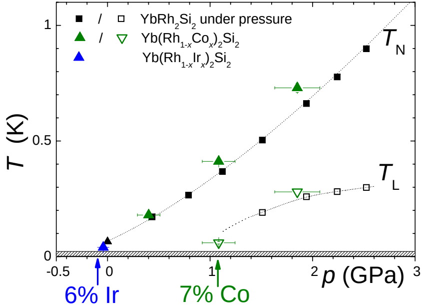
Mederle et al., JPCM **14**, 10731 (2002)
M. Macovei et al., JPCM **20**, 505205 (2008)

$Yb(Rh_{1-x}M_x)_2Si_2$

7 % Co volume decrease
stabilizes magnetism

Pressure and Substitution Effects





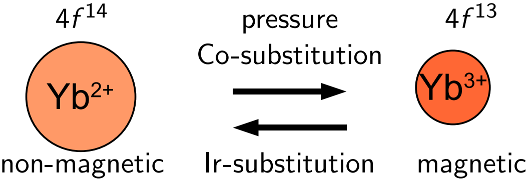
Mederle et al., JPCM **14**, 10731 (2002)
M. Macovei et al., JPCM **20**, 505205 (2008)

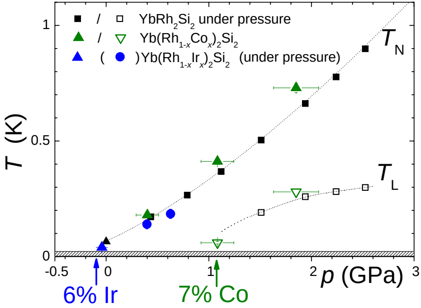
$Yb(Rh_{1-x}M_x)_2Si_2$

7 % Co volume decrease stabilizes magnetism

6 % Ir volume increase suppresses magnetism

Pressure and Substitution Effects





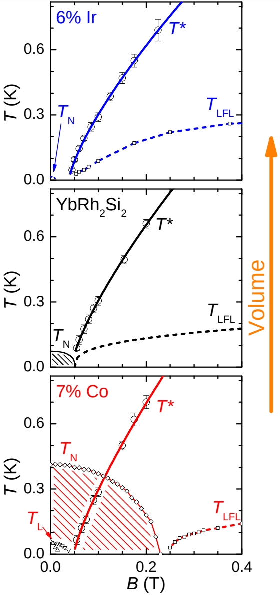
Mederle et al., JPCM **14**, 10731 (2002)
M. Macovei et al., JPCM **20**, 505205 (2008)

$Yb(Rh_{1-x}M_x)_2Si_2$

7 % Co volume decrease stabilizes magnetism

6 % Ir volume increase suppresses magnetism

Energy Scales under Pressure

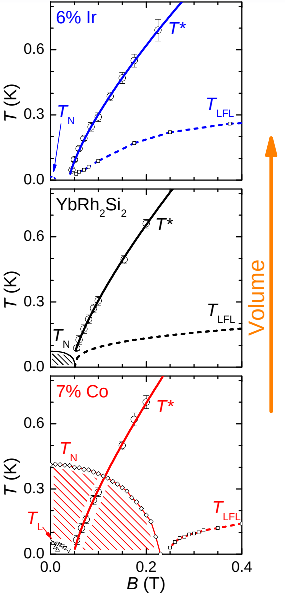


- AFM stabilized under chemical pressure
- Kondo breakdown not affected

↷ coincidence lifted

SF *et al.*, Nature Phys. **5**, 465-469 (2009)

Energy Scales under Pressure



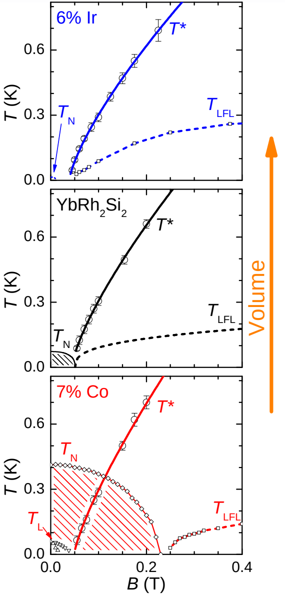
- AFM stabilized under chemical pressure
- Kondo breakdown not affected

↷ coincidence lifted

6 % Ir detachment of AFM from Kondo breakdown

SF *et al.*, Nature Phys. **5**, 465-469 (2009)

Energy Scales under Pressure



- AFM stabilized under chemical pressure
- Kondo breakdown not affected

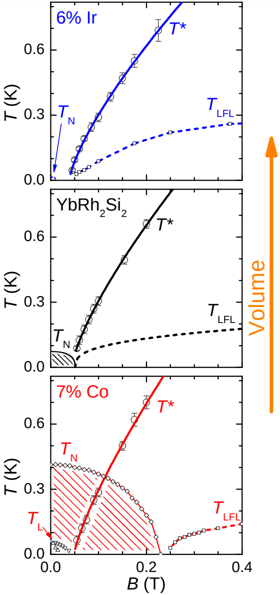
↷ coincidence lifted

6 % Ir detachment of AFM from Kondo breakdown

6 % Ir metallic spin liquid?
also in Ge-substituted $YbRh_2Si_2$
J. Custers *et al.*, PRL, **104** 186402 (2010)

SF *et al.*, Nature Phys. **5**, 465-469 (2009)

Energy Scales under Pressure



- AFM stabilized under chemical pressure
- Kondo breakdown not affected

↷ coincidence lifted

6 % Ir detachment of AFM from Kondo breakdown

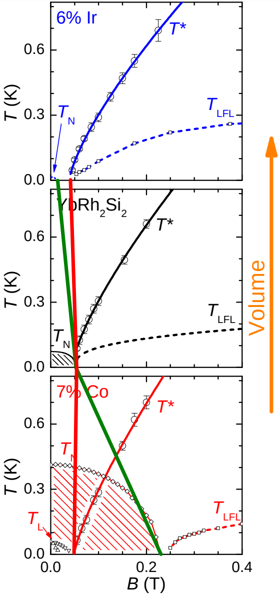
6 % Ir metallic spin liquid?
also in Ge-substituted $YbRh_2Si_2$
J. Custers *et al.*, PRL, **104** 186402 (2010)

7 % Co $T^\star(B)$ and $T_N(B)$ intersect confirmed under pressure
Y. Tokiwa *et al.*, JPSJ, **78** 123708 (2009)

7 % Co AFM within Kondo regime

SF *et al.*, Nature Phys. **5**, 465-469 (2009)

Energy Scales under Pressure



- AFM stabilized under chemical pressure
- Kondo breakdown not affected

↷ coincidence lifted

6 % Ir detachment of AFM from Kondo breakdown

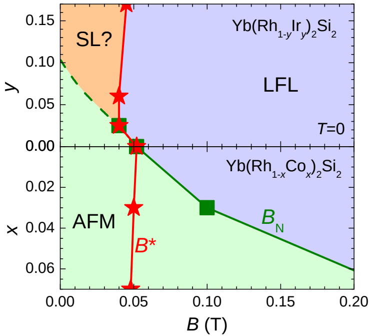
6 % Ir metallic spin liquid?
also in Ge-substituted $YbRh_2Si_2$
J. Custers *et al.*, PRL, **104** 186402 (2010)

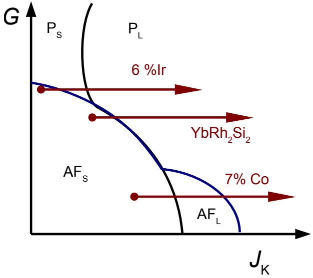
7 % Co $T^\star(B)$ and $T_N(B)$ intersect
confirmed under pressure
Y. Tokiwa *et al.*, JPSJ, **78** 123708 (2009)

7 % Co AFM within Kondo regime

SF *et al.*, Nature Phys. **5**, 465-469 (2009)

Global Phase Diagram





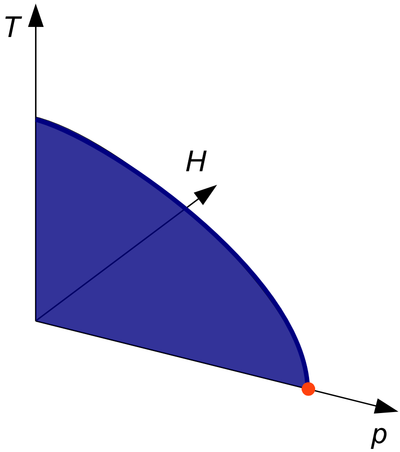
Q. Si, PSS B **247**, 476–484 (2010)

Detachment of Magnetism and Kondo Breakdown

- 7 % Co: AFM within Kondo regime
- 6 % Ir: Detachment of magnetic and electronic QCP ↷ SL?
- $YbRh_2Si_2$: accidental coincidence?

Outline

Ferromagnetic Quantum Criticality in Metals

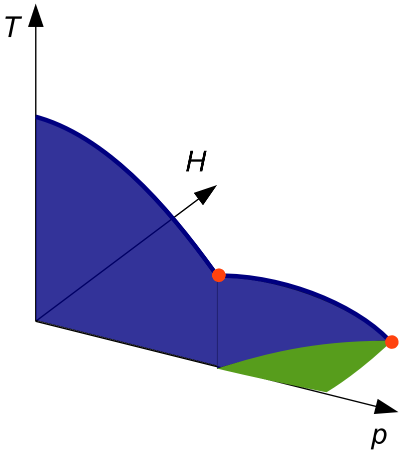


Theory

1. FM QCP in metals

   JA Hertz, PRB **14** 1165 (1976)

Ferromagnetic Quantum Criticality in Metals



Theory

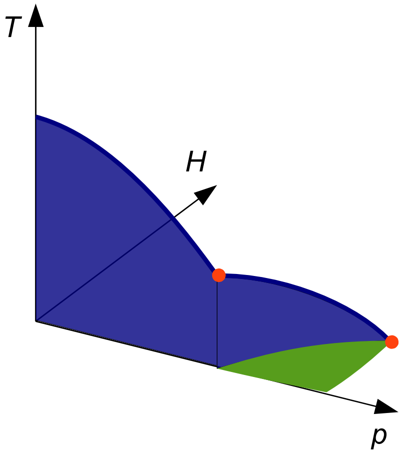
1. FM QCP in metals

   JA Hertz, PRB **14** 1165 (1976)

2. No FM QCP in clean metals with itinerant magnetism in $d \geq 2$

   D Belitz, et al., PRL **82** 4707 (1999)

Ferromagnetic Quantum Criticality in Metals



Theory

1. FM QCP in metals

   JA Hertz, PRB **14** 1165 (1976)

2. No FM QCP in clean metals with itinerant magnetism in $d \geq 2$

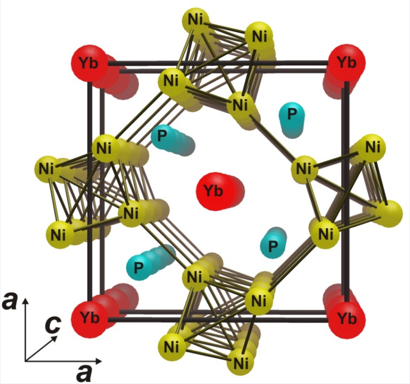
   D Belitz, et al., PRL **82** 4707 (1999)

3. No FM QCP in metal with uniform magnetisation (Ferro-, Ferri-, Canted Ferromagnets, and local moment FM)

   TR Kirkpatrick and D Belitz, arxiv:1203.3826 (2012)

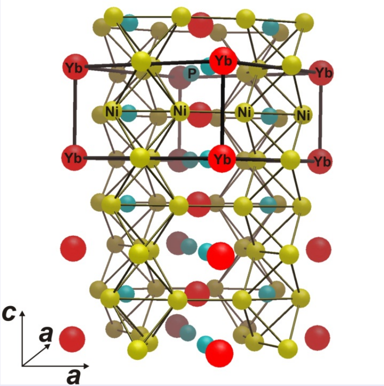
$YbNi_4P_2$

Projection along *c*



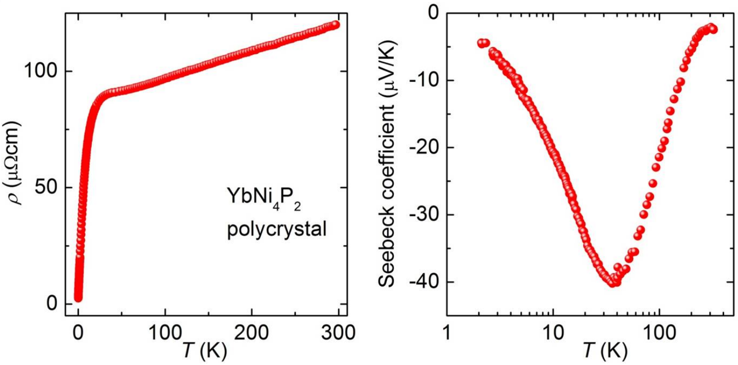
- $ZrFe_4Si_2$ structure type $P4_2/mnm$

Projection along (110)



- isolated Yb chains along *c*-direction

$YbNi_4P_2$ – Kondo lattice



C Krellner et al., New Journal of Physics 13, 103014 (2011)

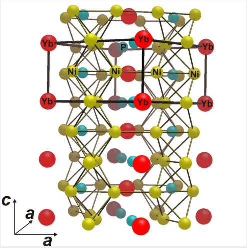
- Kondo coherence in resistivity below 30 K
- Large Thermopower peak around 30 K

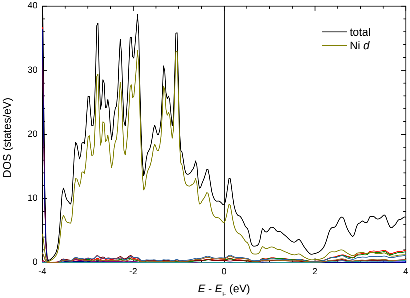
→ Kondo lattice with strong correlations

- Kondo temperature $T_K \approx 8\,K$ (from entropy)

$YbNi_4P_2$ – LDA calculations

crystal structure
1D Yb chains

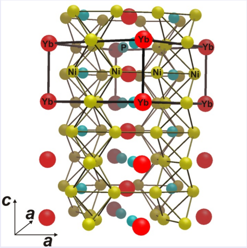


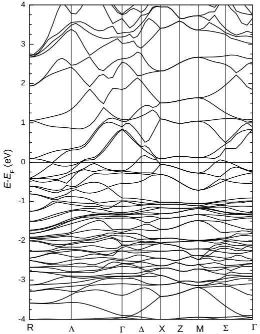


- LDA calculations with spin-orbit corrections
- frozen 4*f* core – uncorrelated band structure
- strong contribution from Ni-3*d* states
- yet no magnetism arising from Ni

$YbNi_4P_2$ – LDA calculations

crystal structure
1D Yb chains

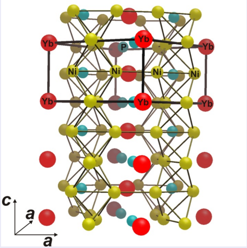




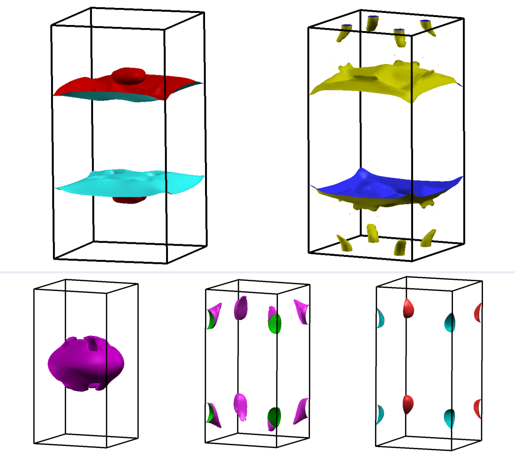
- LDA calculations with spin-orbit corrections
- frozen 4*f* core – uncorrelated band structure
- strong contribution from Ni-3*d* states
- yet no magnetism arising from Ni

$YbNi_4P_2$ – quasi 1D electronic structure

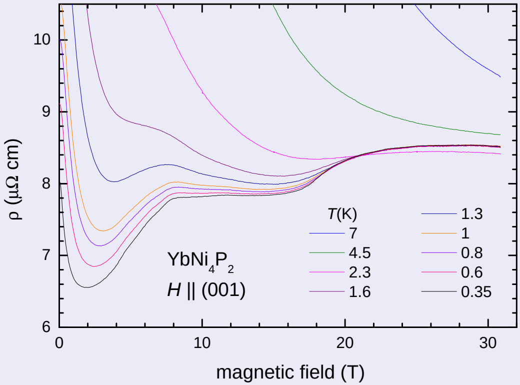
crystal structure
1D Yb chains



quasi 1D Fermi surfaces

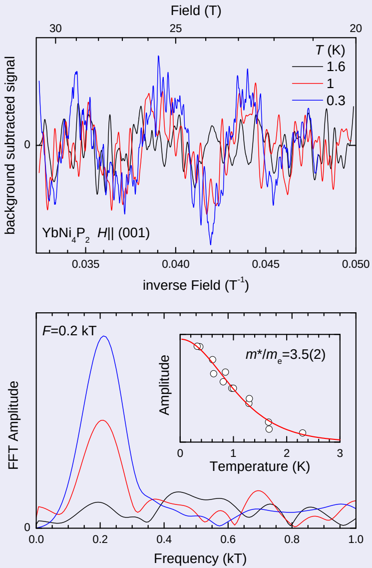


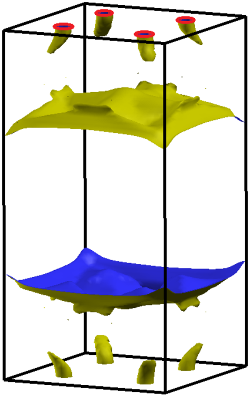
$YbNi_4P_2$ – Magnetoresistance



- pronounced plateaus
- steps at 6 T and 18 T
- possibly Lifshitz transitions

$YbNi_4P_2$ – Shubnikov de Haas Oscillations

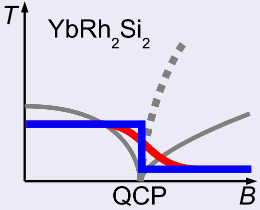




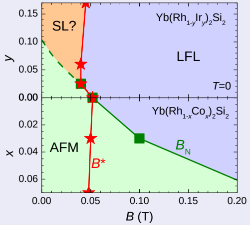
	exp.	calc.
$F(T)$	200	60
$m(m_e)$	3.5	0.25

Summary

Quasiparticle Breakup

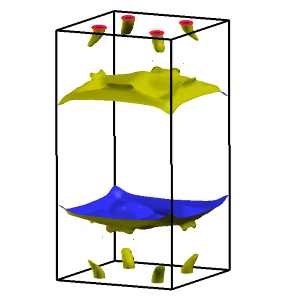


Novel Spin-Liquid Phase



1D FM QCP

- $YbNi_4P_2$
- quasi 1D Fermi surface
- dimensionality key to FM QCP



Acknowledgement

T Westerkamp
M Brando
C Krellner
S Wirth
S Kirchner
S Paschen
P Gegenwart
Q Si
F Steglich

S Goh
L Klintbert
T Murphy
C Geibel
C Pfleiderer
F M Grosche
H Rosner
G Zwicknagl
G Lonzarich

UNIVERSITY OF CAMBRIDGE
Cavendish Laboratory

NATIONAL HIGH MAGNETIC FIELD LABORATORY
FSU · UF · LANL

easyLab
science under pressure

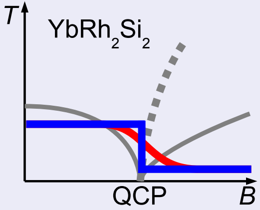
PEOPLE

Unterstützt von / Supported by
Alexander von Humboldt
Stiftung / Foundation

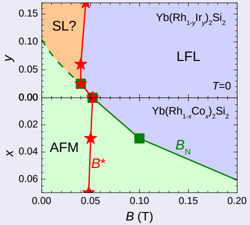
Thank you for your attention

Summary

Quasiparticle Breakup



Novel Spin-Liquid Phase



1D FM QCP

- $YbNi_4P_2$
- quasi 1D Fermi surface
- dimensionality key to FM QCP