



## Field Induced Quantum Critical Point in YbAgGe

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## Ames Laboratory



Mid-sized DOE Laboratory with ~ 400 employees  
Organized in 1947 as a part of Manhattan Project

**Now:**

Applied Mathematics and Computational Sciences  
Chemical and Biological Sciences  
**Condensed Matter Physics**  
Environmental and Protection Sciences  
Granular and Multiphase Systems  
Materials Chemistry  
Materials and Engineering Physics  
Non-Destructive Evaluation

**Also:**  
Renewable Resources Consortium  
Materials Preparation Center

**Iowa State University**  
**Large Land Grant University**

~25,000 Students

**Known for Ag. (not Silver), Vet.,  
and, in our circles, Physics and  
Chemistry associated with  
Ames Lab.**



In collaboration with:

Emilia Morosan, Yuri Janssen, Yurij Mozhariovskyj, Stephanie Law (ISU);

Björn Fåk (CEA/Grenoble), Desmond McMorrow (Univ. College /London);

Philipp Niklowitz, Jacques Flouquet (CEA/Grenoble)

Discussions with:

Jörg Schmalian, Maxim Dzero (ISU) **and I hope many of you here at the workshop.**

Also thanks to:

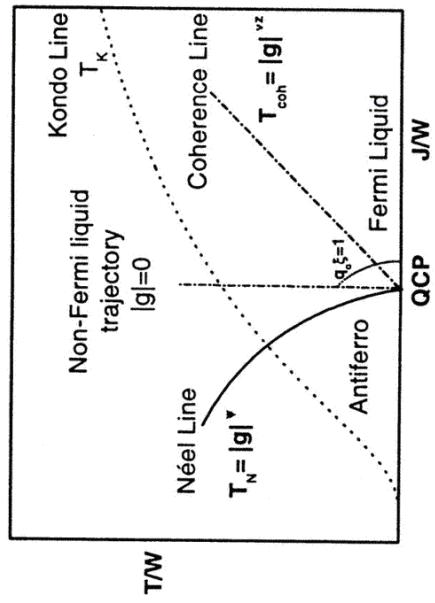
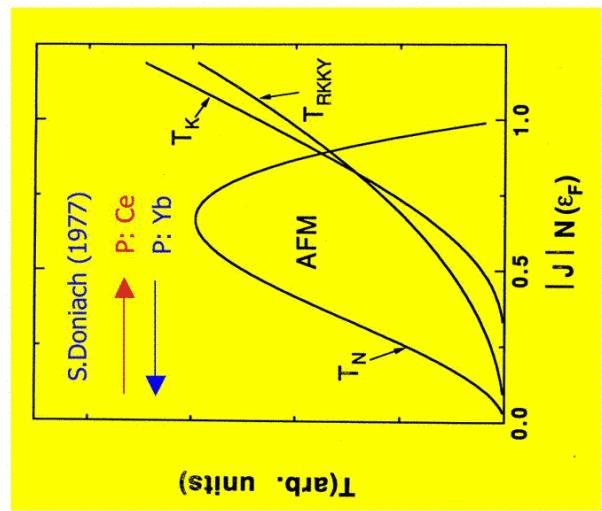


and A. Paul Ness, Marc D. McGinn (ISU)

## Outline and salient papers

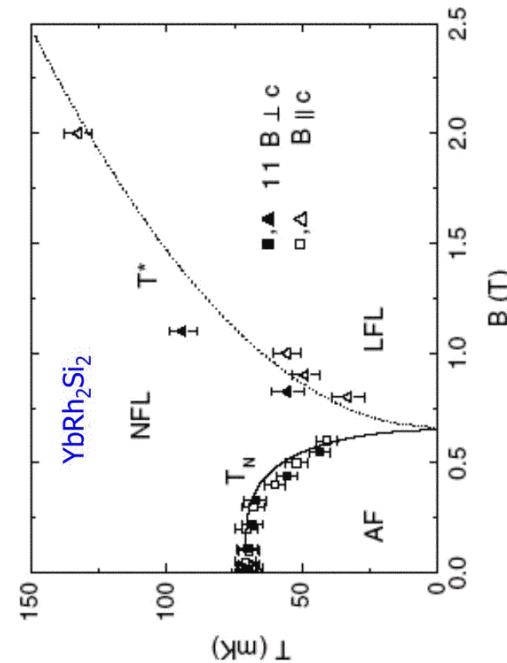
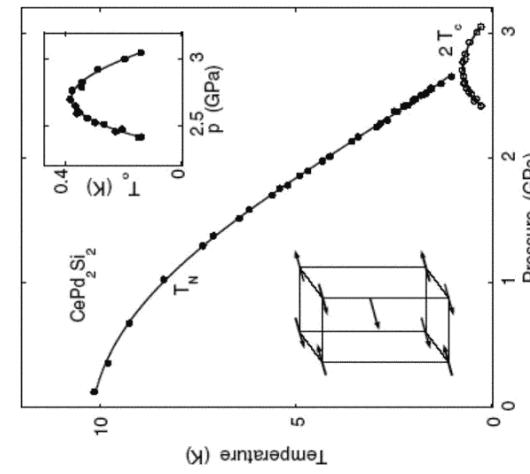
- Thermodynamic and Transport Properties of RAgGe ( $R = \text{Tb} - \text{Lu}$ ) single crystals, E. Morosan et al., *JMMM* 277 (2004) 298. (*cond-mat/0309327*)
- Angular-dependent planar metamagnetism in the hexagonal compounds TbPtIn and TmAgGe, E. Morosan et al., *PRB* 71 (2005) xxxx. (*cond-mat/0408121*)
- Magnetic field induced non-Fermi-liquid behavior in YbAgGe single crystals, S. L. Bud'ko et al., *PRB* 69 (2004) 014415. (*cond-mat/0308517*)
- Hall effect in single crystal heavy Fermion YbAgGe, S. L. Bud'ko et al., *PRB* 71 (2005) xxxx. (*cond-mat/0406435*)
- Inelastic neutron scattering study of single crystal heavy fermion YbAgGe, B. Fak et al., *J. Phys. Cond. Matter* 17 (2005) 301
- Low temperature transport properties of YbAgGe near a quantum critical point, P. Niklowitz et al., unpublished.

## Doniach's phase diagram and QCP



M. Continentino (1989) and many others before and mostly after...

## QCP – experimental examples ( $P, x, H$ )

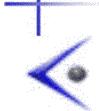


Gegenwart et al., PRL 89 (2002)  
056402.

Grosche et al., JPCM 13  
(2001) 2845  
(Similar results for CeIn<sub>3</sub>)

pressure

applied field



## QCP – experimental examples

Problems: **substitution**  $\Rightarrow$  disorder  
**pressure:** discontinuity, difficult

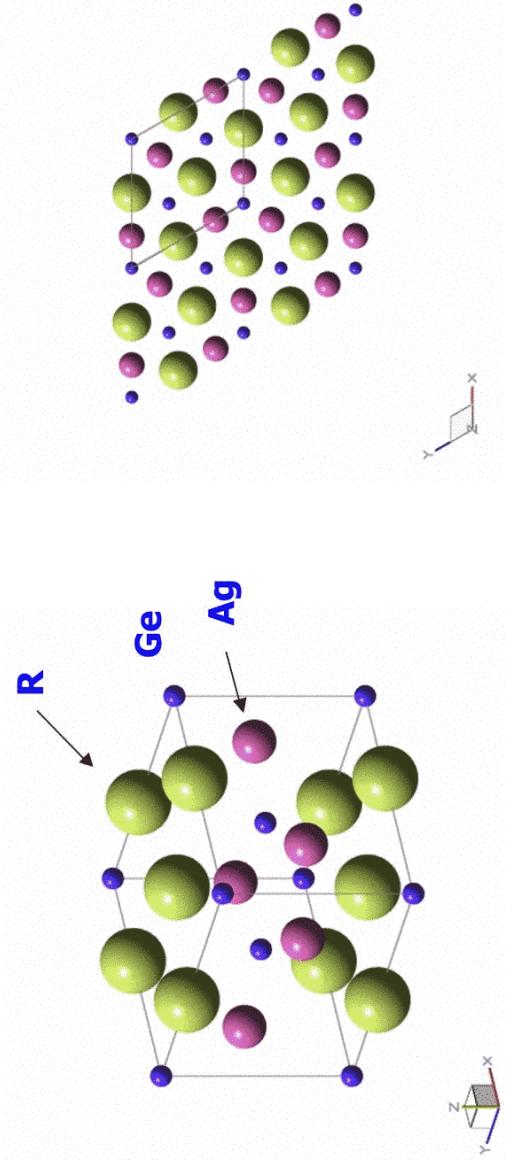
**Magnetic field:** continuous, more measurements are accessible.

**Are P, x, H "equivalent"? Is there any single, "universal" picture?**

**More, "clean" examples needed!**



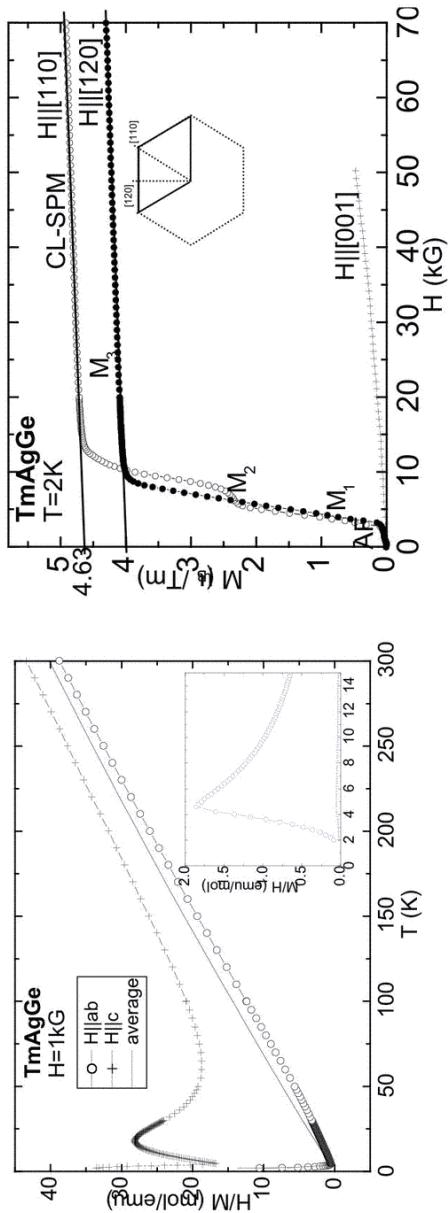
## R<sub>Ag</sub>Ge - structure



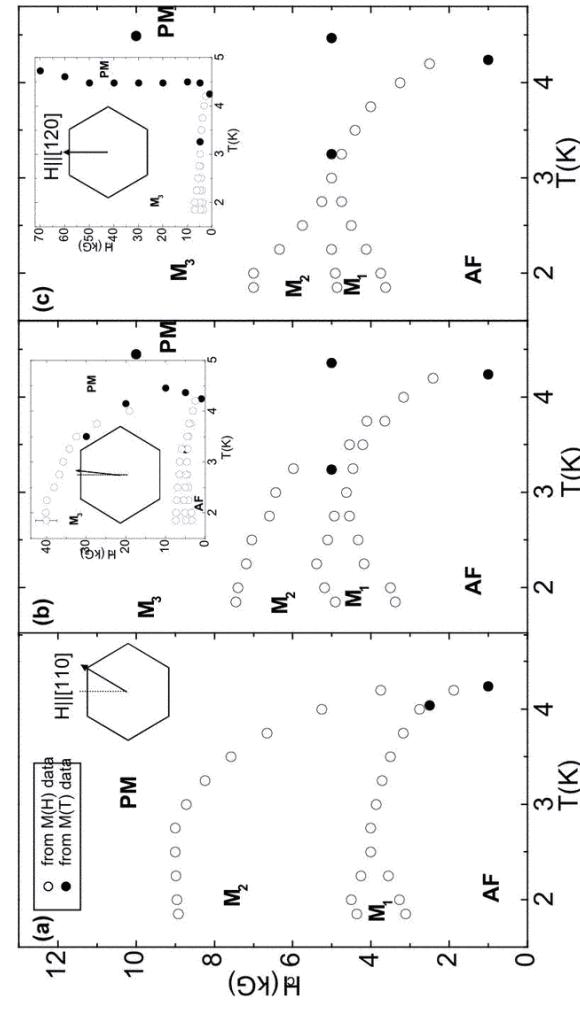
Hexagonal P-62m, R in orthorhombic point symmetry  
For RAgGe overview see E.Morosan et al. JMM 277 (2004) 298.  
Lots of curious stuff: metamagnetism, "unconventional" resistivity, etc. for R = Tb-Tm.

- “Thermodynamic and transport properties of RAgGe ( $R = Tb - Lu$ ) single crystals”, E. Morosan *et al.*, J. Magn. Magn. Mater. 277 (2004) 298 and cond-mat/0309327
- “Angular dependent planar metamagnetism in the hexagonal compounds TbPtIn and TmAgGe”, E. Morosan *et al.*, Phys. Rev. B (in press) and cond-mat/0408121.

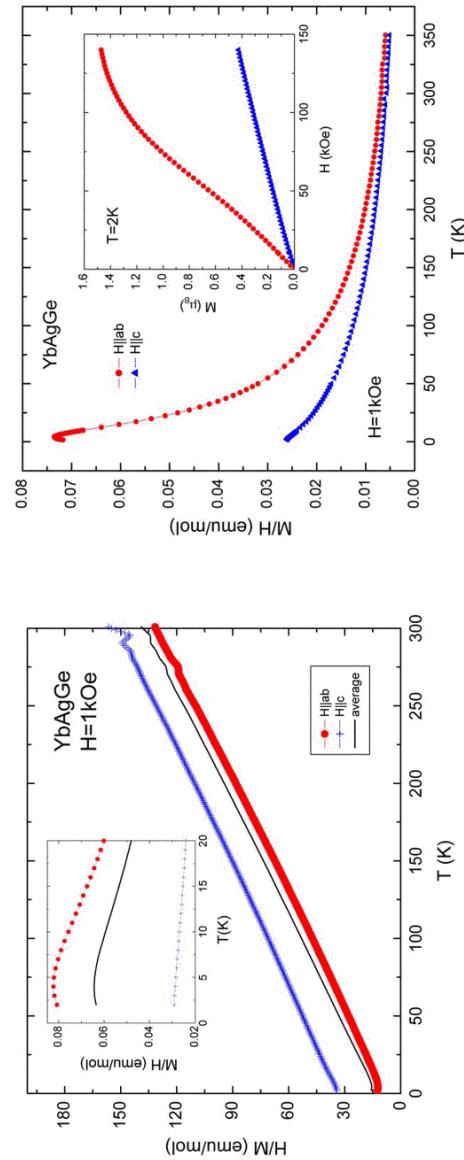
### TmAgGe:



### TmAgGe:

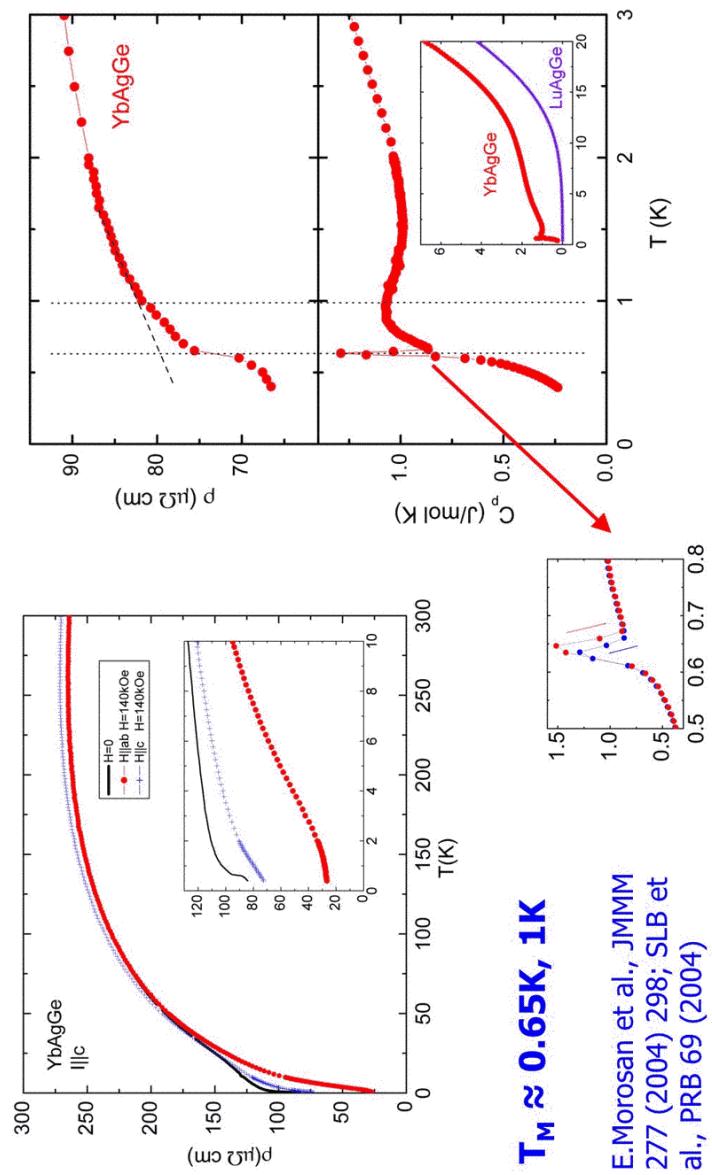


## YbAgGe – basic properties

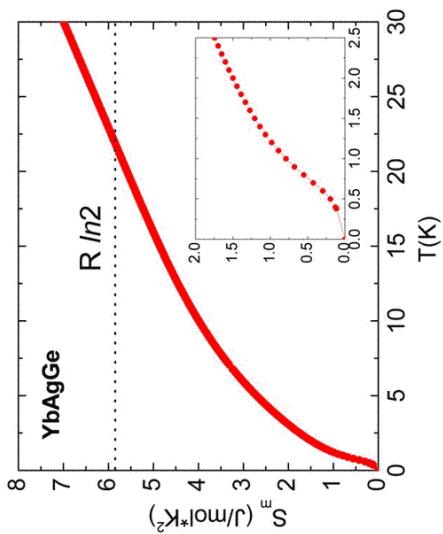
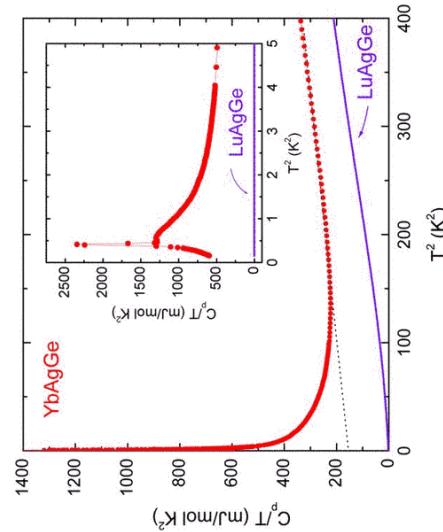


E.Morosan et al., Jmmm 277  
(2004) 298

## YbAgGe – basic properties



## YbAgGe – basic properties



$\gamma \approx 150 \text{ mJ/mol K}^2$  from 10K-20K range extrapolation. More realistic estimate:  $150 \text{ mJ/mol K}^2 \leq \gamma \leq 1 \text{ J/mol K}^2$

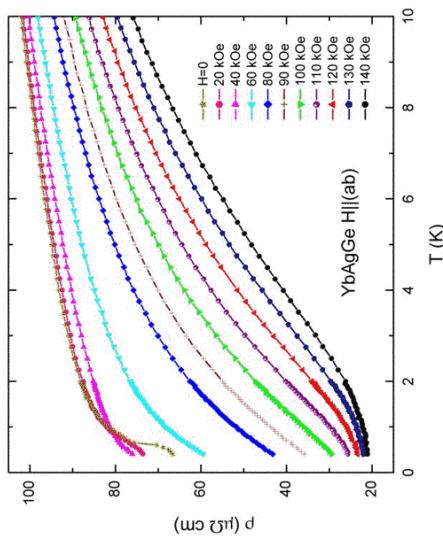
- (i) YbAgGe is new Yb-based HF (or close to being HF)
- (ii) LRO below 1K, probably small moment ordering  
⇒ good candidate for suppression of  $T_N$  to QCP

## YbAgGe – estimate of some parameters

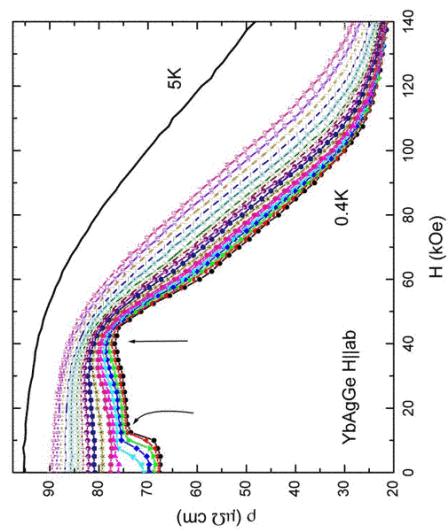
- ◆ **150 mJ/mol K<sup>2</sup> ≤ γ ≤ 1J/mol K<sup>2</sup>**
- ◆  $\Theta_{\text{ave}} \approx -30 \text{ K}$ ,  $\Theta/10 \leq T_K \leq \Theta \Rightarrow 3\text{K} \leq T_K \leq 30 \text{ K}$
- ◆  $T_K = W_N \pi^3 R / 6\gamma$   
 $W_N = 0.4107$  (Wilson number), R – gas constant ⇒ **15K ≤ T<sub>K</sub> ≤ 120 K**
- ◆ Wilson ratio:  $R = 4\chi\pi^2 k_B^2 / 3\gamma\mu_{\text{eff}}^2 \approx 1.8$   
(R = 1 for non-interacting electrons, R = 2 for heavy fermions)



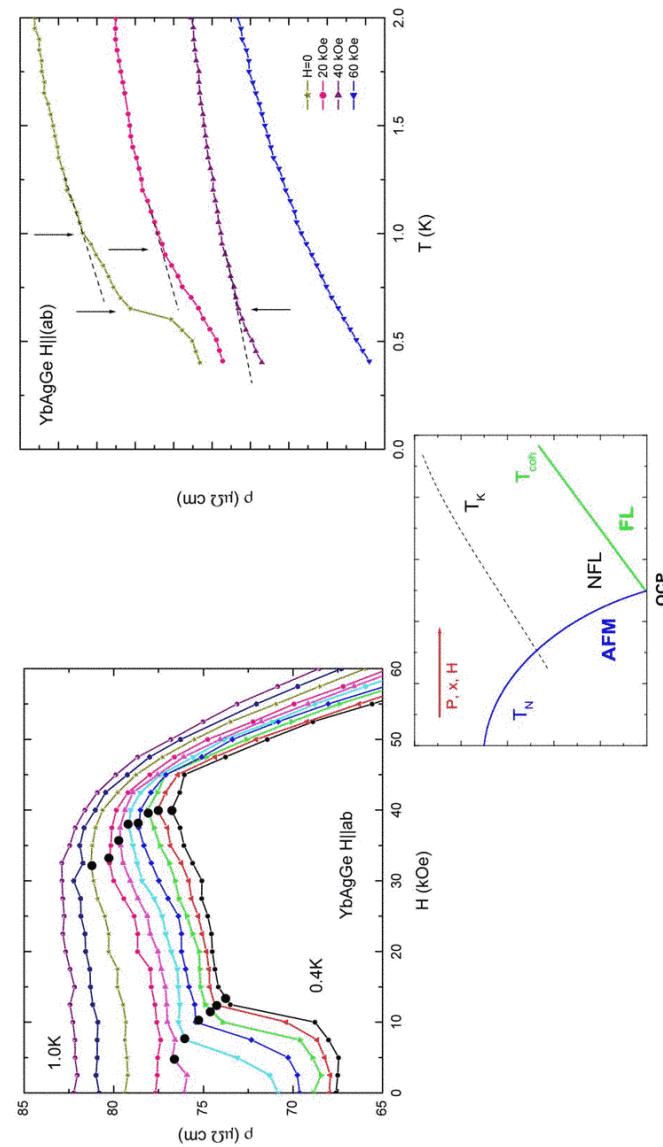
YbAgGe – resistivity in applied field



Let us look in more detail

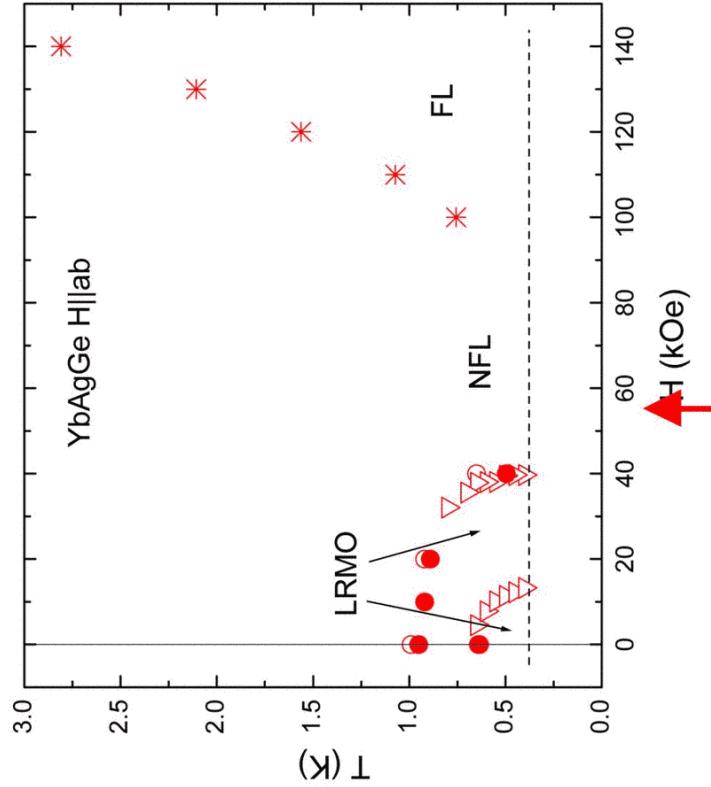


YbAgGe -  $\rho(T,H)$ : shift of magnetic transitions in applied field

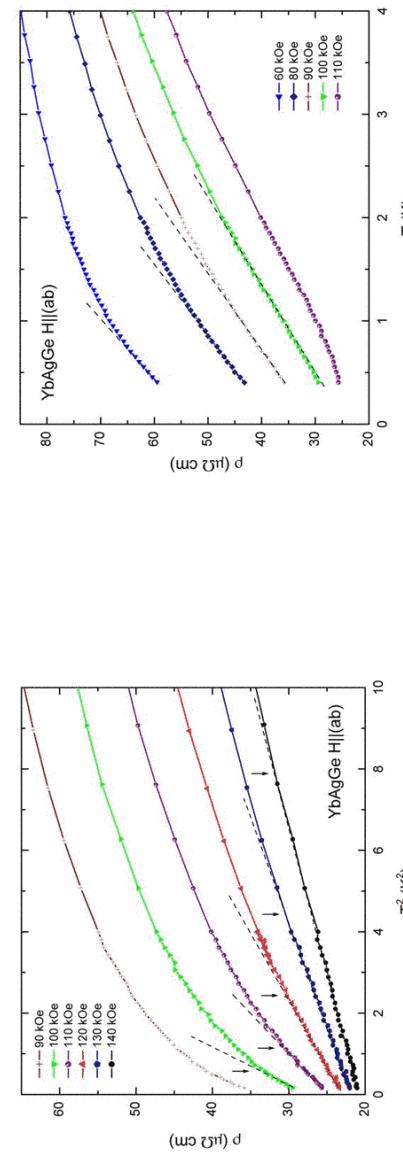




## YbAgGe – phase diagrams

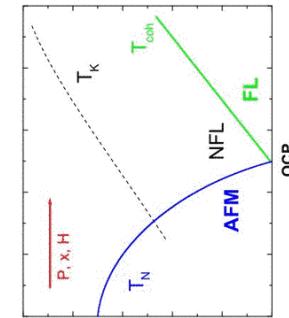


## YbAgGe - $\rho(T,H)$ : Fermi-liquid vs. non-Fermi-liquid

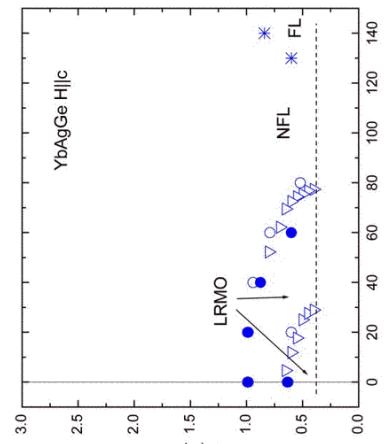
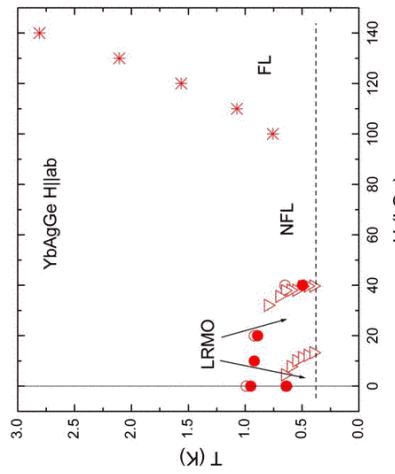


High fields:  
 $\rho = \rho_0 + AT^2$ ,  
**FL - like**

Intermediate fields:  
 $\rho = \rho_0 + BT$ : **NFL**



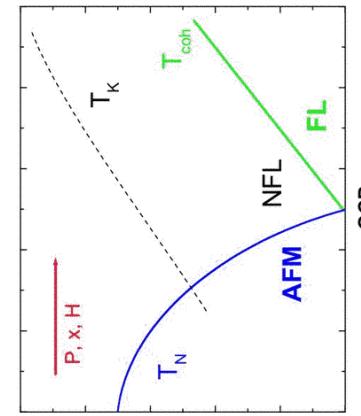
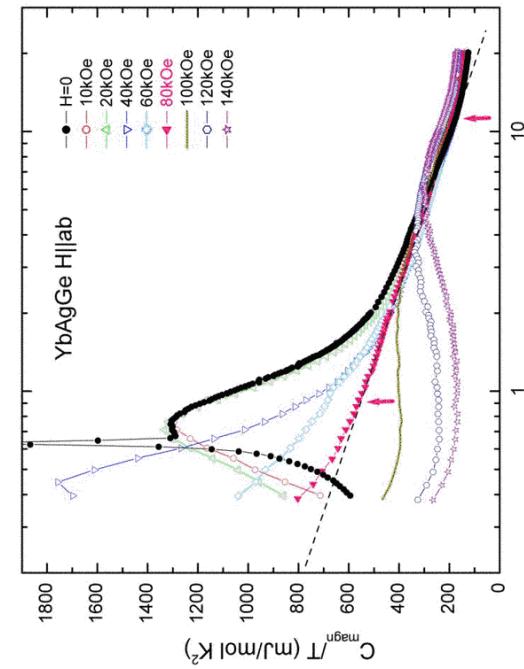
## YbAgGe – phase diagrams



- (i) Tuning via simple and clean knob –  $H$  (not  $P$  or  $x$ )
- (ii) Only second stoichiometric Yb-compound to show this
- (iii) Unlike  $\text{YbRh}_2\text{Si}_2$  crystals can be BIG



## YbAgGe – heat capacity in applied field

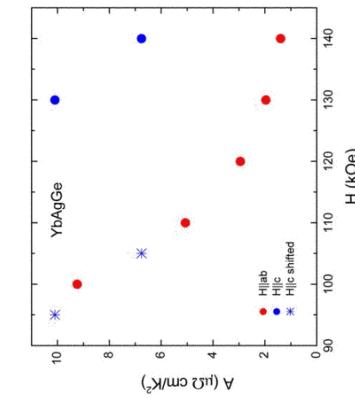
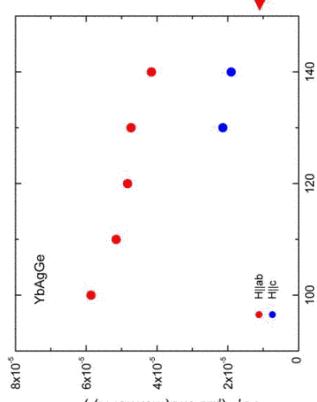
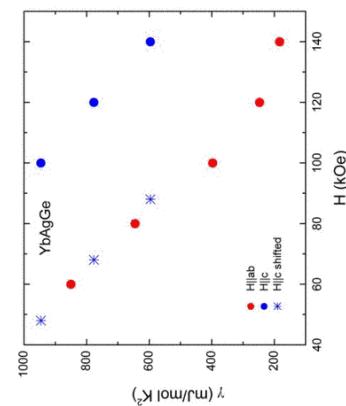


Also: scaling of the specific heat:  
 $[C(H) - C(H=0)]$  vs.  $H/T^\beta$ ,  
 $\beta = 1.15$   
 (observed in a number of materials with NFL properties)

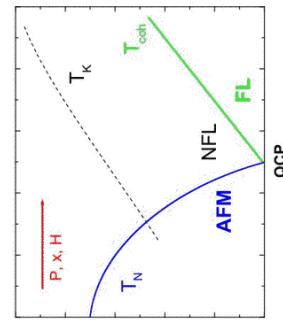
$H = 80$  kOe:  $C_{\text{magn}}/T \propto -\ln T$  for over a decade in temperature

$$C_{\text{magn}}/T = \gamma'_0 \ln(T_0/T); \gamma'_0 \approx 144 \text{ mJ/mol K}^2; T_0 \approx 41 \text{ K}$$

# YbAgGe: resistivity and heat capacity coefficients



Higher KW ratio close to magnetic instability – Takimoto & Moriya, SSC 99 (1996) 457  
Constant – in local critical regime



## Hall effect at QCP

P.Coleman et al., JPCM 13 (2001) R723

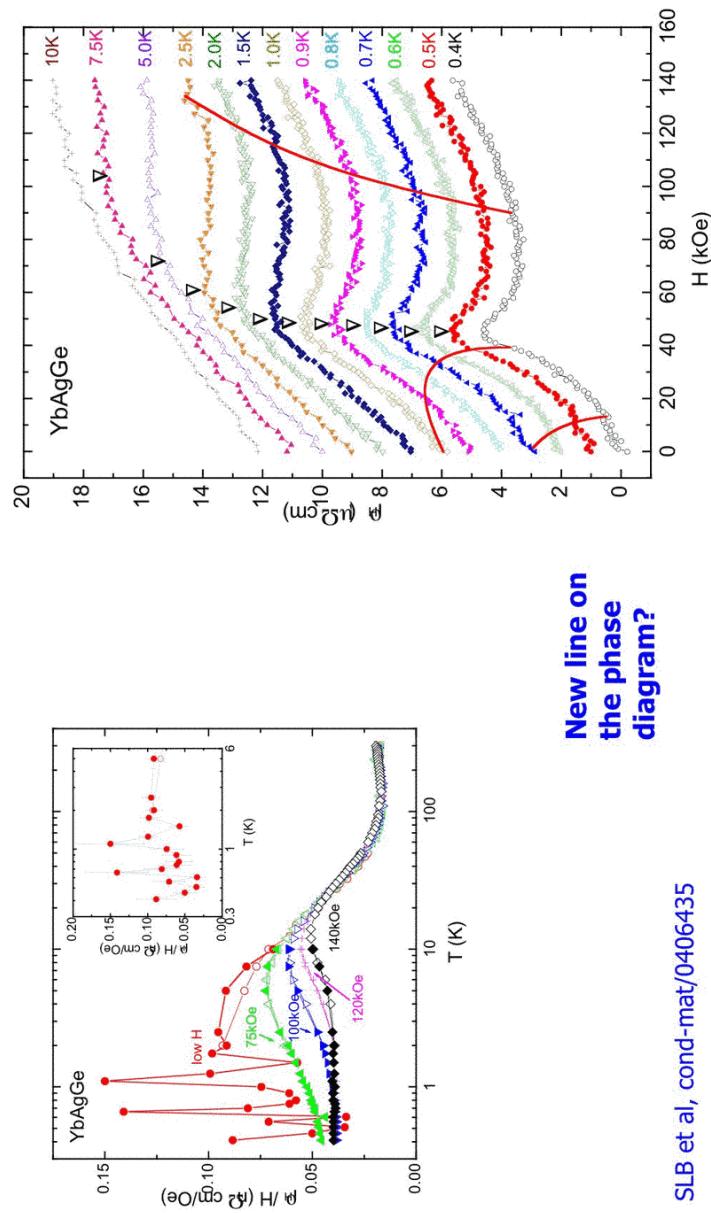
### Two scenarios of quantum critical behavior:

- SDW
- breakdown of composite HF

### Hall effect as a test:

Mechanism	$R_H$
S.D. W.	$R_H$ constant, $\Delta R_H \propto M^2 \sim  P - P_c $
Breakdown of composite Fermions	$\Delta R_H \neq 0, \lambda = 0$ , $\Delta R_H \propto M \sim  P - P_c ^{1/2}, \lambda \neq 0$

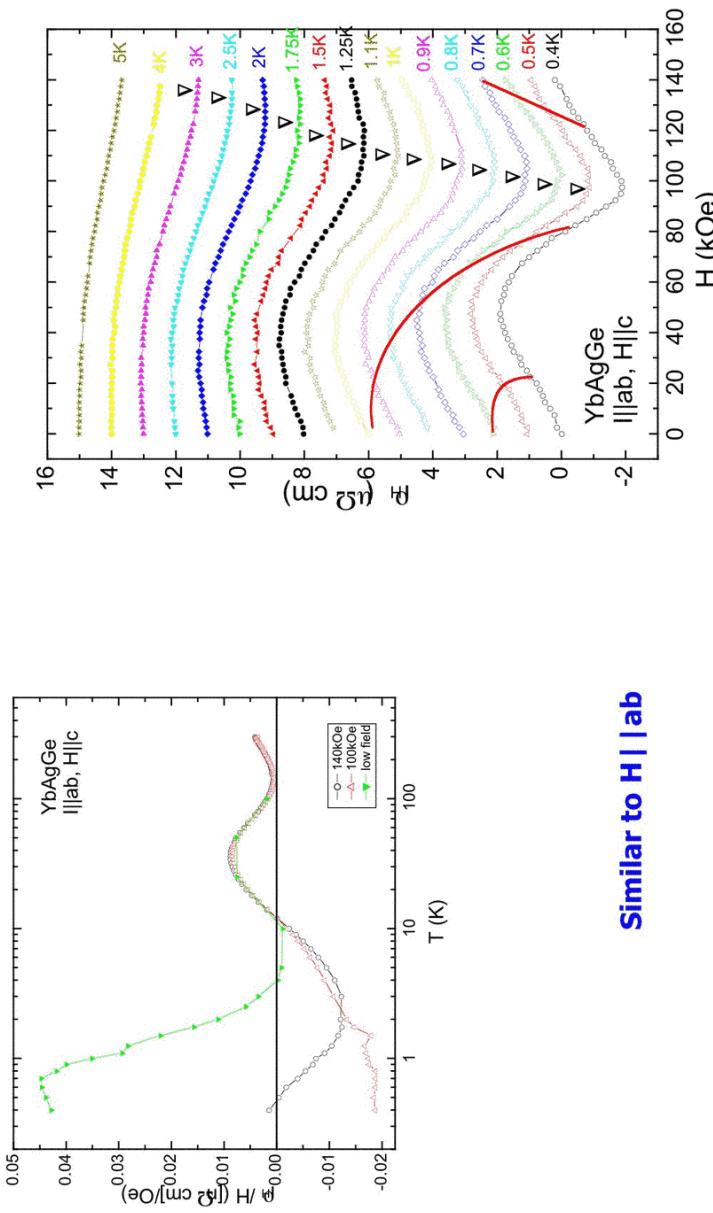
## YbAgGe – Hall effect ( $H \parallel \text{lab}$ )



SLB et al, cond-mat/0406435

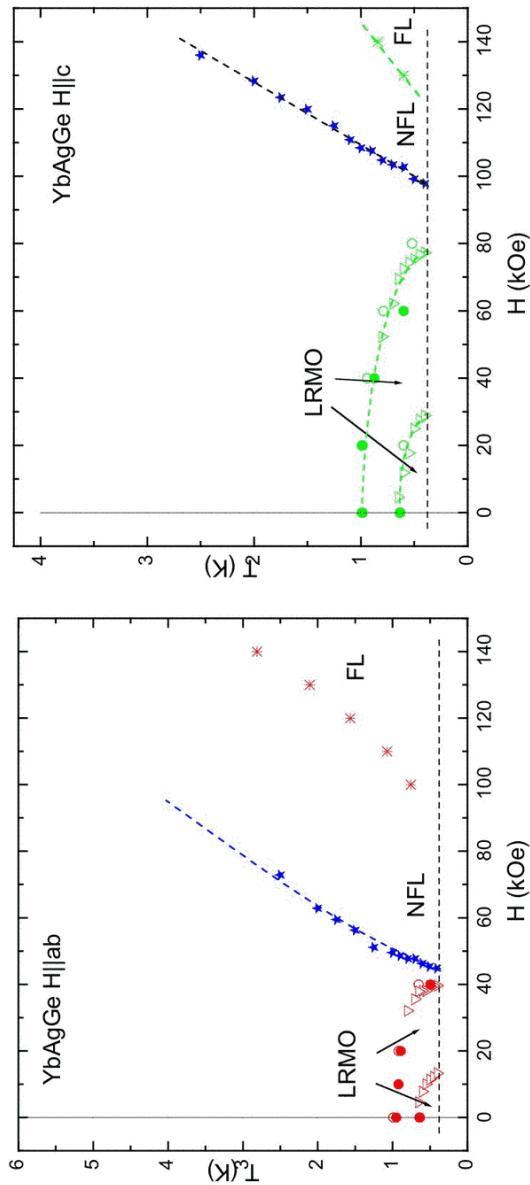
New line on  
the phase  
diagram?

## YbAgGe – Hall effect ( $H \parallel c$ )



Similar to  $H \parallel \text{lab}$

## YbAgGe – “revised” phase diagrams

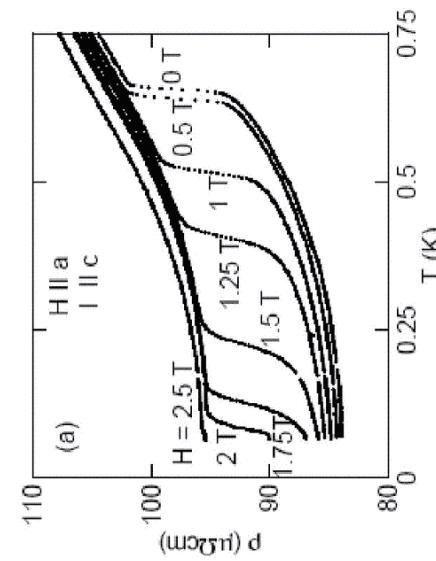


For both field orientations  $\rho_H(H)$  define a new line.

From  $\rho_H(H)$  no unambiguous choice between the two QCP models.

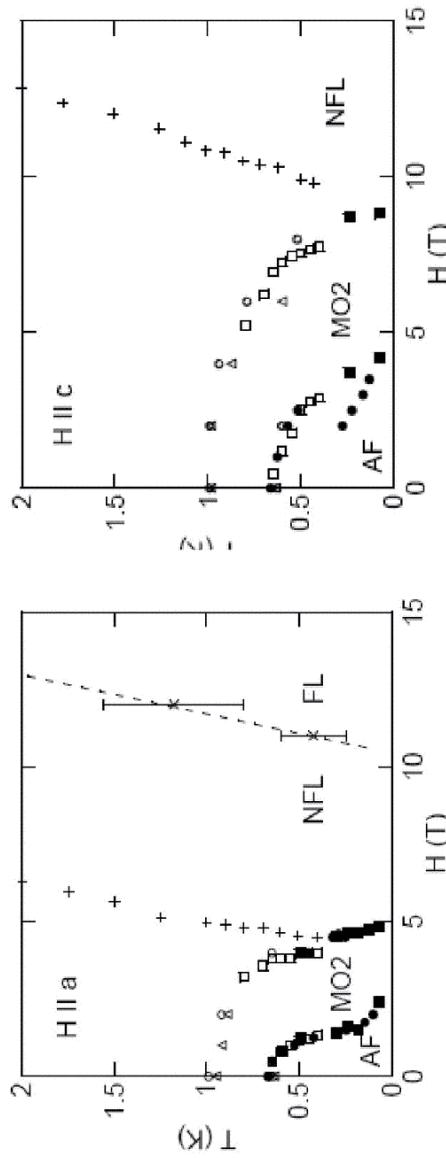
## Possible FIQCP in YbAgGe – next steps

- ▶ Lower temperatures
- ▶ Neutron scattering measurements



Philippe Niklowitz, Jacques Flouquet  
(CEA/Grenoble)

## YbAgGe H-T Phase diagrams



**Extended temperature range data from Philipp Nicklowitz et al., CEA Grenoble. These data further support identification of field induced QCP.**

## Possible FIQCP in YbAgGe – next steps

### Other techniques:

#### NEUTRON SCATTERING:

- (i) Find and confirm ordering (partially done) and fully determine ordered structure (ongoing).
- (ii) Look at inelastic scattering near QCP (ongoing with several runs scheduled for the first quarter of '05)

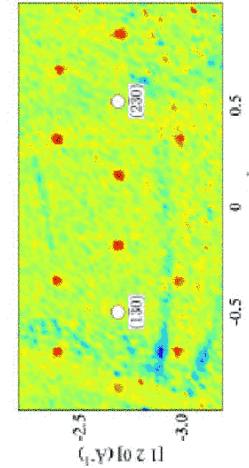


Figure 2. Color map of the low- $T$  magnetic scattering in YbAgGe, taken as the difference between data at  $T = 0.32$  and  $2.0$  K, in the  $(hk)$  scattering plane for  $l = 1/3$ . The six-fold symmetry of the magnetic satellites characterized by a propagation vector of  $\mathbf{k}=(1/3,0,1/3)$  is easily seen.

Below 0.6 K a  $(1/3,0,1/3)$  wave vector evolves.

Björn Fåk, Desmond McMorrow, et al.

JPCM 17 (2005) 301



## YbAgGe – Stoichiometric FIQCP compound

- Resistivity: decrease of  $T_{\text{magn}}$   $\Rightarrow$  linear LT resistivity  $\Rightarrow$  recovery of  $T^2$  (FL) behavior
  - Heat capacity: decrease of  $T_{\text{magn}}$   $\Rightarrow C_{\text{magn}}/T \propto -\ln T \Rightarrow$  recovery of FL behavior. Scaling of  $[C(H)-C(H=0)]$  vs.  $H/T^\beta$
  - Anomaly in Hall resistivity data very clear and apparently associated with FIQCP
  - FIQCP in accessible fields ( $\leq 11\text{T}$ ) associated with a  $H = 0$   $T_N$  that is also very accessible.
  - One of the few **stoichiometric** compounds possibly showing FIQCP
    - Effects are anisotropic



## Conclusions:

- Yb-based heavy fermions offer fertile ground for QCP research
- They allow to address “key” question of how can correlated electron state evolve out of local moment. One can be a voyeur and watch how it happens.
- Few properties are curious and entertaining (for some).
- Potentially can shed light on few open questions in HF physics (if samples and “knobs” are under control).
- Can we find a few more so as to identify unifying trends?



## Group: Novel Materials and Ground States

### Two permanent members:

<http://cmp.ameslab.gov/personnel/canfield/>

### Paul C. Canfield and Sergey L. Bud'ko

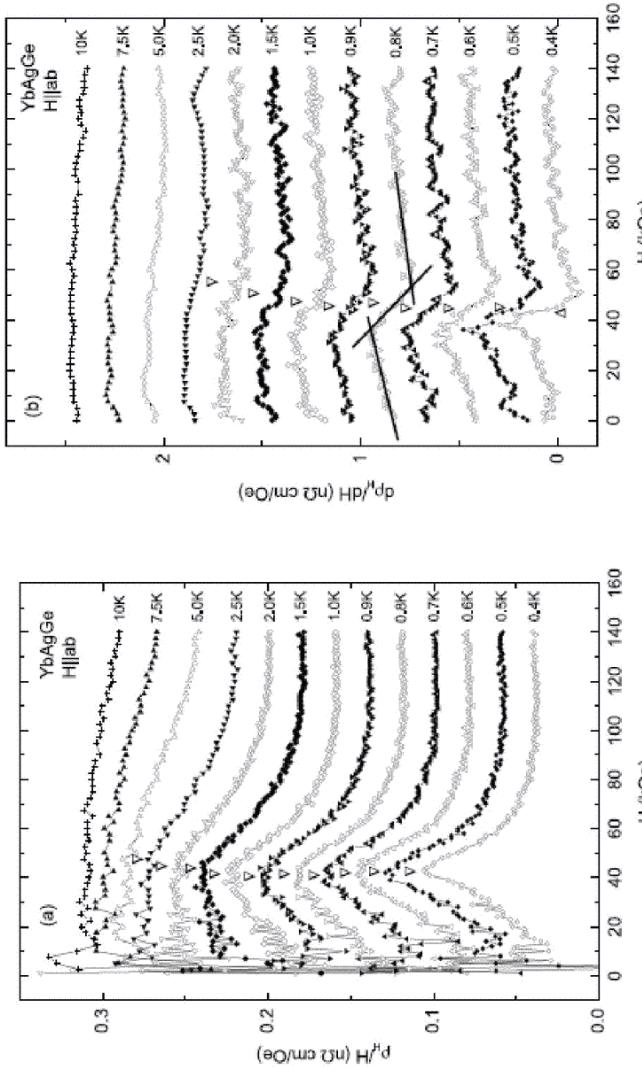
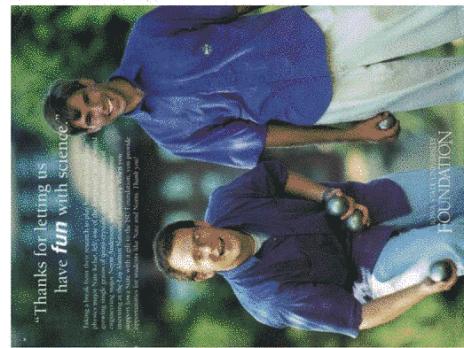
in a steady state:

- 2-3 post-docs / visiting scientists
- 2-4 graduate students
- 1-3 (hourly) undergraduates

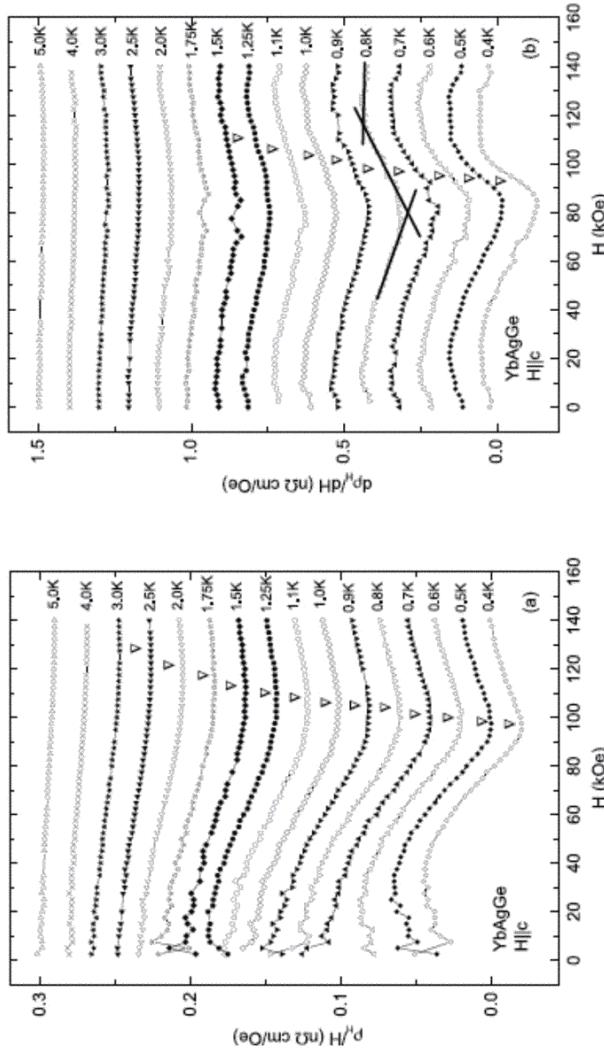
### Toys:

- Furnaces, arc-melter
- Powder diffractometer
- 2\_ QD MPMS magnetometers
- 1\_ QD PPMS systems (with a few widgets and gadgets)
- Polishers, wire & diamond saws, press, etc.

Easy access to Ames Lab resources



➤ S. L. Bud'ko et al., PRB 71 (2005) xxxx. (cond-mat./0406435)



► S. L. Bud'ko et al., PRB 71 (2005) xxxx. (cond-mat/0406435)

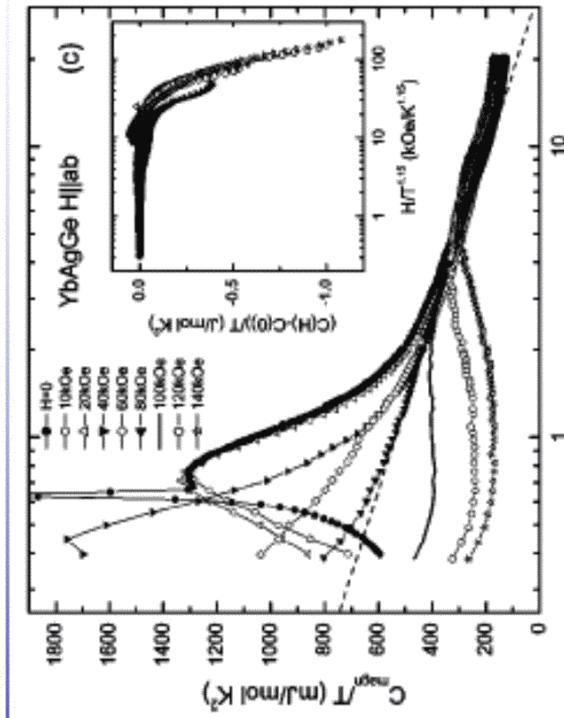


FIG. 5. (a) Low-temperature part of the heat-capacity curves for YbAgGe taken at different applied fields  $H \parallel ab$ , arrows indicate peaks associated with magnetic ordering. (b) low-temperature part of  $C_p$  vs  $T^2$  curves; (c) semi-log plot of the magnetic part [ $C_p^{\text{magn}} = C_p(\text{YbAgGe}) - C_p(\text{LuAgGe})$ ] of the heat capacity,  $C_p^{\text{magn}}/T$  vs  $T$ , for different applied magnetic fields, dashed line is a guide to the eye, it delineates linear region of the  $H = 80$  kOe curve; inset: semi-log plot of  $[C(H) - C(H=0)]/T$  vs  $H/T^{1.15}$  ( $T \geq 0.8$  K), note approximate scaling of the data for  $H \geq 60$  kOe.

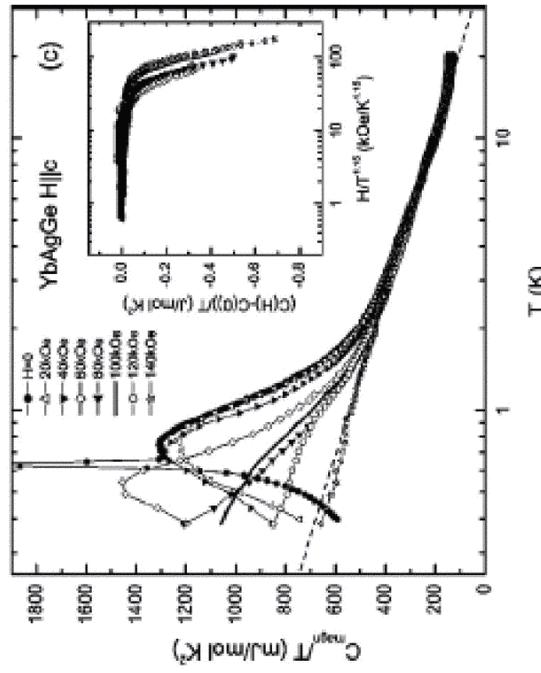


FIG. 8. (a) Low-temperature part of the heat-capacity curves for YbAgGe taken at different applied fields  $H \parallel c$ , arrows indicate peaks associated with magnetic ordering; (b) low-temperature part of  $C_p$  vs  $T^2$  curves; (c) semi-log plot of the magnetic part [ $C_{\text{magn}} = C_p(\text{YbAgGe}) - C_p(\text{LuAgGe})$ ] of the heat capacity,  $C_{\text{magn}}/T$  vs  $T$ , for different applied magnetic fields, dashed line, a guide to the eye, it delineates linear region of the  $H = 140$  kOe curve; inset: semi-log plot of  $[C(H) - C(H=0)]/T$  vs  $H/T^{1/3}$  ( $T \geq 0.8$  K), note approximate scaling of the data for  $H \geq 100$  kOe.

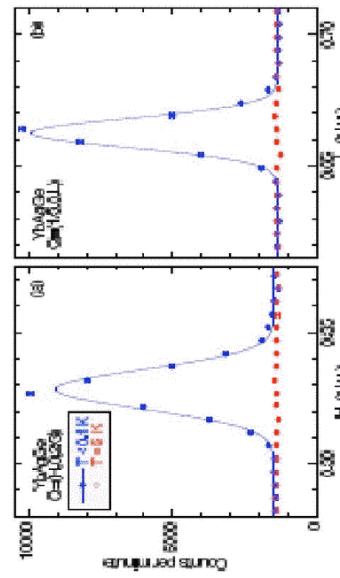


Figure 3. Scans at zero energy transfer along the (a)  $h$  and (b)  $l$  direction of the  $Q=(1/3, 0, 2/3)$  magnetic Bragg peak of YbAgGe measured on IN14 using  $k_f = 1.3$   $\text{\AA}^{-1}$ . Closed and open circles correspond to temperatures of 0.1 and 5.0 K, respectively. The lines are Gaussian fits.

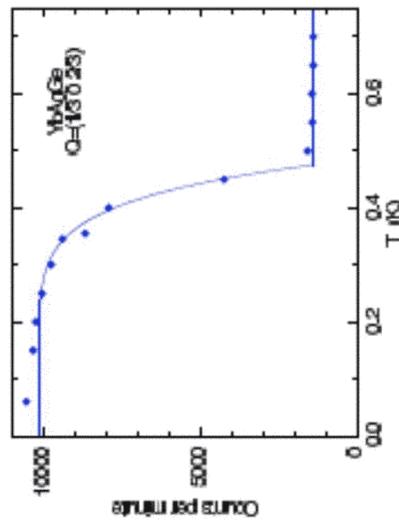


Figure 4. Temperature dependence of the magnetic Bragg peak intensity at  $\mathbf{Q} = (1/3, 0, 2/3)$  of YbAgGe measured on IN14 using  $k_f = 1.3 \text{ \AA}^{-1}$ . The line is a guide to the eye.

### Scattering study of YbAgGe

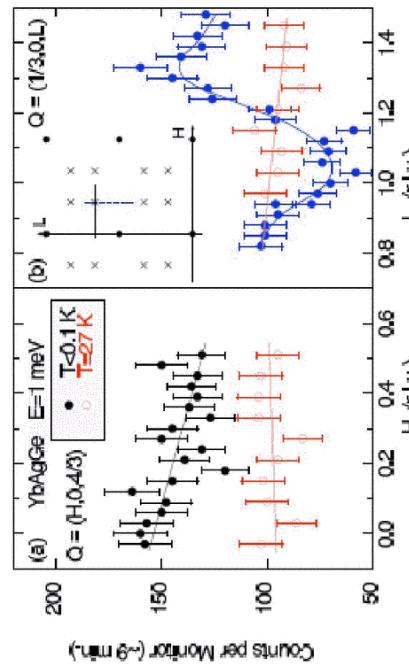


Figure 6. Scans in wave vector  $\mathbf{Q}$  along the (a)  $h$  and (b)  $l$  direction of the spin-fluctuation scattering at an energy transfer of  $E = 1 \text{ meV}$ , measured on IN14 using  $k_f = 1.30 \text{ \AA}^{-1}$ . Closed and open circles correspond to  $T < 0.1$  and  $T = 27 \text{ K}$ , respectively. The lines are guides to the eye. The inset shows the scan directions in the  $(h0l)$  plane.

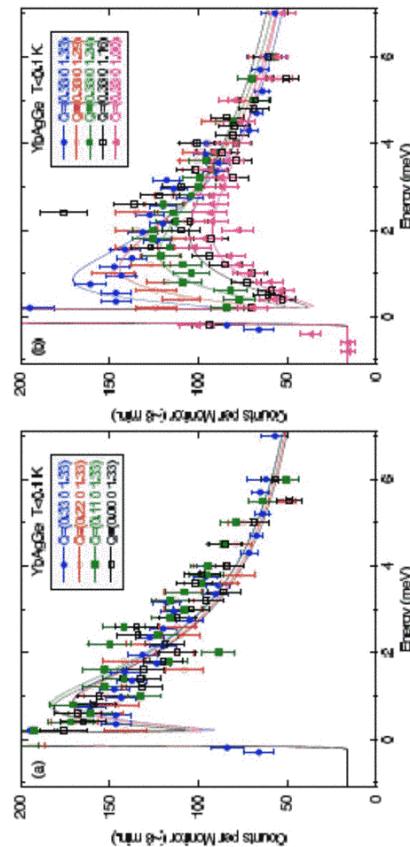


Figure 7. Energy scans of the quasielastic magnetic scattering at low temperatures,  $T < 0.1$  K, for different  $\mathbf{q}$  values along the (a)  $h$  and (b)  $l$  direction, measured on IN14 using  $k_f = 1.30 \text{ \AA}^{-1}$ . The lines are fits to a quasielastic Lorentzian, Eqs. (1-2), plus a Gaussian describing the elastic scattering.

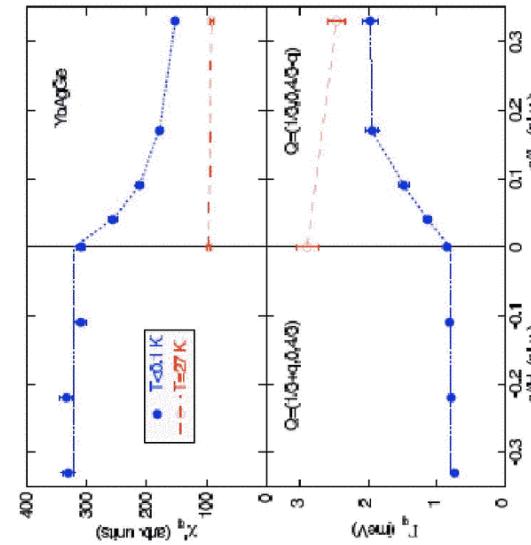


Figure 8. Wave vector dependence of the static susceptibility  $\chi'_q$  and the characteristic energy  $\Gamma_q$  of the quasielastic magnetic scattering along the  $h$  (left part) and  $l$  (right part) direction at  $T < 0.1$  K (closed circles) and  $T = 27$  K (open circles). The lines are guides to the eye.

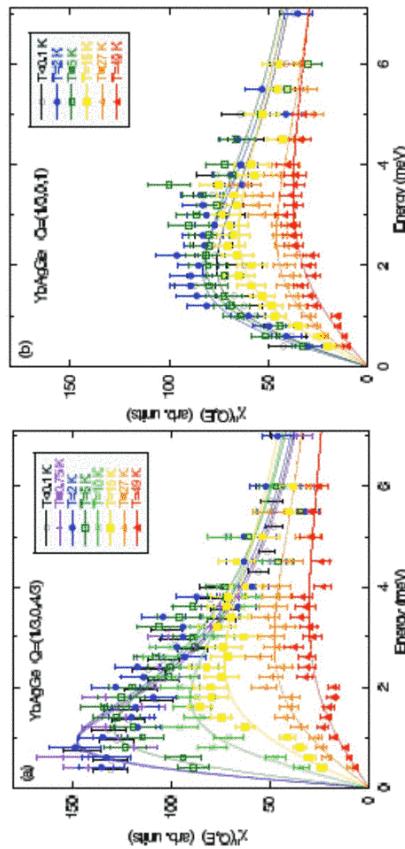


Figure 9. Dynamic magnetic susceptibility for different temperatures at (a) the AFM zone center  $Q = (1/3, 0, 4/3)$  and (b) the AFM zone boundary  $Q = (1/3, 0, 1)$ , measured on IN14 using  $k_f = 1.30 \text{ \AA}^{-1}$ . The lines are fits to a quasielastic Lorentzian, Eq. (2).

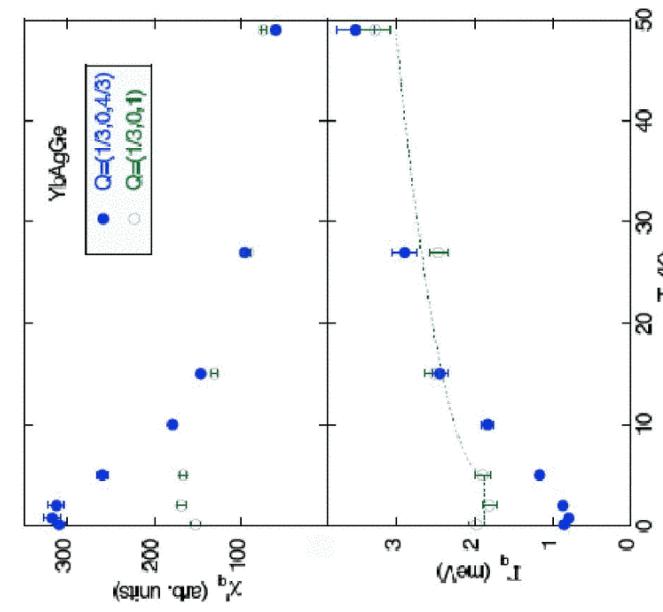


Figure 10. Temperature dependence of the static susceptibility  $\chi'_Q(T)$  and the characteristic energy  $T_Q(T)$  of the quasielastic magnetic scattering at the AFM zone center  $Q = (1/3, 0, 4/3)$  (solid circles) and at the AFM zone boundary  $Q = (1/3, 0, 1)$  (open circles). The dashed line shows a fit of Eq. (3) to the zone boundary energy  $\Gamma_0$ .

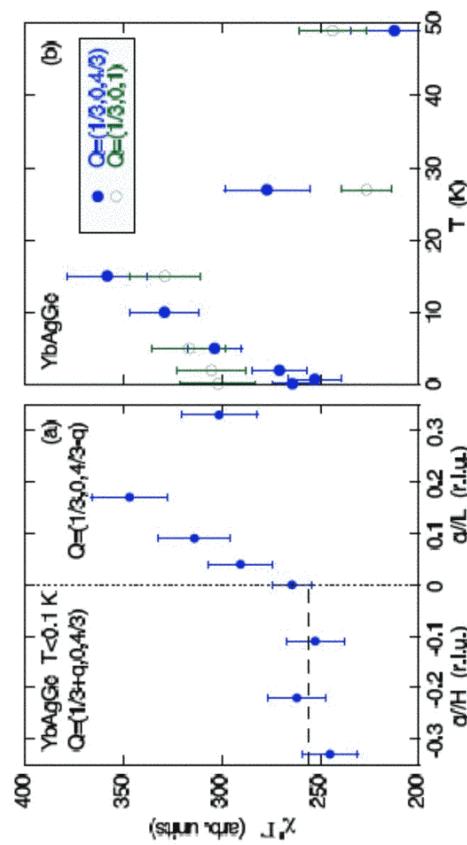


Figure 11. The product  $\chi' \Gamma$  of the static susceptibility  $\chi_q(T)$  and the characteristic energy  $\Gamma_q(T)$  of the quasielastic magnetic scattering. (a)  $\chi' \Gamma$  as a function of  $q$  along  $h$  (left part) and  $l$  (right part). (b)  $\chi' \Gamma$  as a function of temperature for  $q$  at the antiferromagnetic zone center and at the zone boundary.

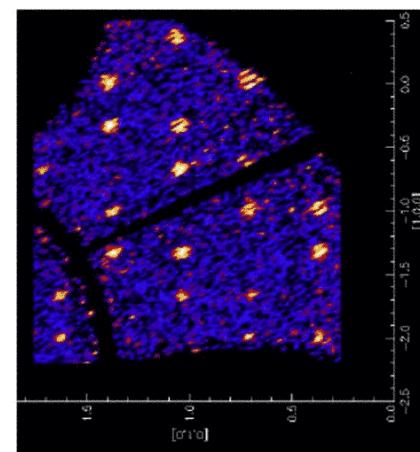


Figure 1:  $(h, k)$  scattering plane of YbAgGe. Shown is the difference in intensity between  $T = 0.32$  and  $2.0$  K.