Localized Excitation in the Hybridization Gap in $YbAl_3$

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Intermediate Valence Materials

- Materials where the 4f level is close to the Fermi level($4f^n$ and $4f^{n-1}$ are degenerate)
- Homogenous mixed valent-both configurations contribute to the IV wave function (schematically $|\psi\rangle = a_n|f^n\rangle + a_{n-1}|f^{n-1}\rangle$)
- Elements where IV behavior is found: Ce, Sm, Eu, Tm, and Yb
- Examples: $CePd_3$, $CeSn_3$, $EuPd_2Si_2$, SmB6, TmSe, YbB_{12}, $YbAl_3$, etc.
- Why IV materials? Opportunity to explore the physics of strong electron correlations without some of the complications found in other strongly correlated systems

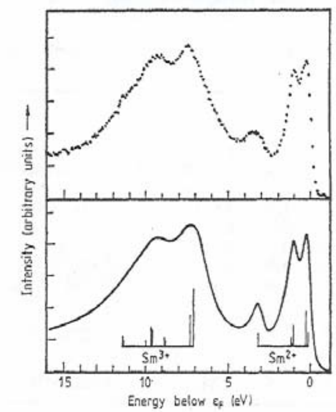
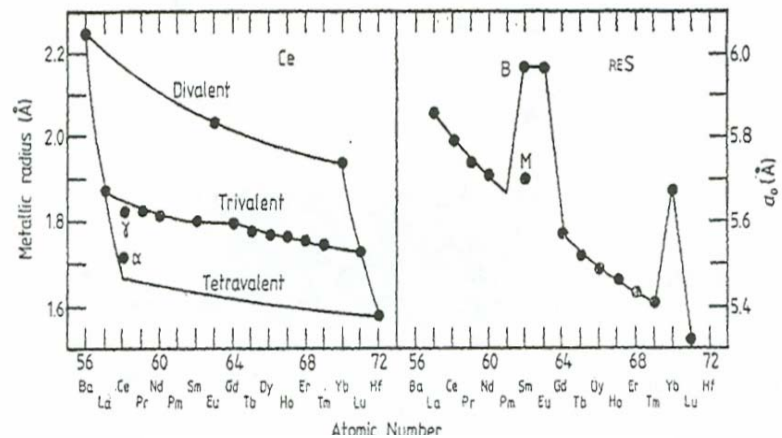


Figure 4. Valence band XPS spectrum of SmB_6. The theoretical curve was calculated as described in §2.4.1 (from Chazalviel *et al* 1976).

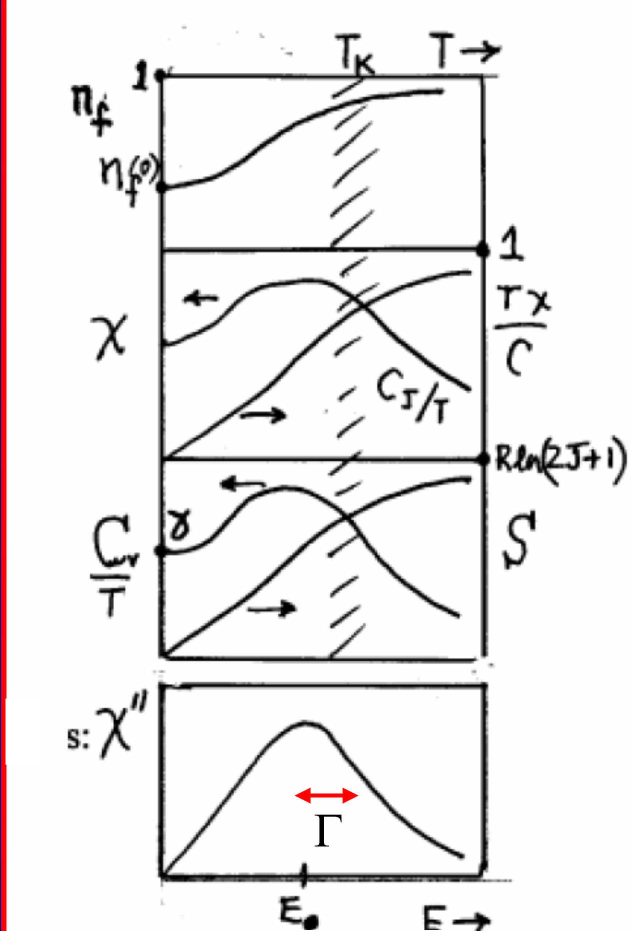
From J. M. Lawrence, *et al.*, Rep. Prog. Phys. **44**, 1 (1981).



From J. M. Lawrence, *et al.*, Rep. Prog. Phys. **44**, 1 (1981).

Characteristics of IV Systems

- High Temperature Local moment behavior (Curie-Weiss susceptibility)
- Low Temperature Fermi liquid (Pauli Susceptibility)
- Specific heat
  - Full Ground state multiplet entropy is recovered Rln(2J+1)
  - Large γ
- The INS response of polycrystal samples is a broadened Lorentzian
  - $\Gamma \sim T_K$
- Behavior qualitatively consistent with Anderson impurity model
- Anderson Lattice is the appropriate theoretical model

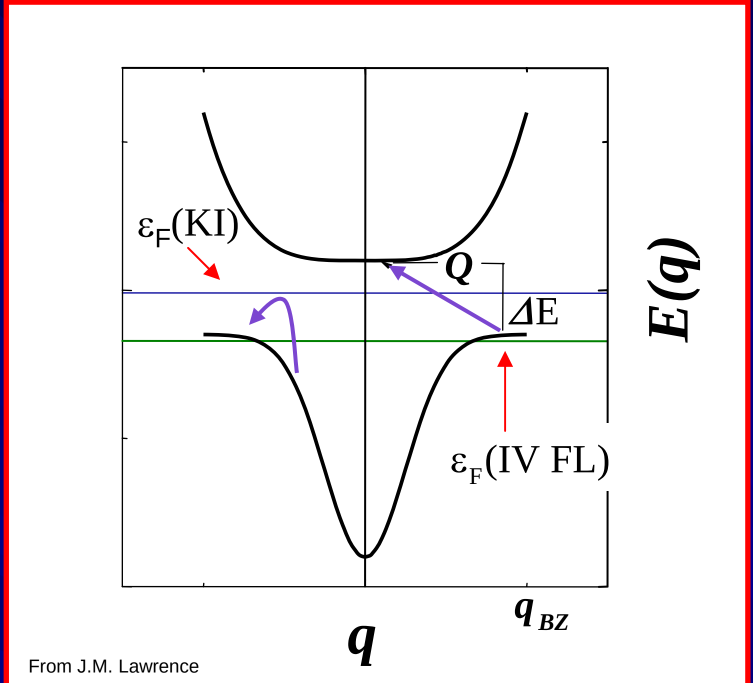


From J.M. Lawrence

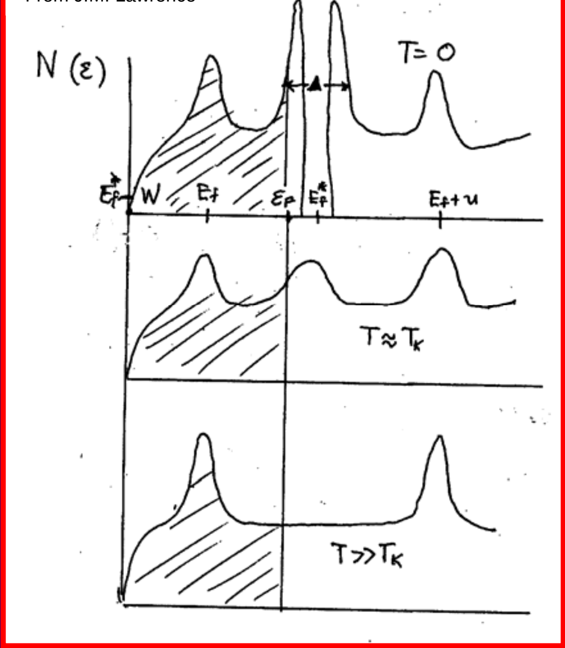
The Anderson Lattice

- Anderson lattice

  $H = \Sigma_k \varepsilon_k \mathbf{n}_k + \Sigma_i \{E_f \mathbf{n}_{fi} + U \mathbf{n}_{fi\uparrow} \mathbf{n}_{fi\downarrow} + \Sigma_k [V_{kf} \mathbf{c}^+_k \mathbf{f}_i + cc]\}$
  - Hard calculations
  - Sometimes use Anderson impurity model
- Expectations for neutrons
  - Fermi liquid scattering
  - Indirect gap scattering
- Examples
  - IV metals
  - Kondo insulators



From J.M. Lawrence



From J.M. Lawrence

The structure renormalizes away with increasing temperature:

For very low T << T_K
Fully hybridized bands
Gap

For T ~ $T_{K,}$
No gap
Incoherent Kondo resonances

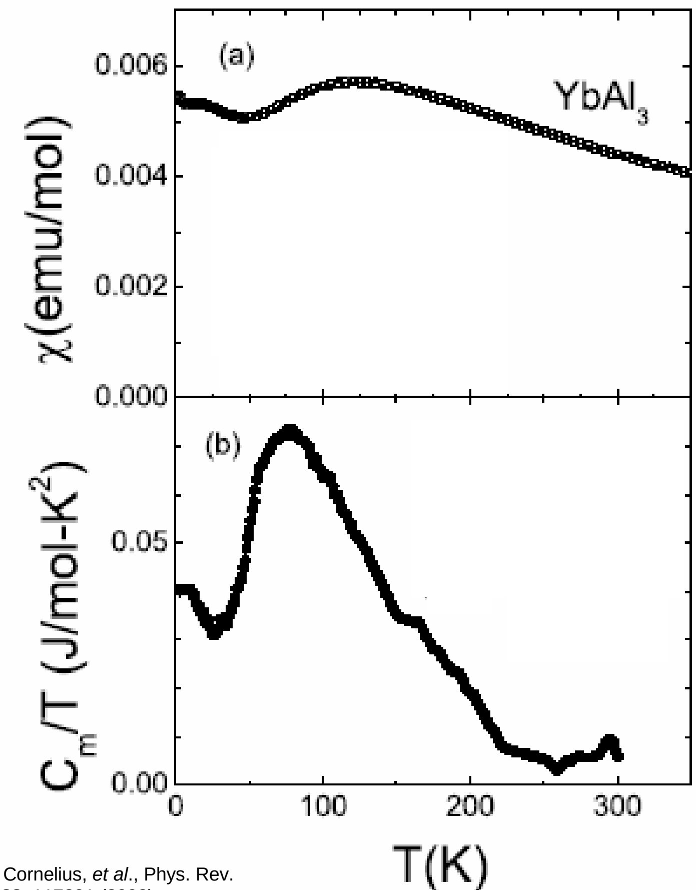
For T >> T_K
Local moments uncoupled from band electrons

For IV metals we expect to see both Fermi liquid and the indirect gap scattering

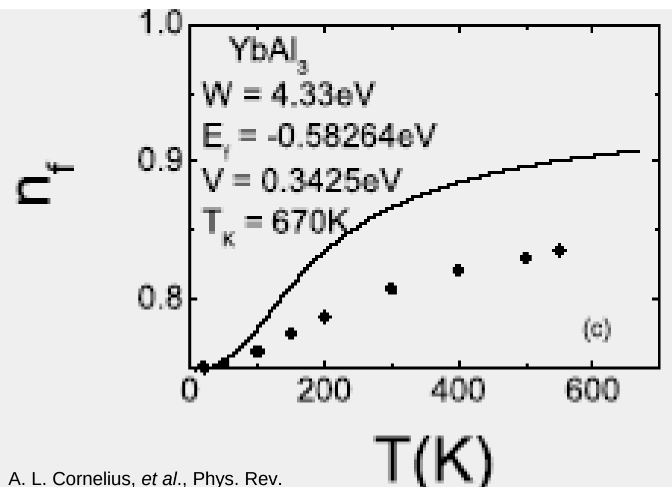
For Kondo Insulators we expect to see the indirect gap scattering

$YbAl_3$

- Started studying in early 1970s
- FCC (magnetic Brillouin zone simple cube)
- $T_K \sim 670$ K
- Physical properties consistent with IV behavior
- Self flux method yields high quality samples
  - dHvA
  - $\rho_0 = 0.5\ \mu\Omega$cm



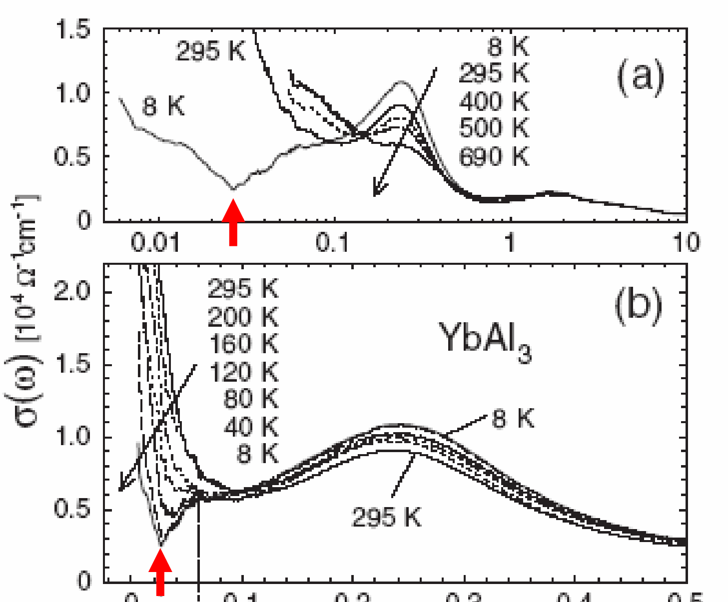
A. L. Cornelius, *et al.*, Phys. Rev. Lett. **88**, 117201 (2002)



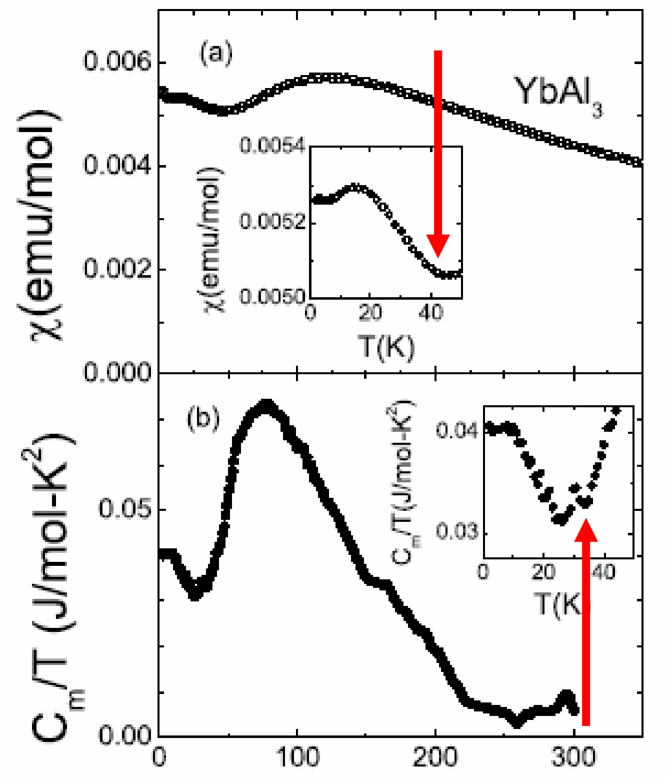
A. L. Cornelius, *et al.*, Phys. Rev. Lett. **88**, 117201 (2002)

A Second Energy Scale

- ~30-40 K anomalies occur in χ and C (R_H also)
- Formation of Hybridization Gap on the same temperature scale in the optical conductivity



H. Okamura, et al., J. Phys. Soc. Japan **73**, 2045 (2004)

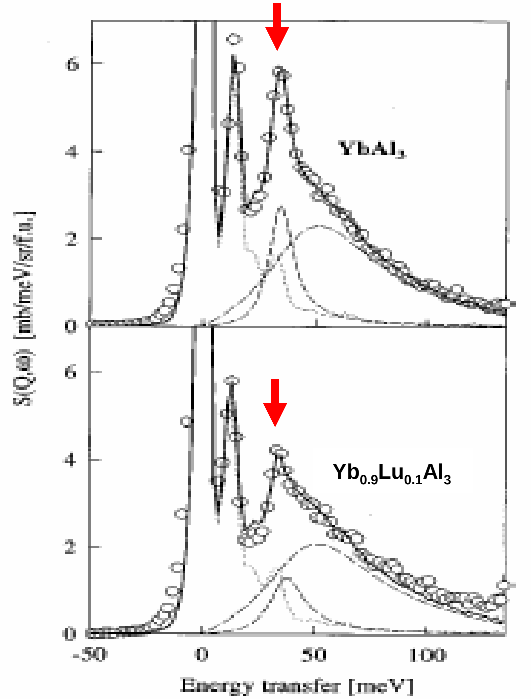


A. L. Cornelius, *et al.*, Phys. Rev. Lett. **88**, 117201 (2002)

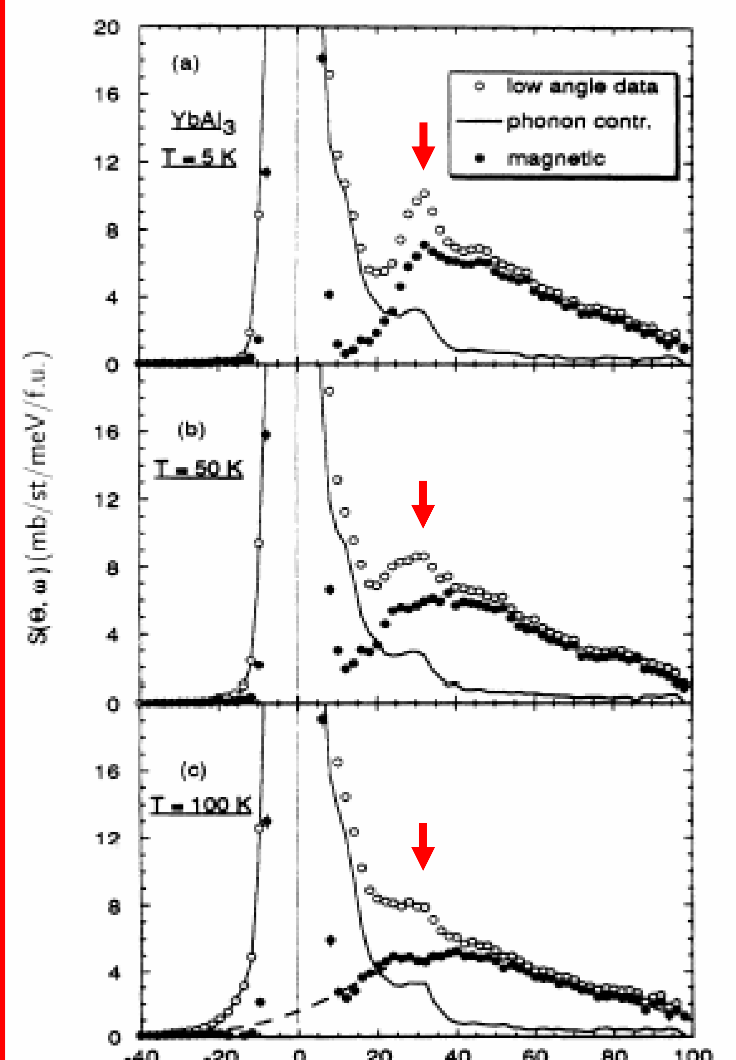
Conclude that the anomalies are due to the formation of a coherent Anderson lattice

A New Excitation in $YbAl_3$

- Magnetic contribution to INS
  - Broadened Lorentzian (E_1 ~ 50 meV)
  - Sharp excitation (E_2 ~ 33 meV) appearing below 50 K
- Strong dependence on Lu doping for E_2 peak, but not E_1 meV peak
- The peak at E_2 is associated with the anomalies at 40 K in the bulk properties



R. Osborn, *et al.*, J. Appl. Phys. **85**, 5344 (1999)

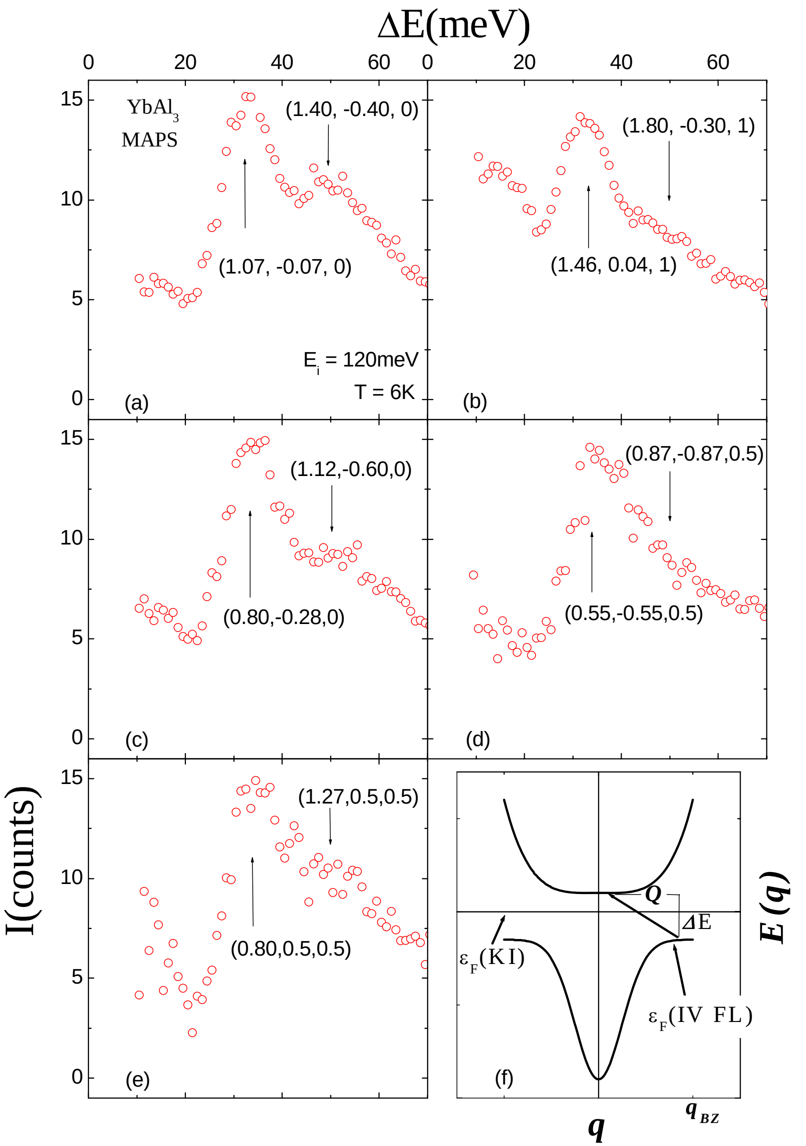


A. P. Murani, Phys. Rev. B **50**, 9882 (1994)

The excitation at E_2 = 33 meV is a property of the coherent Anderson lattice

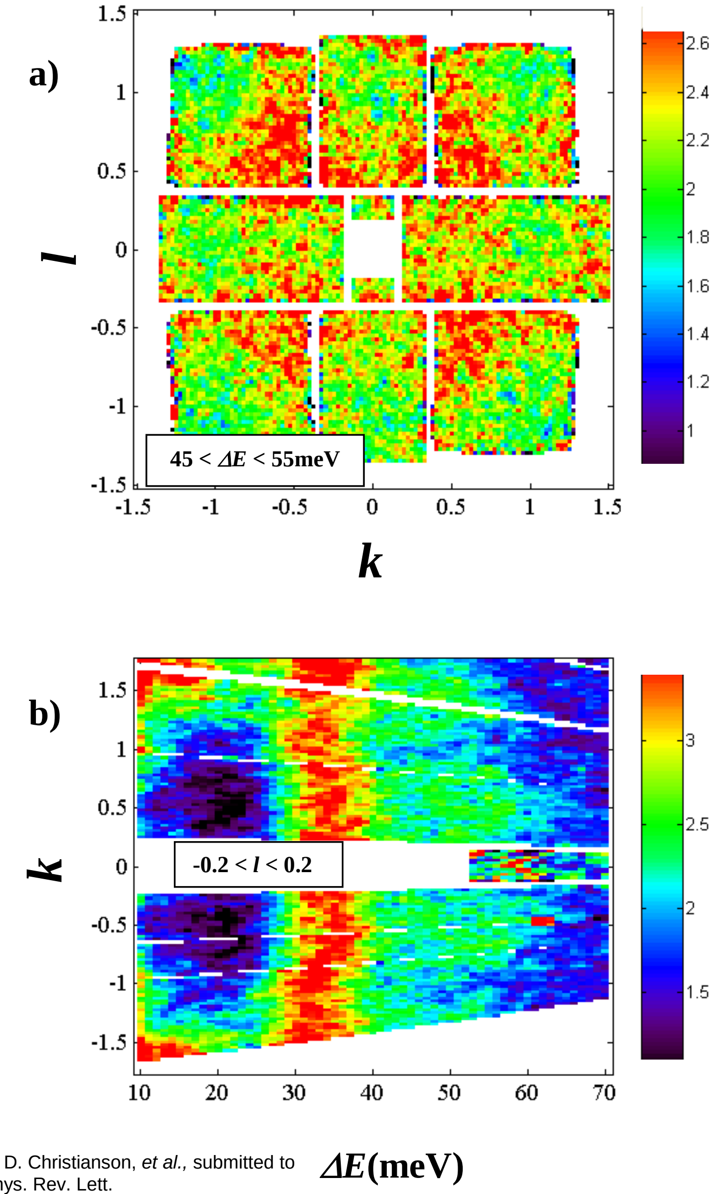
Single Crystal Work: Maps

- 4 crystals total mass ~5 g (mosaic 2.5°)
- E_i=120meV T= 6,100 K
- Two orientations k_i || [1,0,0] and [1,1,0]
- Only three of h,k,l, and ΔE are independent
- E_1 varies significantly in both line shape and intensity
- E_2 is basically independent of Q



A. D. Christianson, *et al.*, submitted to Phys. Rev. Lett.

- Scattering near E_1 = 50 meV depends strongly on Q and is peaked at zone boundary
- Scattering at E_2=33 meV is largely Q independent (spatially localized)
- Scattering at E_1 is indirect gap scattering
- Scattering at E_2 occurs at an energy inside of the gap
- Scattering at E_2 has neither the Q-dependence expected for the indirect gap scattering or the Fermi liquid scattering



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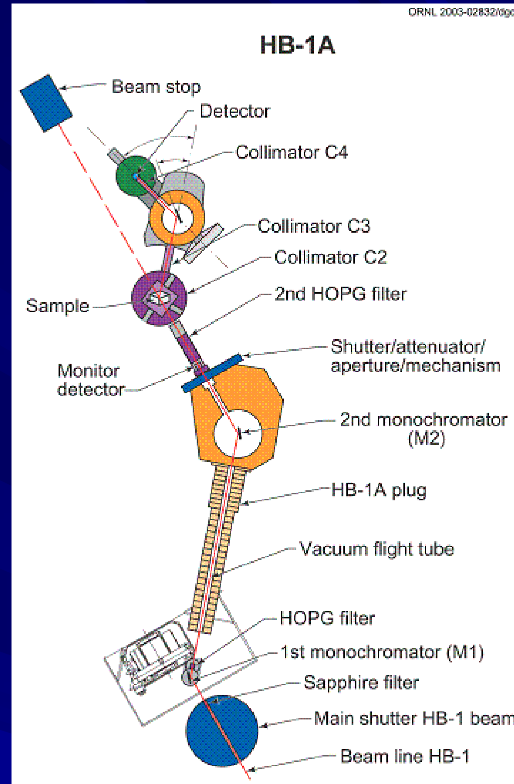
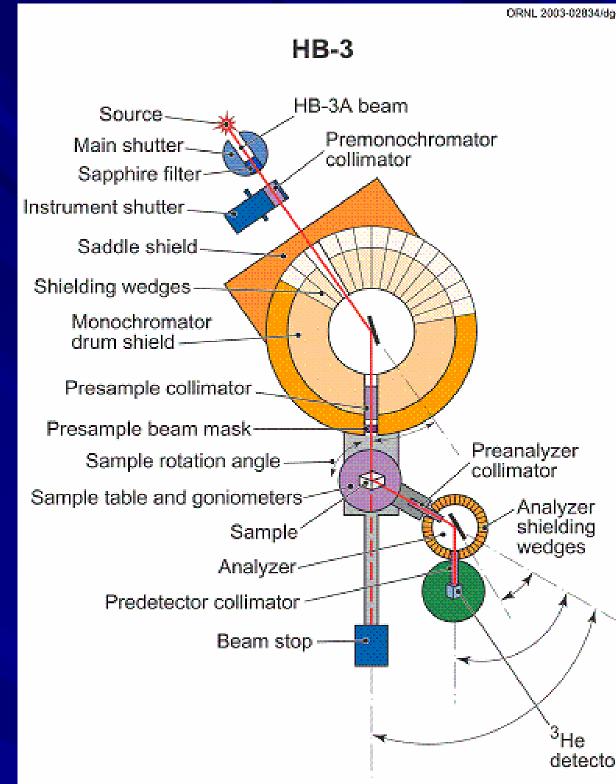
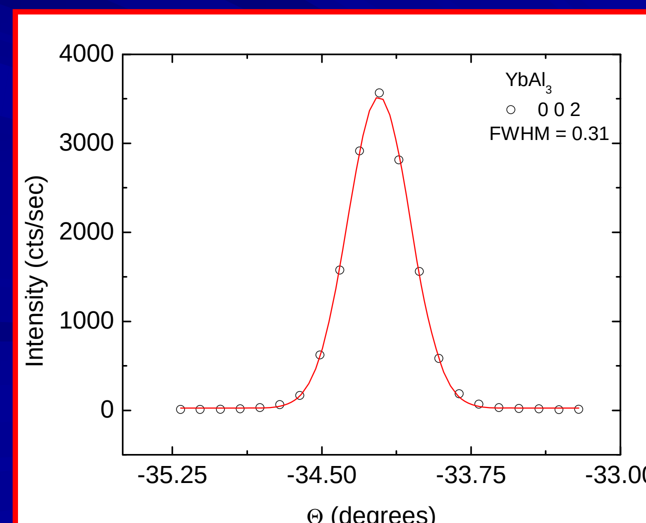
Need constant Q measurements

HFIR – Triple Axis

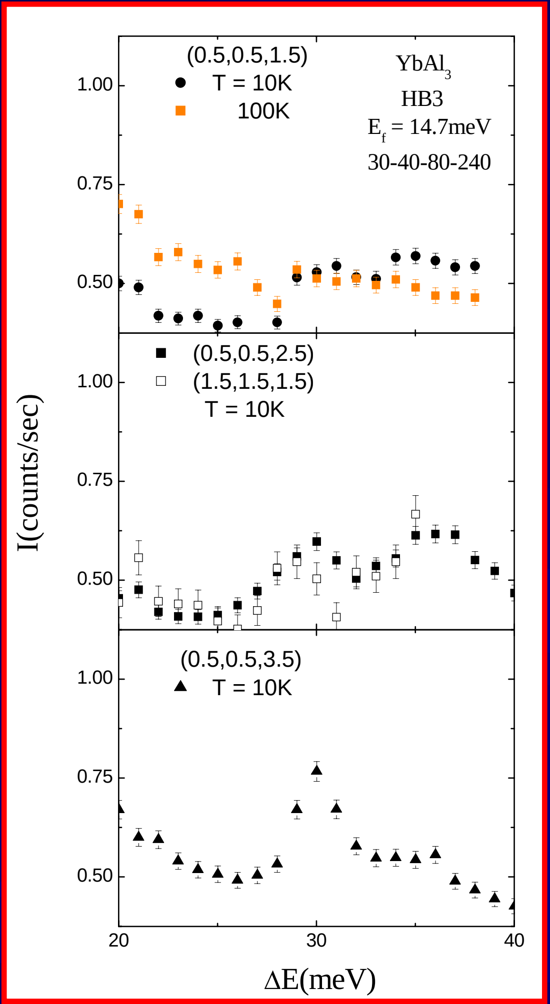


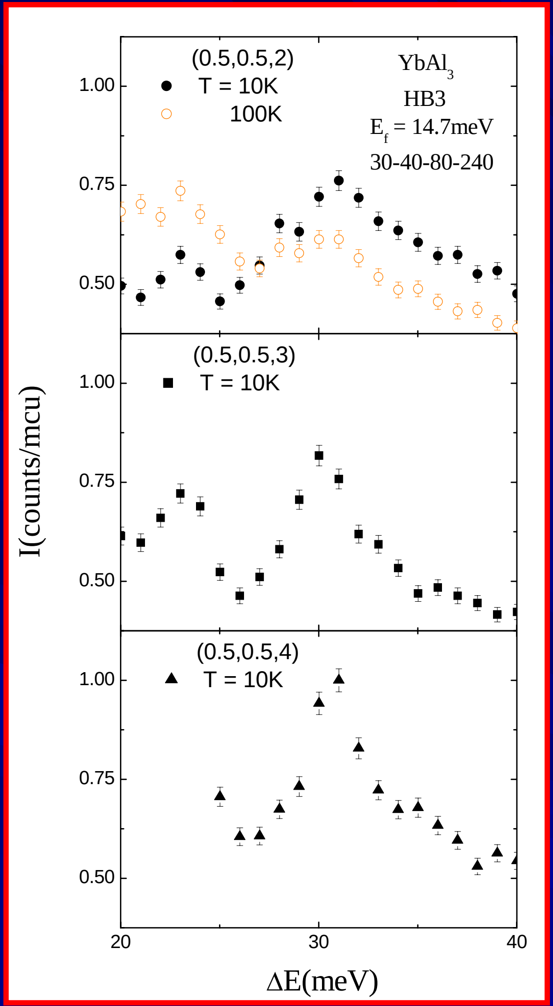


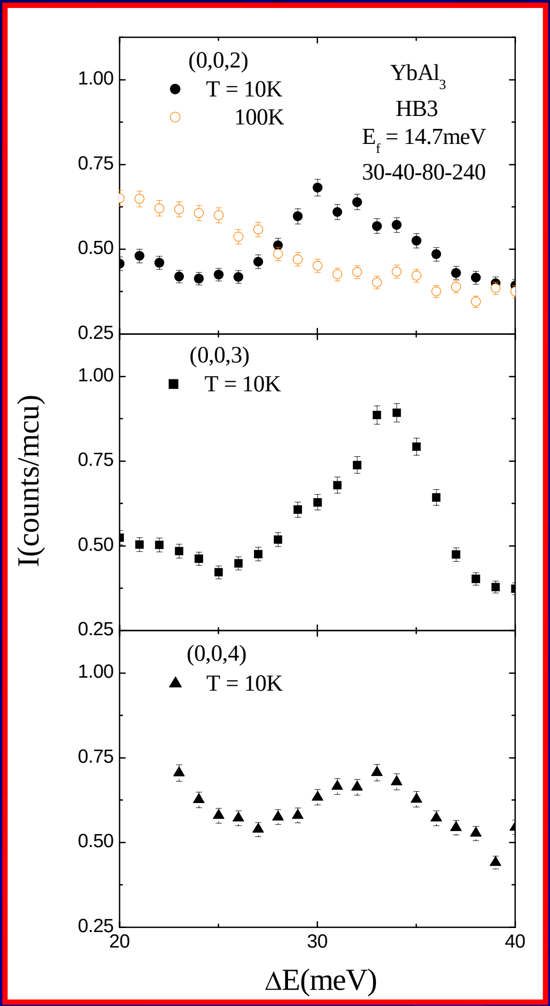
- HB1A for Alignment (Fixed E_i = 14.7 meV)
  - 6 ~1 g single crystals aligned +/- 0.3 degrees
  - Scattering plane (hhl) [1,-1,0] vertical
- HB3 (Fixed E_f = 14.7 meV)
  - Collimation 30’-40’-80’-240’
  - Resolution 1.4 meV at the elastic line
  - Sample Environment displex: Temperatures 10 and 100 K



Raw Data



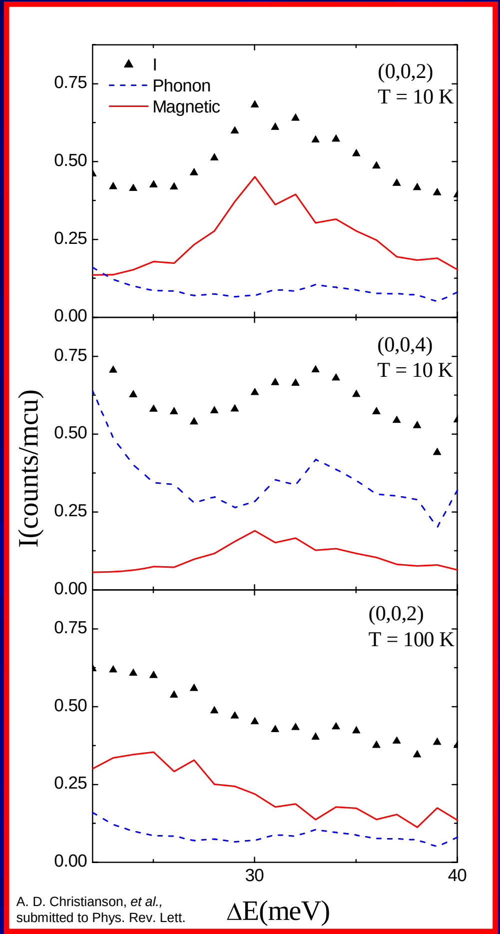


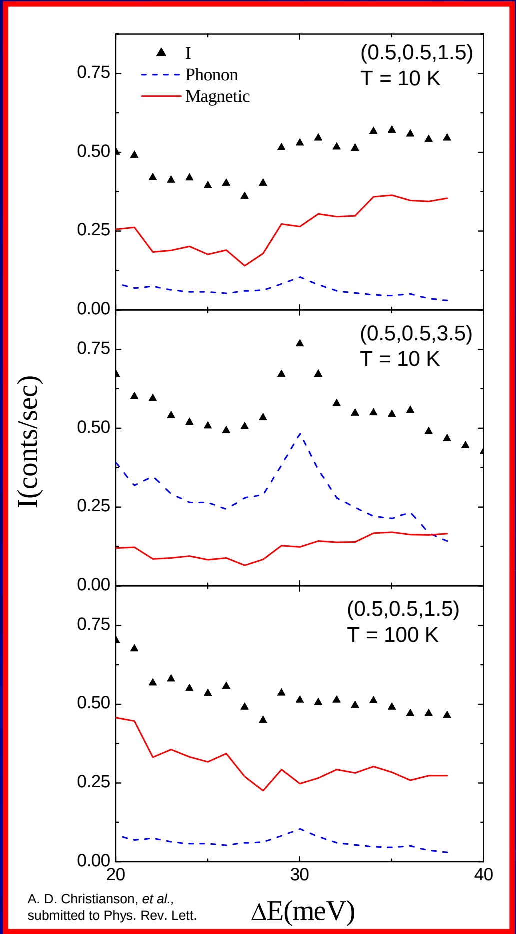


In agreement with earlier studies there is a phonon contribution underneath the magnetic scattering

Analysis

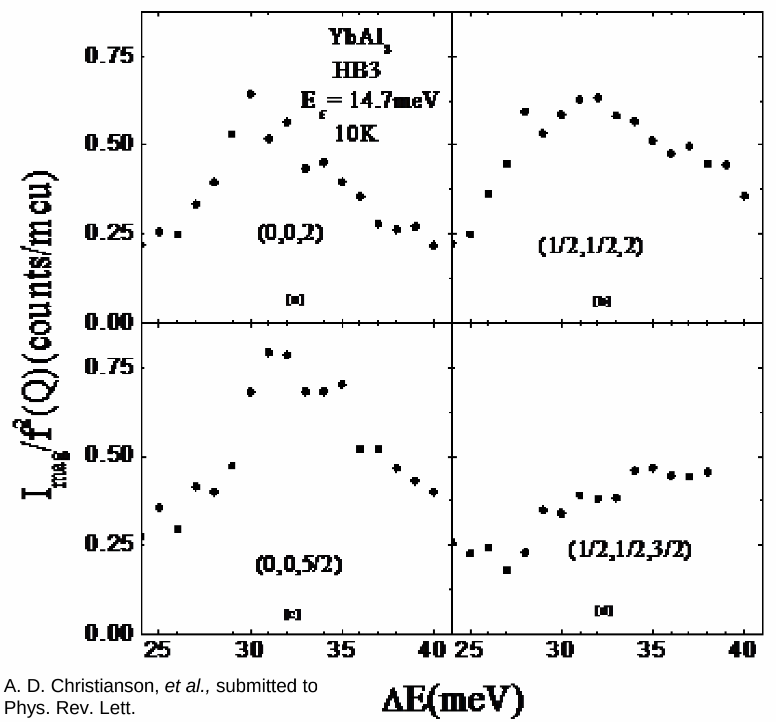
- Phonons scale with Q^2
- Magnetic Scattering scales with form factor
- Check consistency with 100 K data





Magnetic Scattering

- The excitation at E_2 is independent of Q at
  - zone center (0,0,2)
  - zone boundary (1/2,1/2,2)
  - zone boundary (0,0,1/2)
- But not at
  - zone boundary (1/2,1/2,1/2)
- If the scattering at E_1 represents the indirect gap scattering then the scattering at E_2 resides within the gap



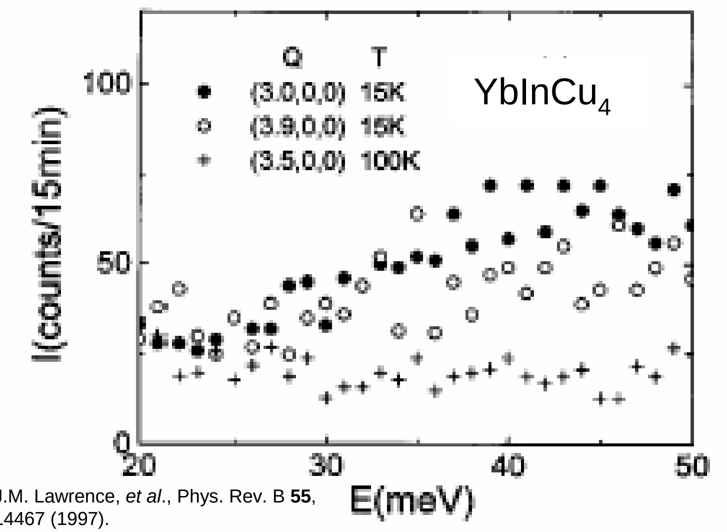
A. D. Christianson, *et al.*, submitted to Phys. Rev. Lett.

The scattering at E_2 is independent of Q for a large part of the zone

IV metals

- Few IV metals single crystal samples have been studied
- $CePd_3$ and $CeSn_3$
  - Some evidence for scattering due to a second energy scale
  - Form factor anomaly
- $YbInCu_4$
  - Very little Q-dependence (neutron absorption?)

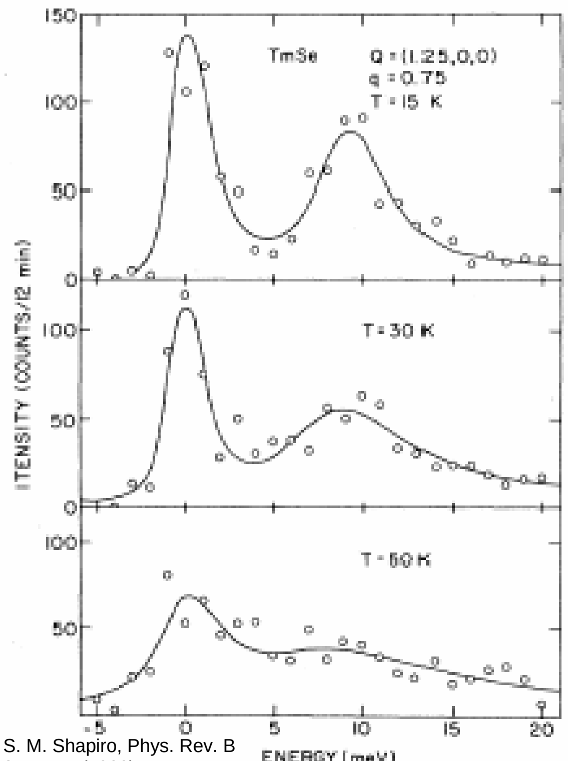
- No form factor anomaly in $YbAl_3$



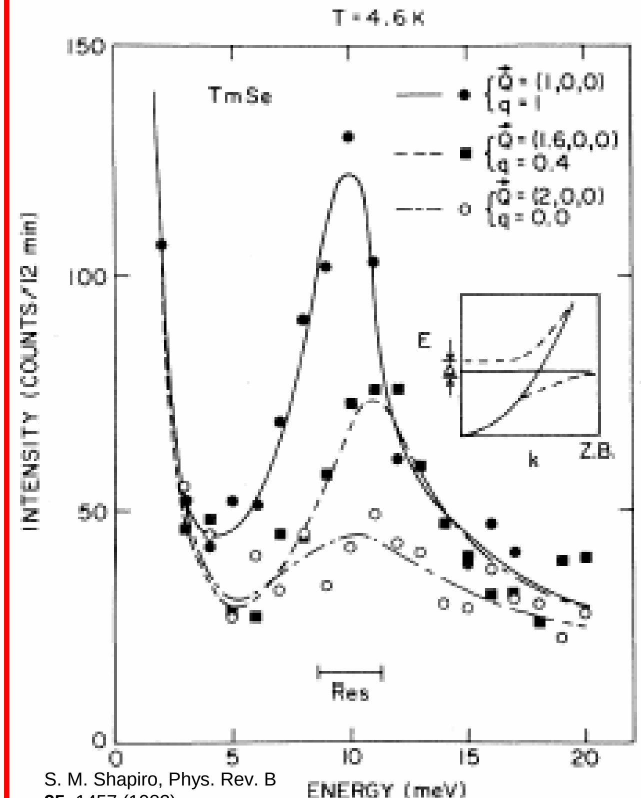
J.M. Lawrence, *et al.*, Phys. Rev. B **55**, 14467 (1997).

Need additional INS studies of single crystal IV metals

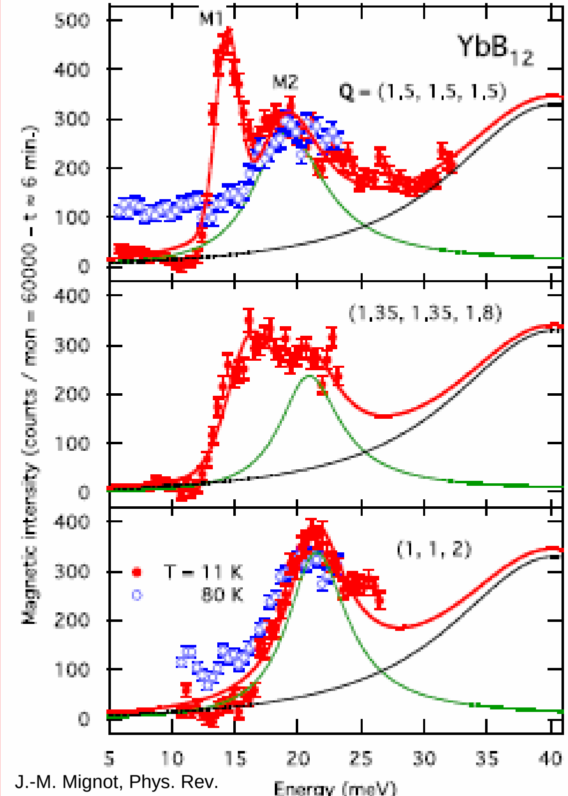
Comparison to Kondo Insulators



S. M. Shapiro, Phys. Rev. B **25**, 1457 (1982).



S. M. Shapiro, Phys. Rev. B **25**, 1457 (1982).



J.-M. Mignot, Phys. Rev. Lett. **94**, 247204 (2005).

- Kondo insulators-Also have deep minimum in optical conductivity
- Sharp excitation strongly dependent on temperature
- Strongly Q-dependent (strongest at zone boundary)

The scattering due to the hybridization gap is similar to the broad scattering at E_1 in $YbAl_3$ NOT the excitation at E_2

Conclusions

- The scattering at E_1 = 50 meV appears related to the hybridization gap scattering as observed in the Kondo insulators.
- The scattering at E_2 = 33 meV is (apart from the 4f form factor) independent of Q over a large fraction of the zone.
- The peak at E_2 in the INS data may arise from a spatially-localized excitation in the hybridization gap.