INSTITUTE FOR **QUANTUM MATTER**

A collaboration between
JOHNS HOPKINS UNIVERSITY
and PRINCETON UNIVERSITY

Magnetic Excitations in the Kondo Insulator SmB_6

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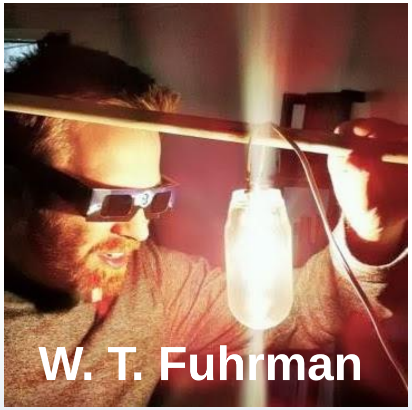


Publications:

W. T. Fuhrman, J. C. Leiner et al., PRL (2015)

W. T. Fuhrman & P. Nikolic PRB (2014)

W. A. Phelan et al. PRX (2014)

SPALLATION NEUTRON SOURCE

Outline

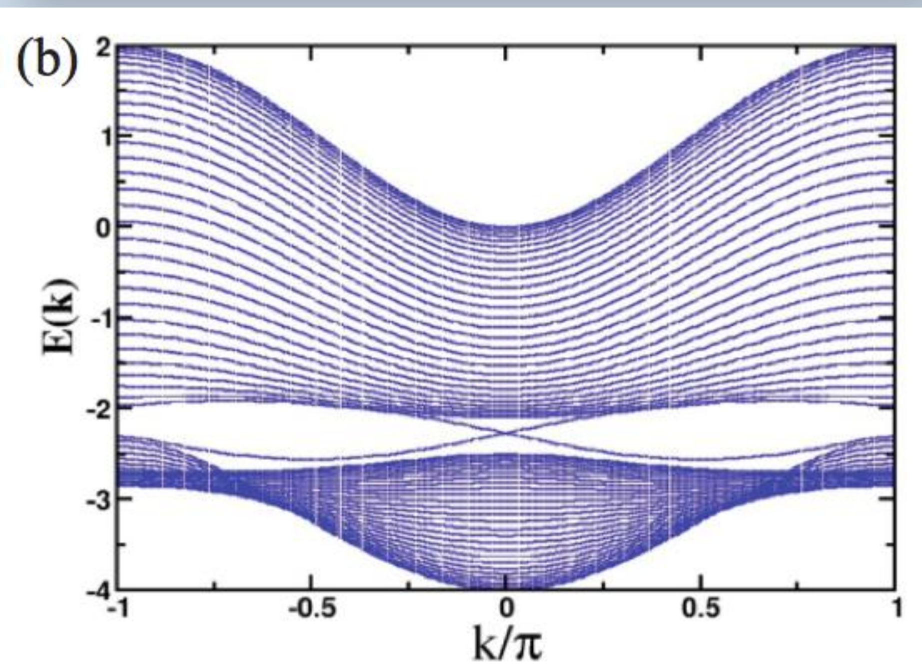
- **Introduction**
  - Kondo Insulators and topology
  - Neutron Scattering
- **The SmB_6 enigma**
  - Transport and thermal properties
  - A resonance with d-form-factor
  - From scattering to Z_2 invariant
- **Resonances & electronic order**
- **Conclusions**

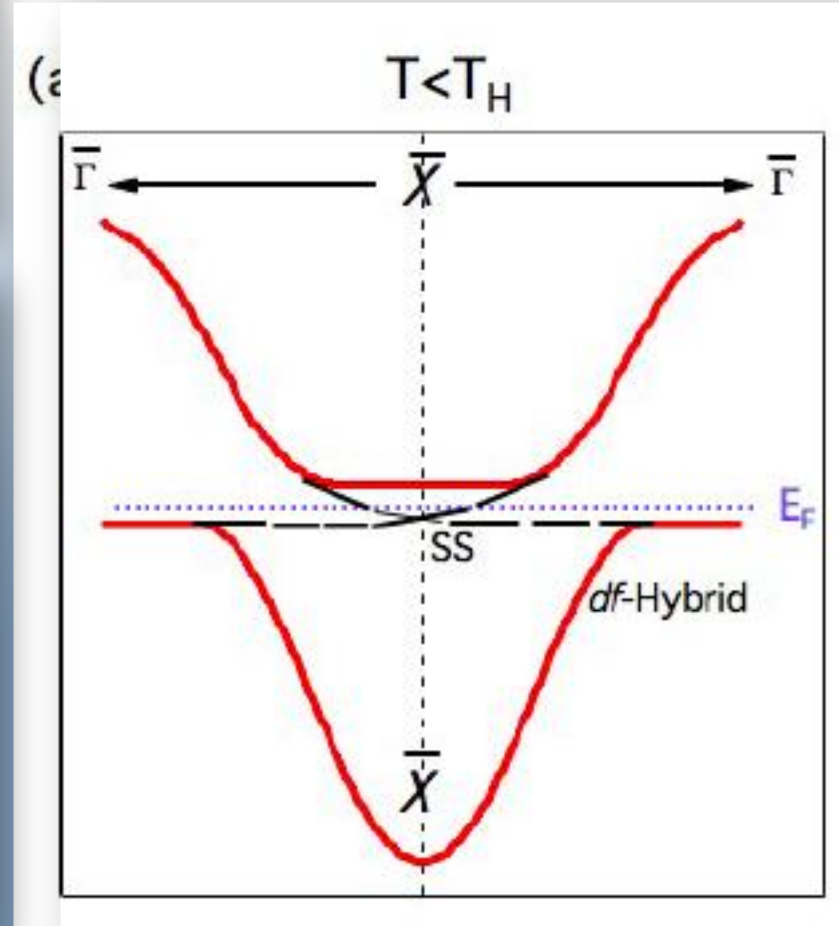
Topological Kondo Insulators

Maxim Dzero,[1] Kai Sun,[1] Victor Galitski,[1] and Piers Coleman[2]

Neuprane et al. (2013)

$$\hat{H} = \sum_{\mathbf{k},\alpha} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + \sum_{j\alpha} [V c^{\dagger}_{j\alpha} f_{j\alpha} + \text{H.c.}] + \sum_{j\alpha} \left[\varepsilon_f^{(0)} n_{f,j\alpha} + \frac{U_f}{2} n_{f,j\alpha} n_{f,j\bar{\alpha}} \right]$$





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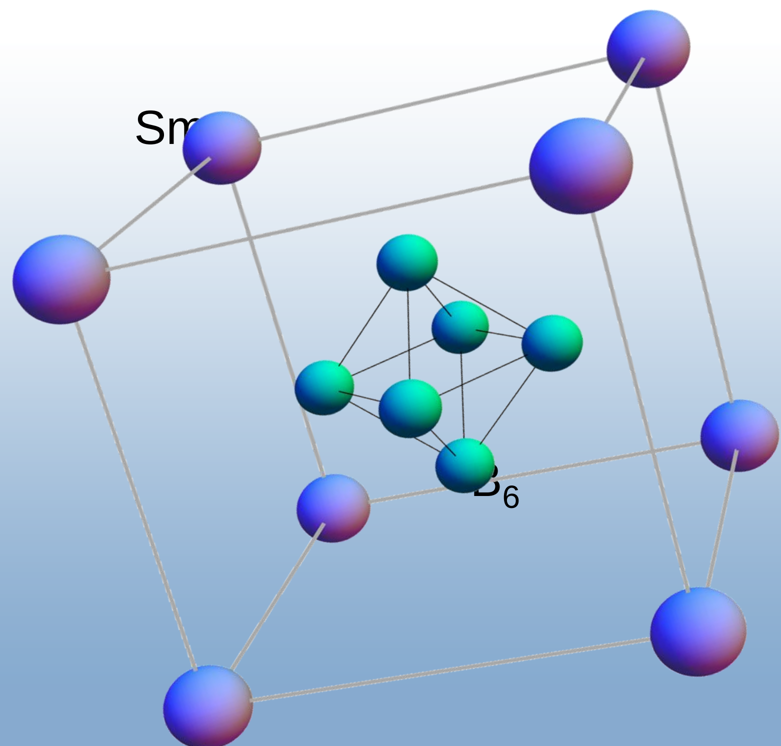
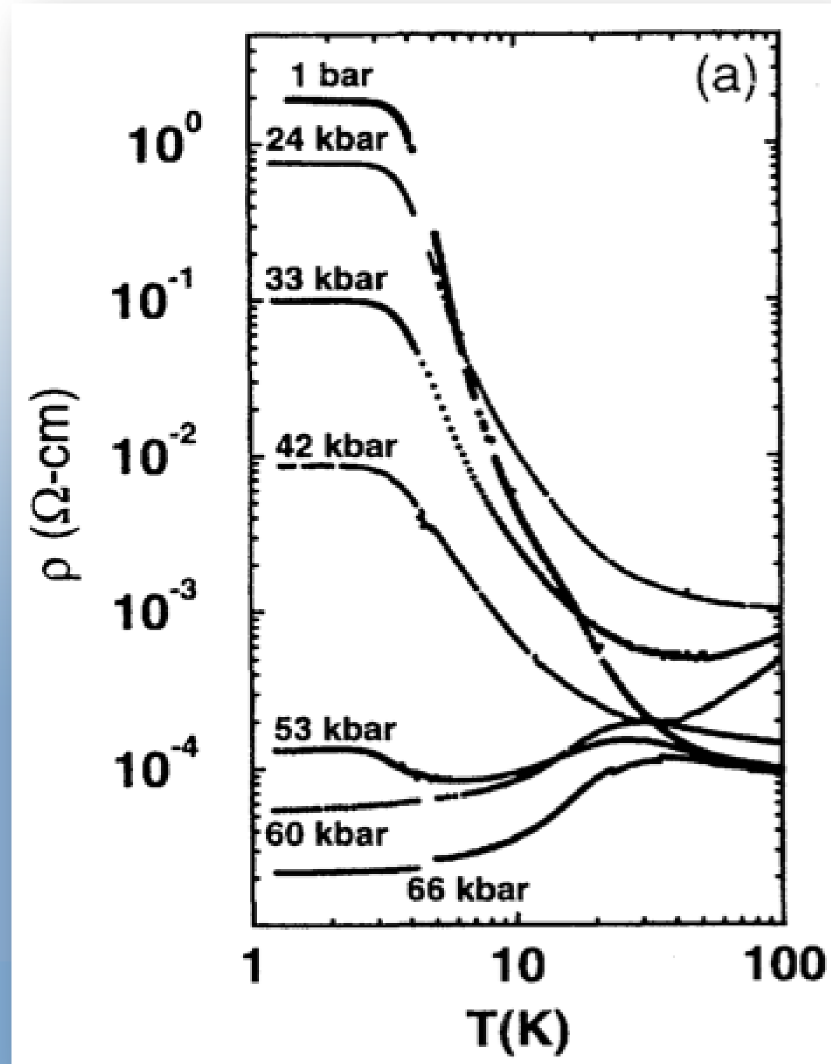
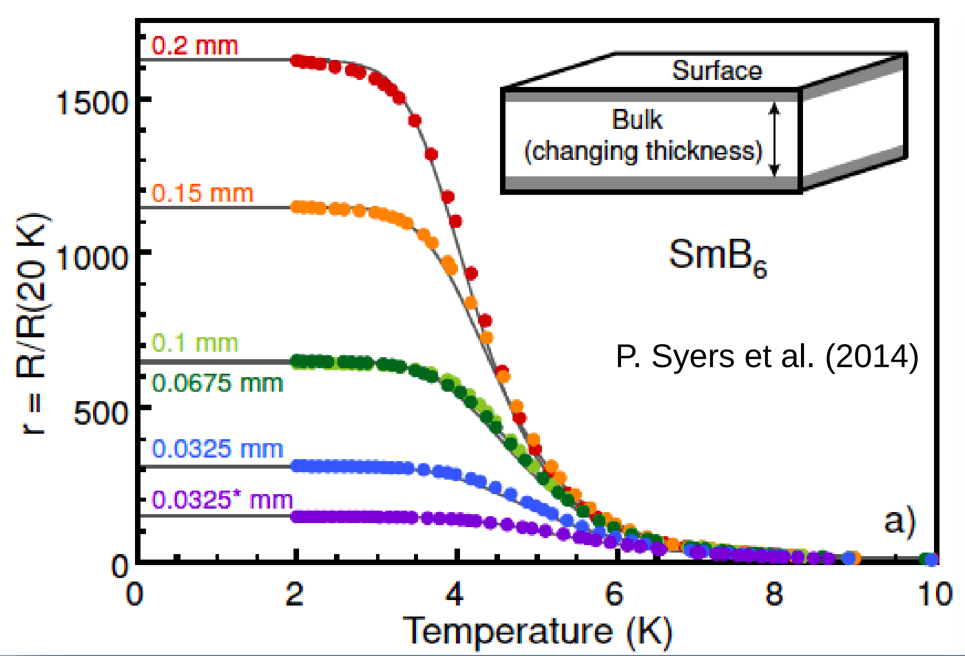
SmB_6: Kondo Insulator or Exotic Metal?

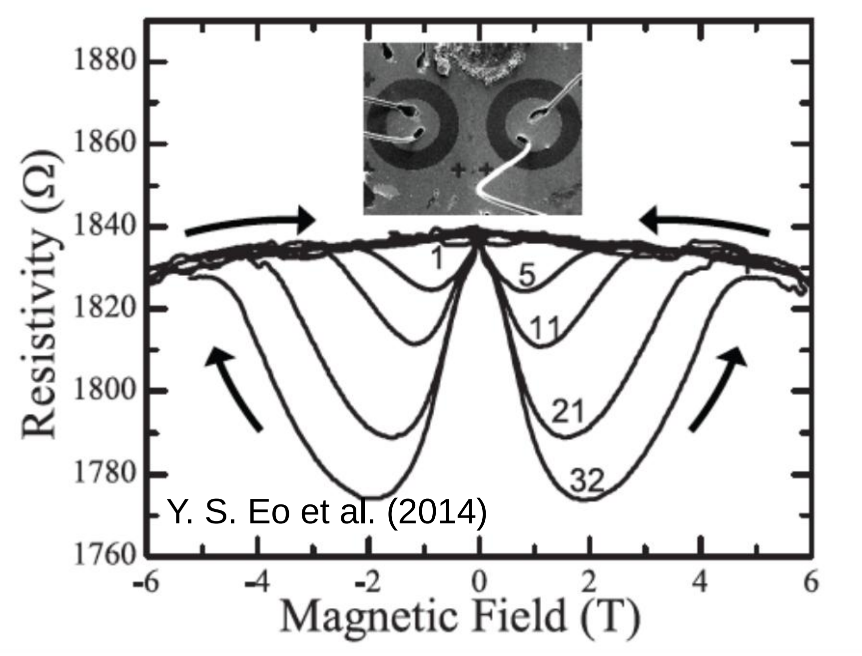
J. C. Cooley,[1] M. C. Aronson,[1] Z. Fisk,[2] and P. C. Canfield[3]





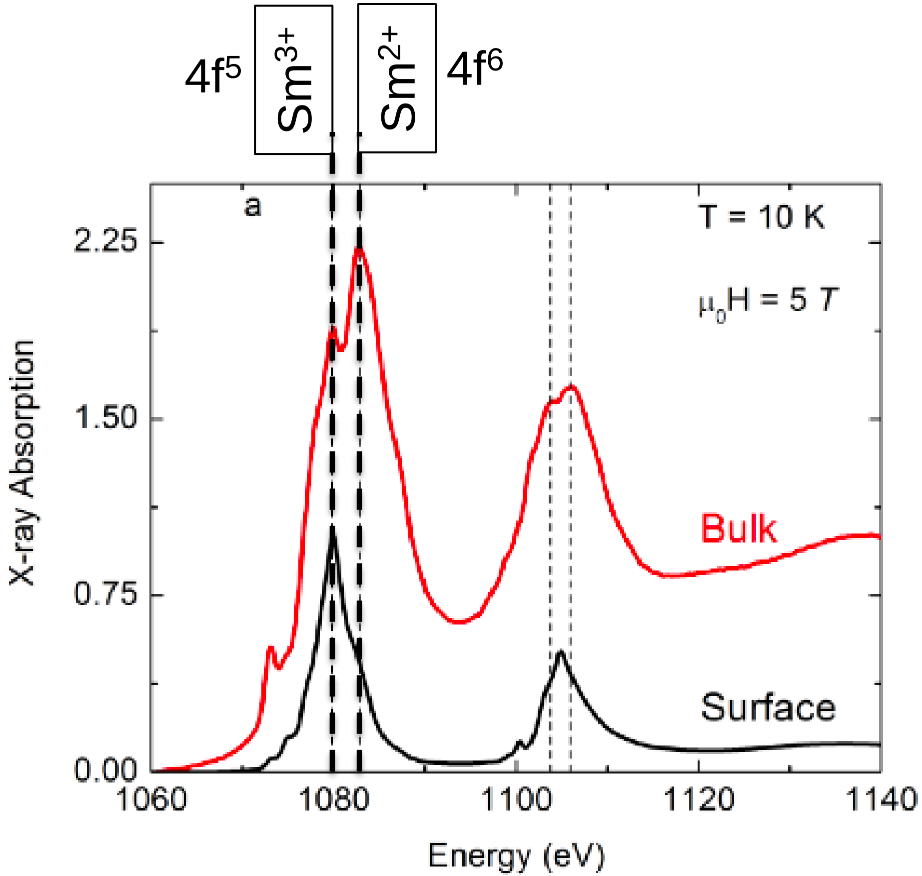
Surface conduction in SmB_6





- The variation of resistance ratio with sample dimensions indicates surface conduction dominates in the low T regime where the bulk insulates
- The hysteretic effects of a magnetic field on surface conduction is indicative of surface magnetism: We are getting what we asked for!

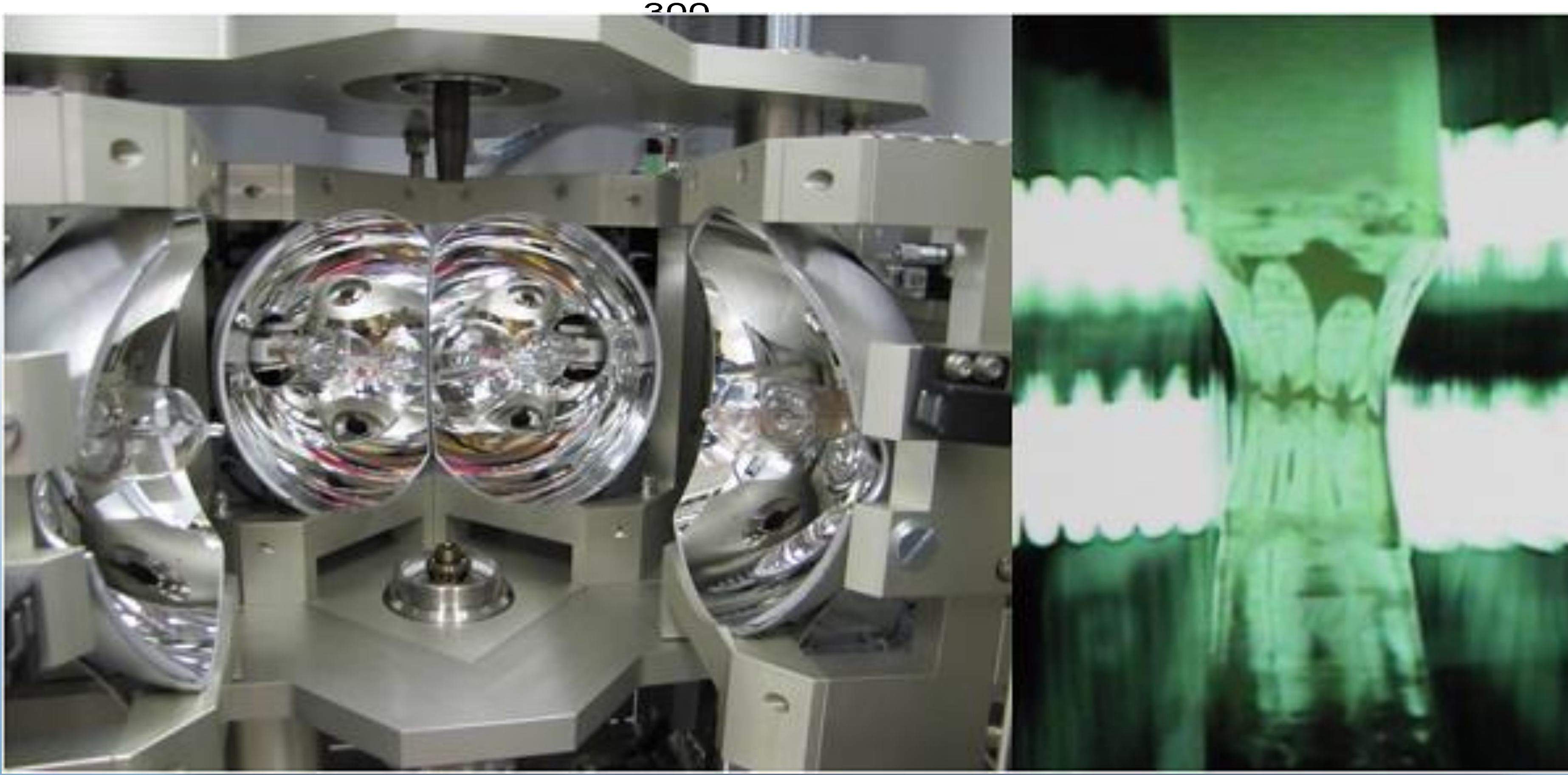
Surface magnetism from Sm^{3+}



$$4f^5 \quad L=5 \quad S=\tfrac{5}{2} \quad J=|L-S|=\tfrac{5}{2}$$

$$4f^6 \quad L=3 \quad S=3 \quad J=|L-S|=0$$

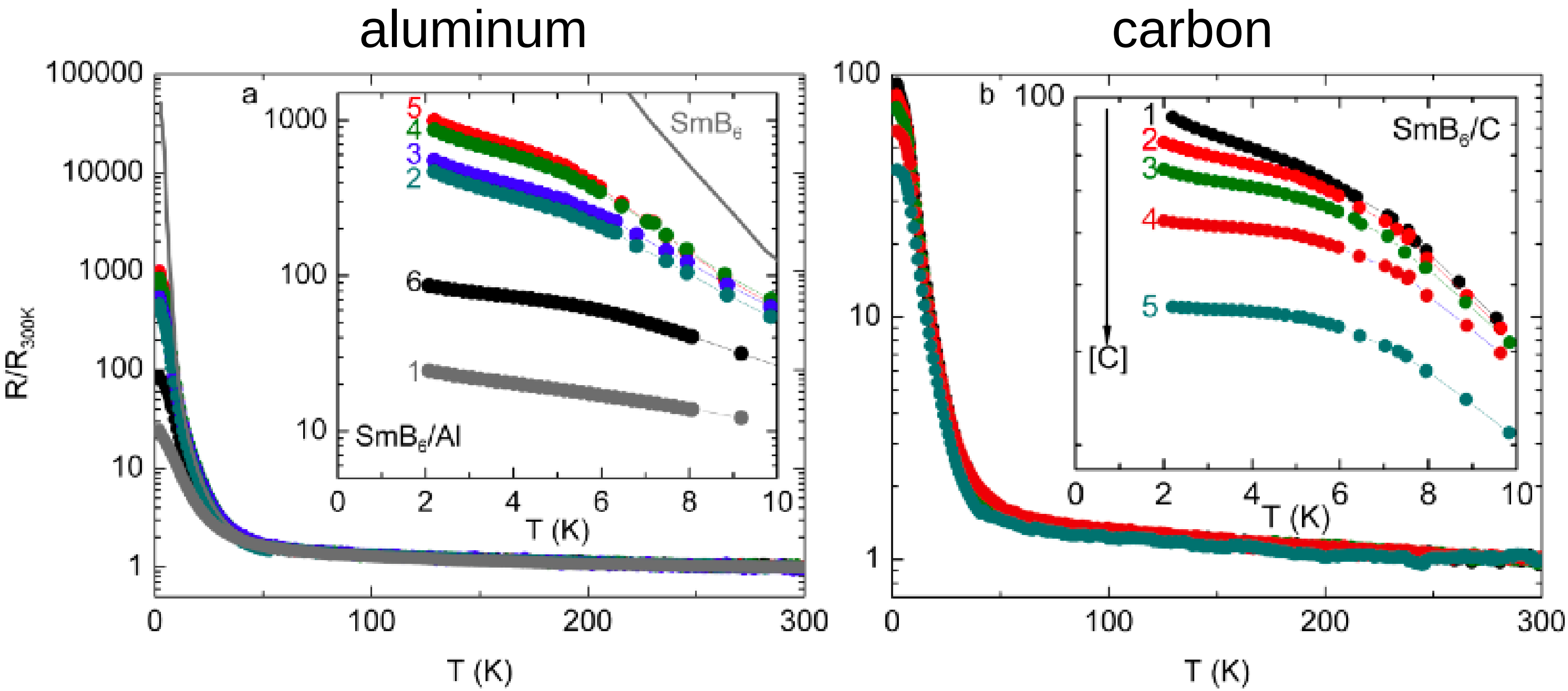
Floating Zone SmB_6



Why different low T sheet resistance in FZ samples:

- Absence of aluminum and carbon in FZ crystals
- Topological: Surface magnetism is different
- Unprotected: surface chemistry or magnetism

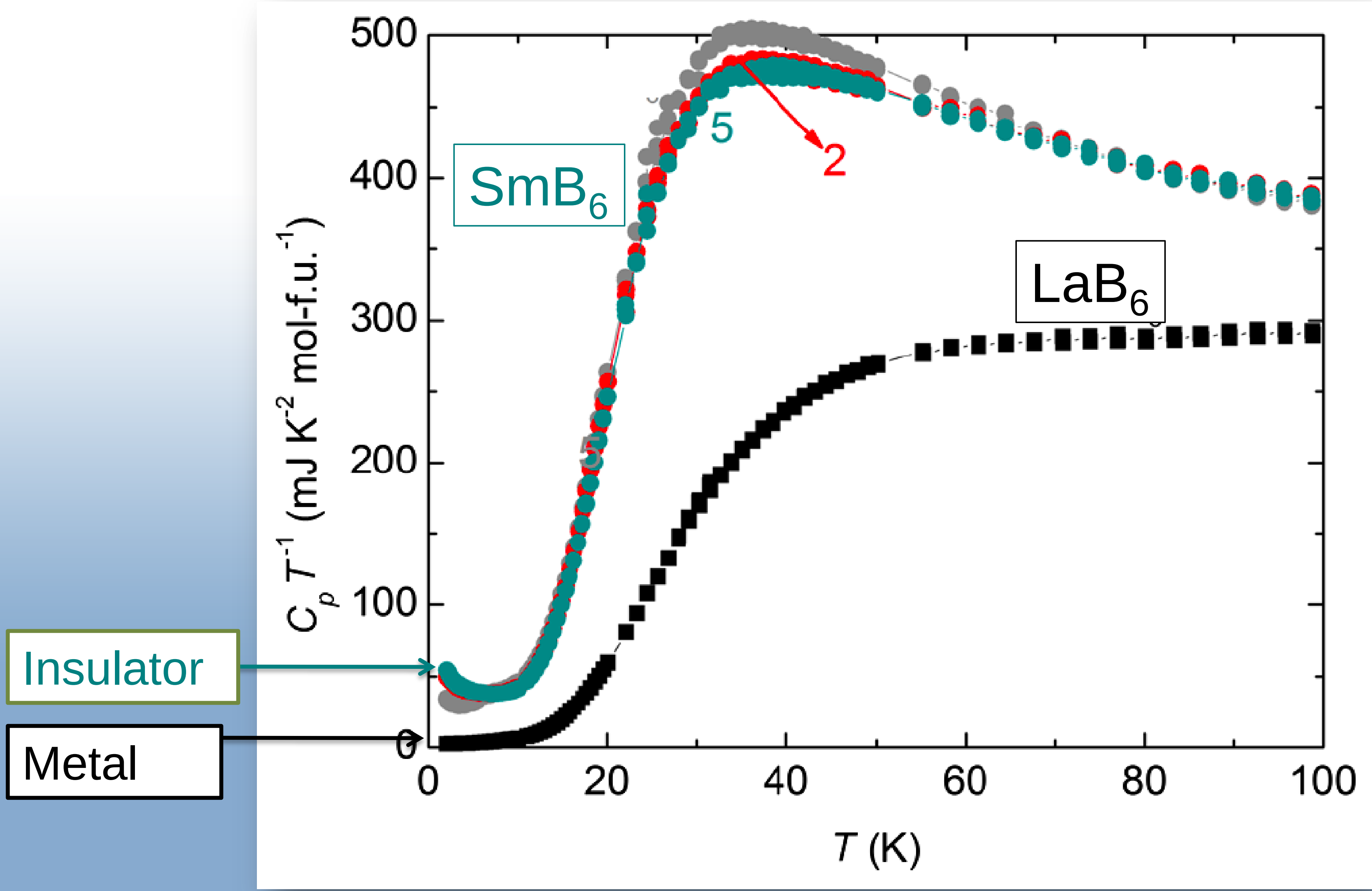
Doping & low T transport



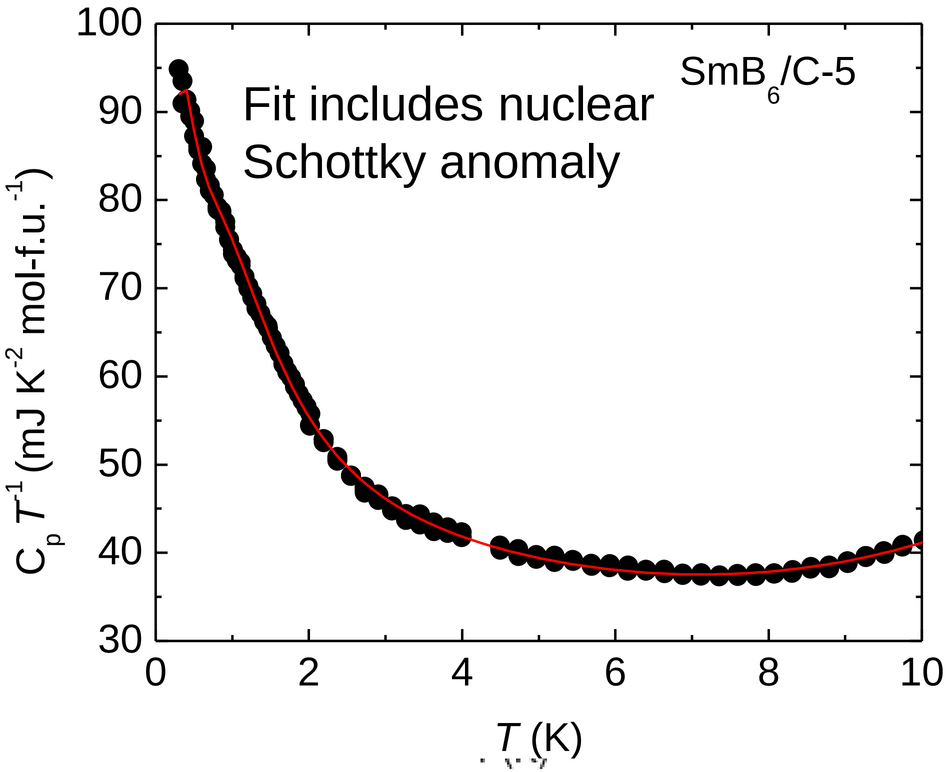
Aluminum: filamentary inclusions observed in flux grown single crystals

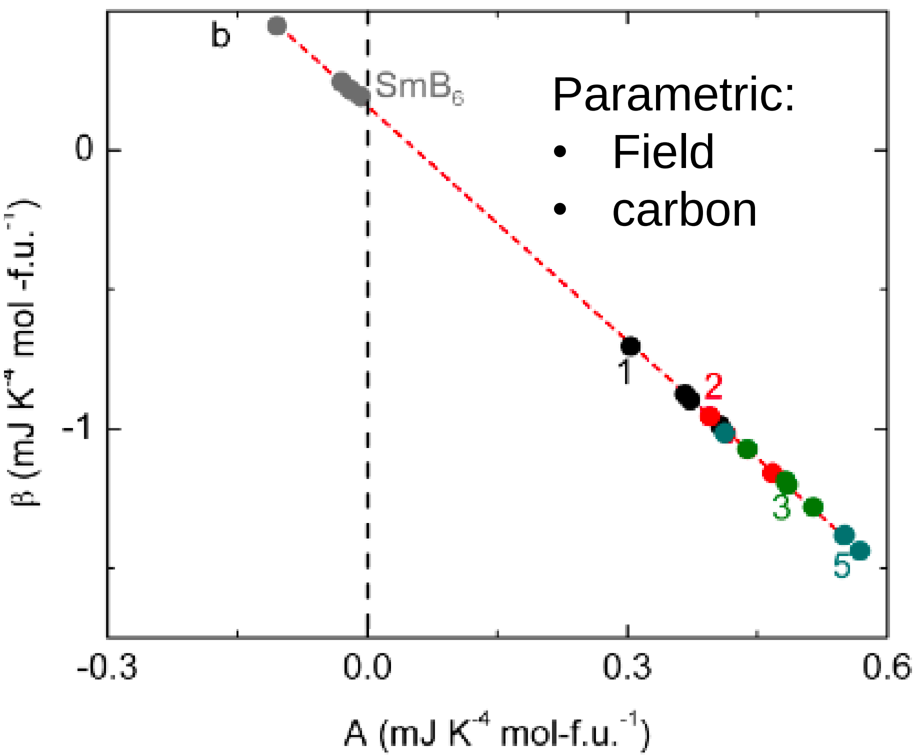
Carbon: Produces a plateau. Carbon is “everywhere” but not in IQM floating zone crystals!

Bulk C(T): Sommerfeld constant in insulator?



Parametric effect of carbon & field



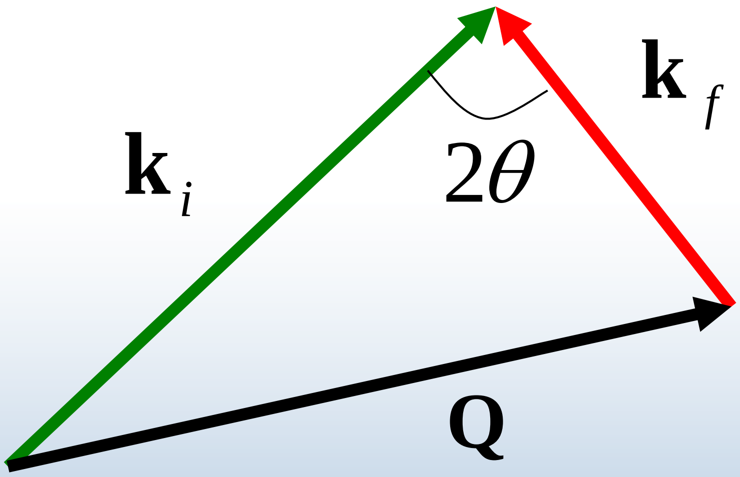


$$Cp/T = g + b_3 T^2 + A T^2 \ln\frac{T}{T^*}$$ for all C-doped samples and fields

$$b = b_3 - A \ln T^* \text{ where } T^* = 17\text{ K and } q_D = 230\text{ K}$$

C-doping & magnetic field shift the chemical potential

Magnetic Neutron Scattering



$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

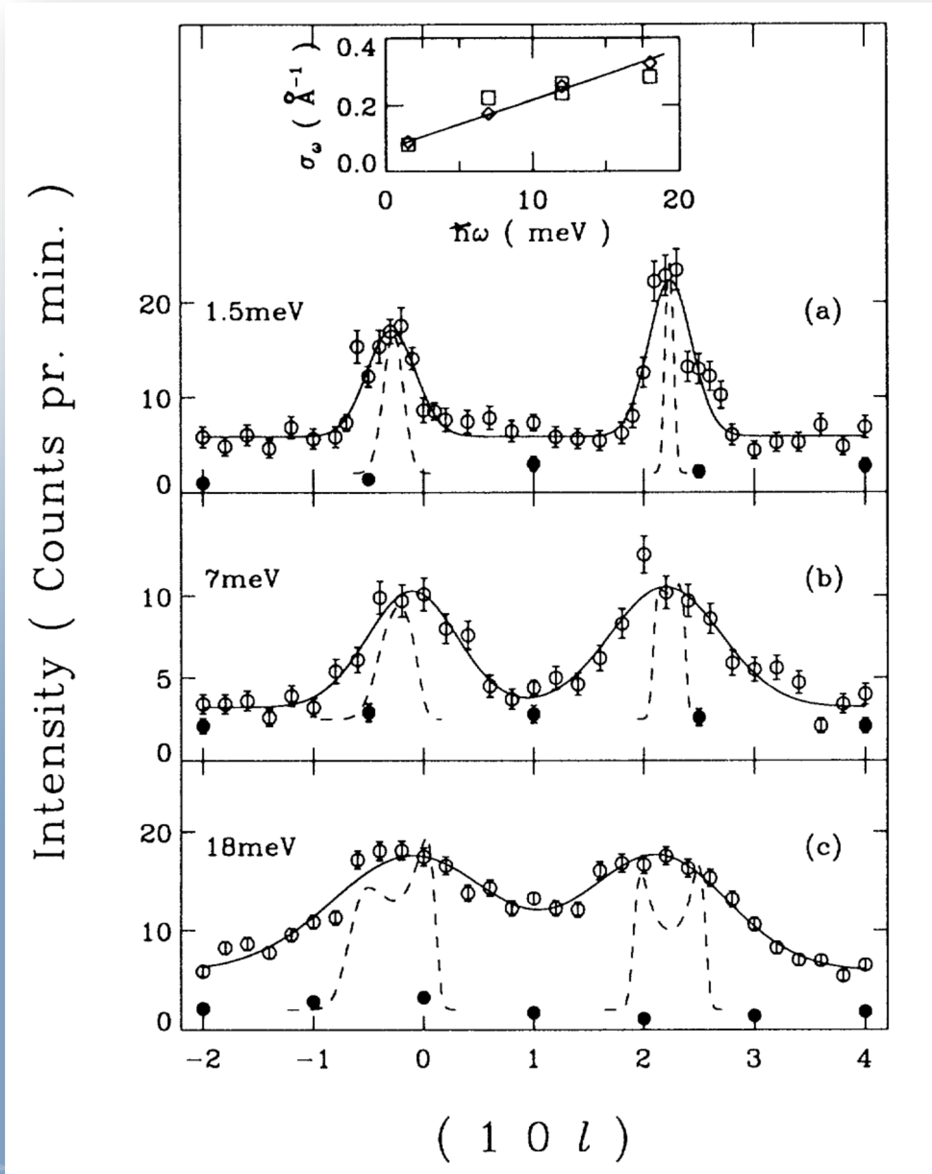
$$\hbar\omega = E_i - E_f$$

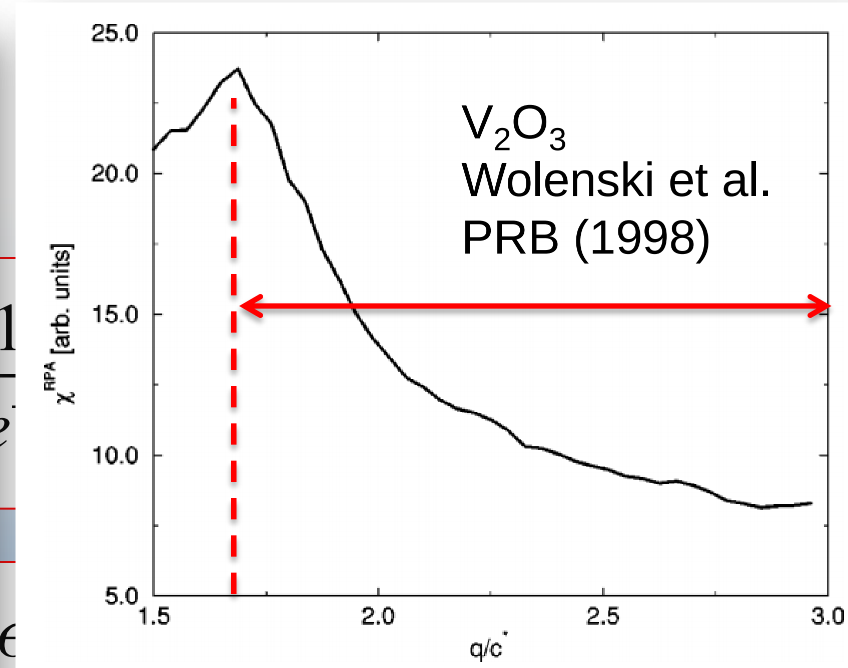
$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i} N r_0^2 \left| \frac{g}{2} F(Q) \right|^2 e^{-2W(Q)} \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta \right) \mathcal{S}^{\alpha\beta}(\mathbf{Q}\omega)$$

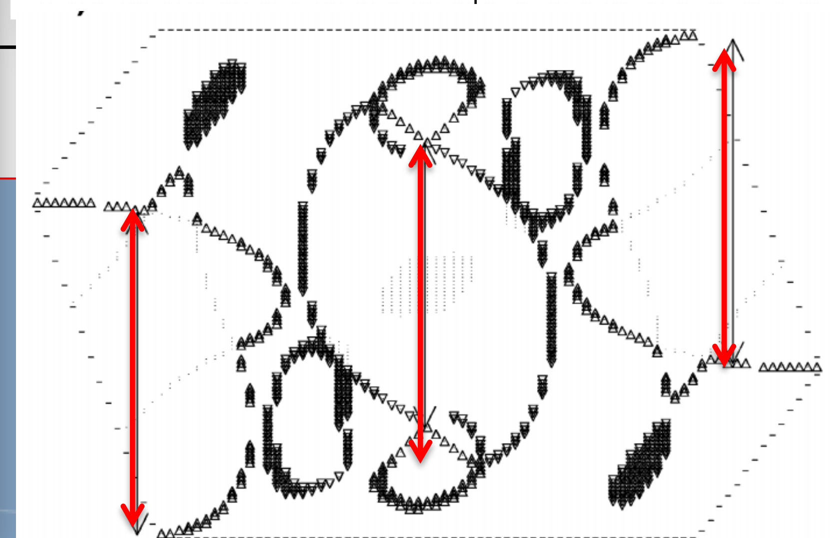
$$\mathcal{S}^{\alpha\beta}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar} \int dt\, e^{-i\omega t} \frac{1}{N} \sum_{\mathbf{RR}'} e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R}')} < S_{\mathbf{R}}^{\alpha}(0) S_{\mathbf{R}'}^{\beta}(t) >$$

Spin Fluctuations & Neutrons Scattering

***$V_{2-y}O_3$** Bao et al. PRL (1993)*



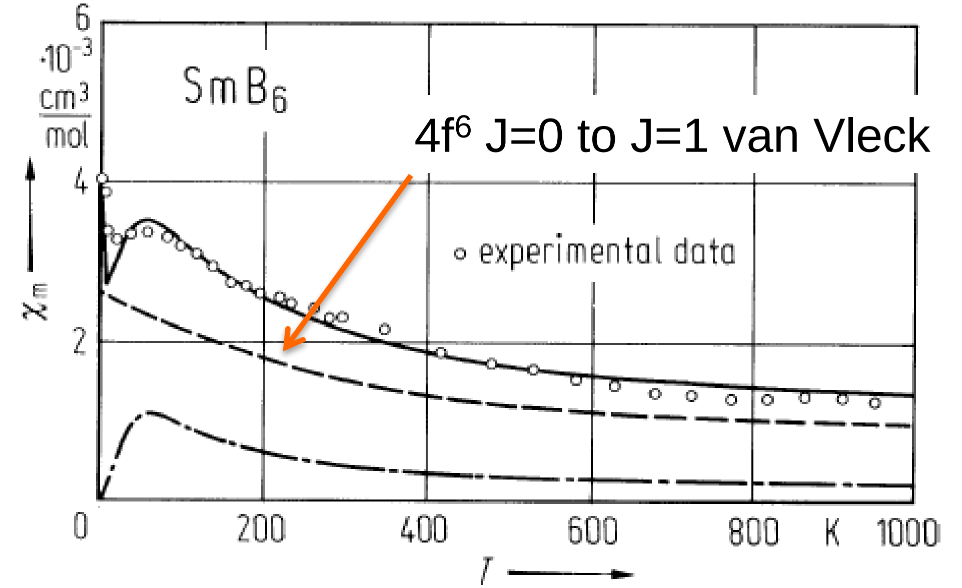


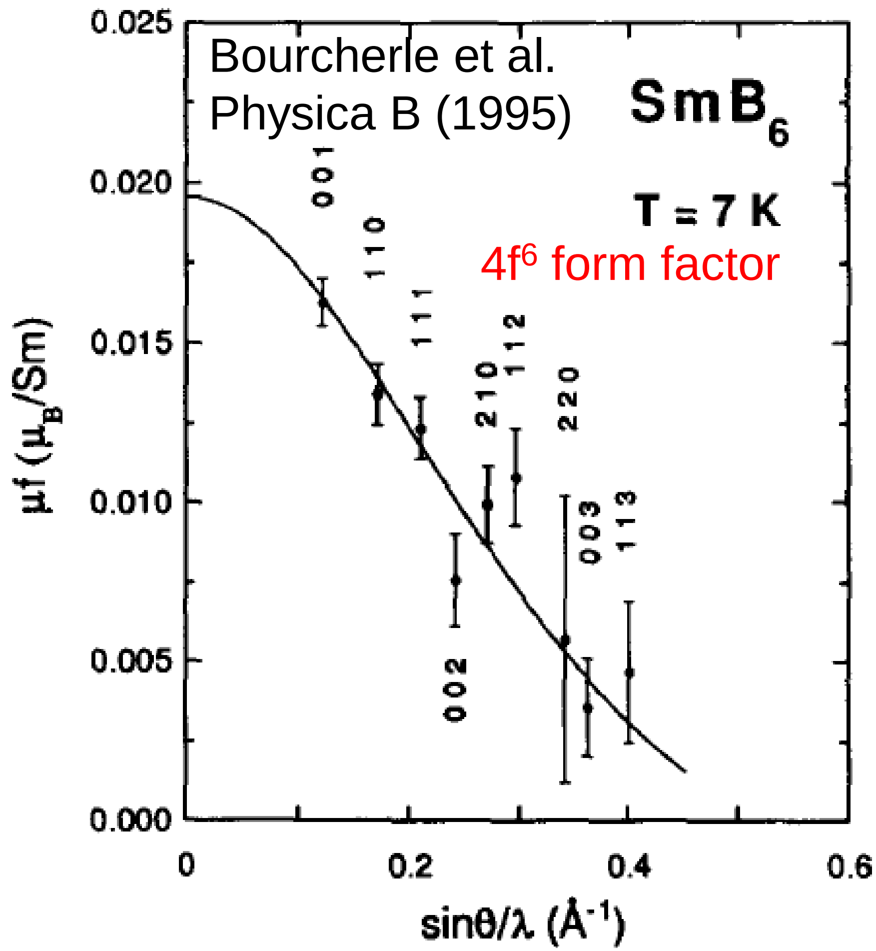


Q=0 Magnetism: Dominated by $4f^6$

$$F(\mathbf{Q}) = \langle j_0(Qr) \rangle + \left(1 - \frac{2}{g_J}\right) \langle j_2(Qr) \rangle$$

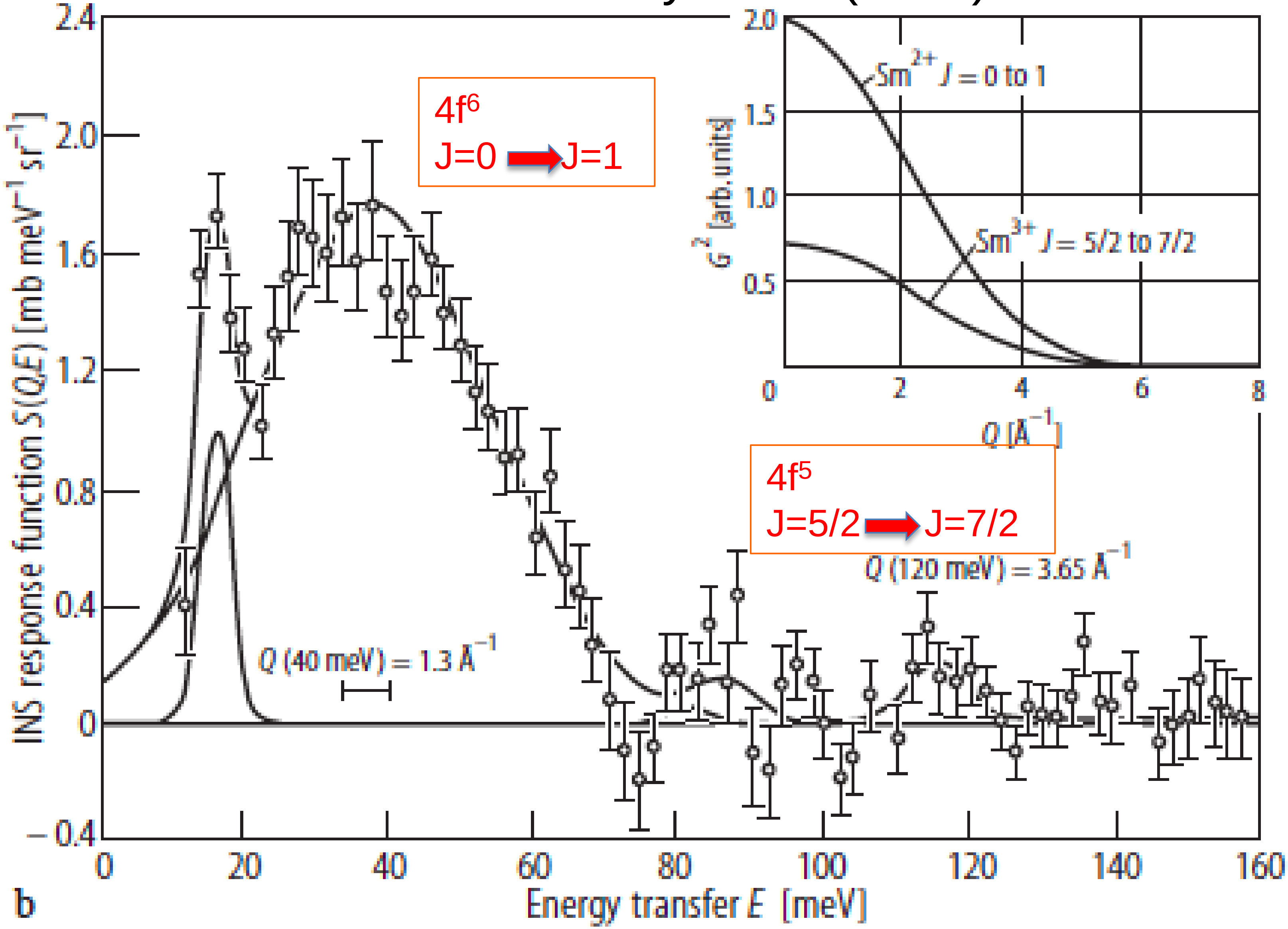
Nickerson et al. PRB (1971)





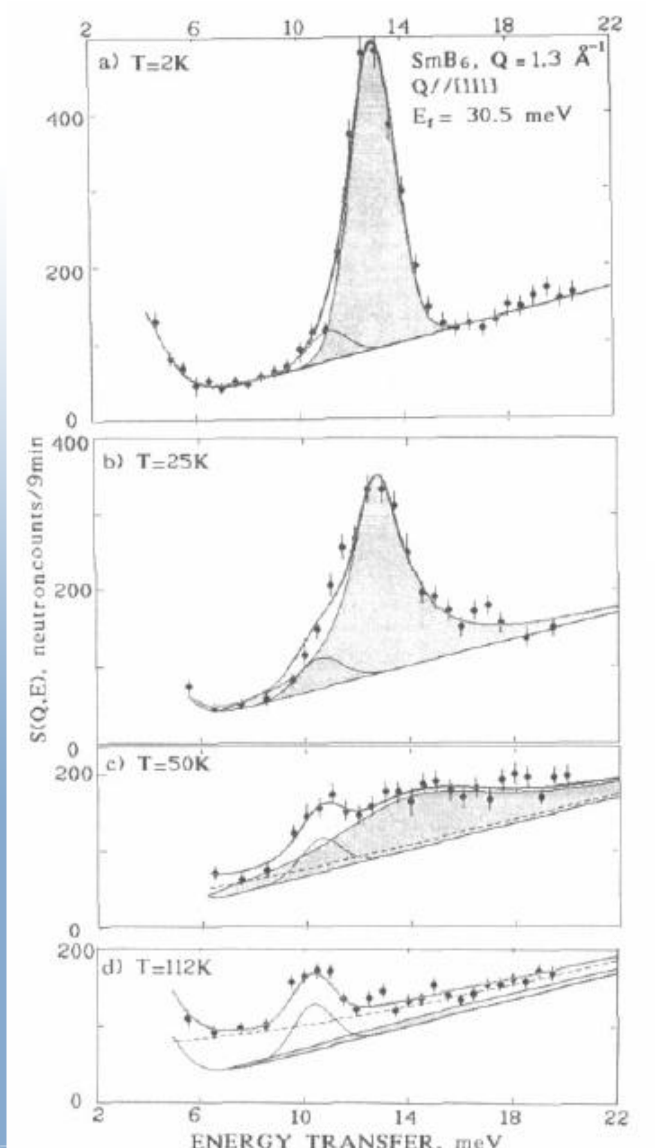
Inter J-multiplet Excitations

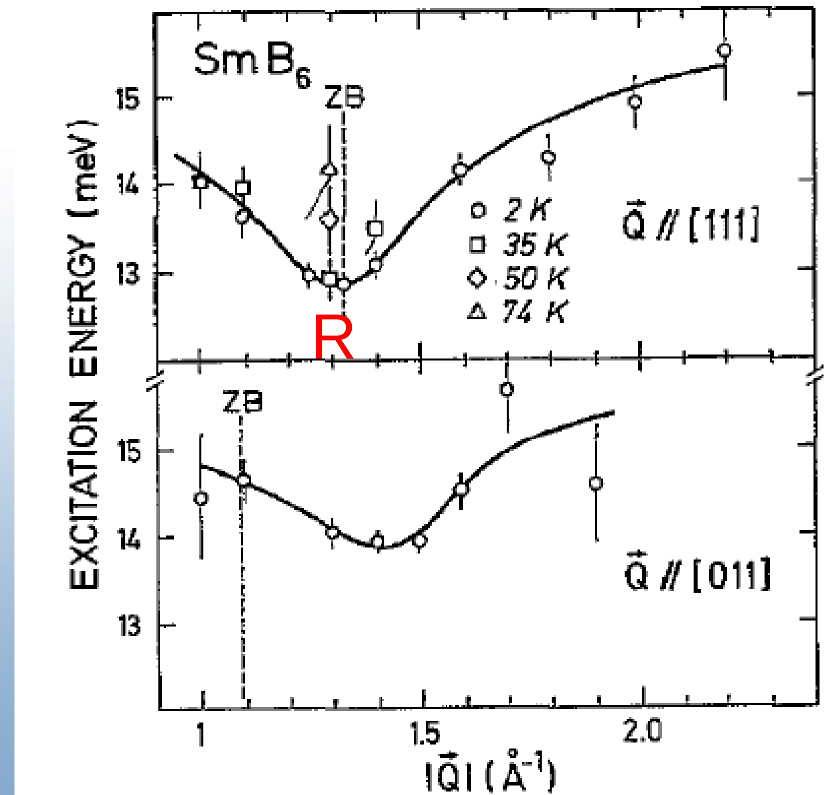
Alekseev et al. Physica B (1993)



Discovery of 14 meV Collective mode

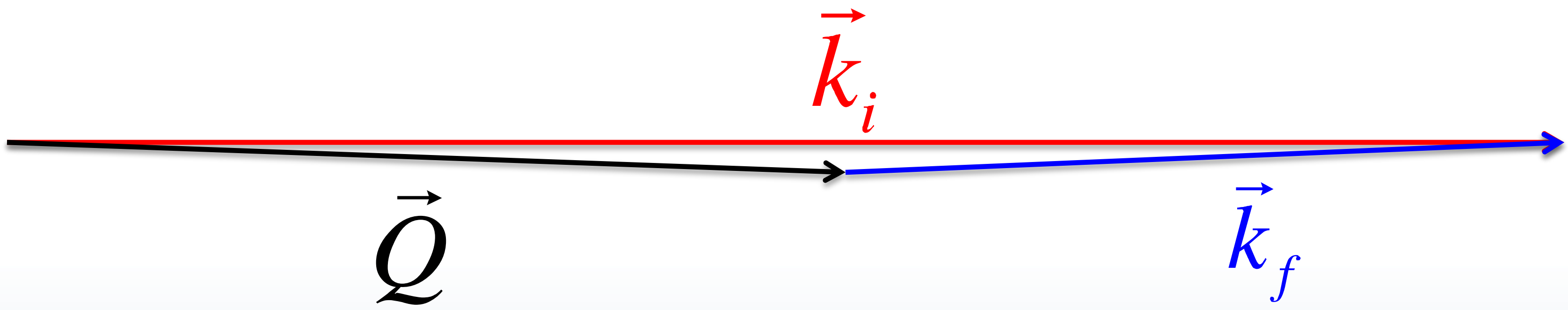
Alekseev, Mignot et al. (1995)

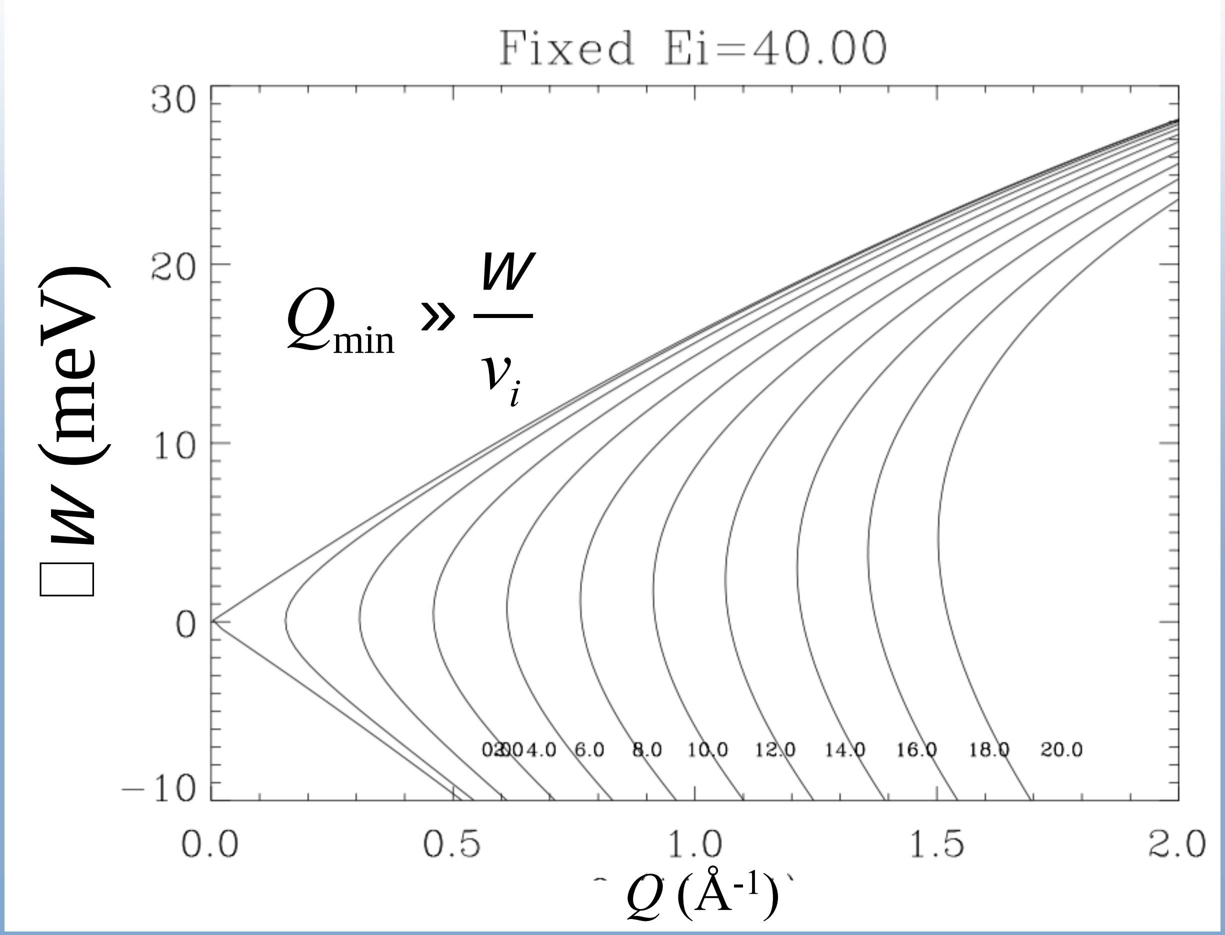




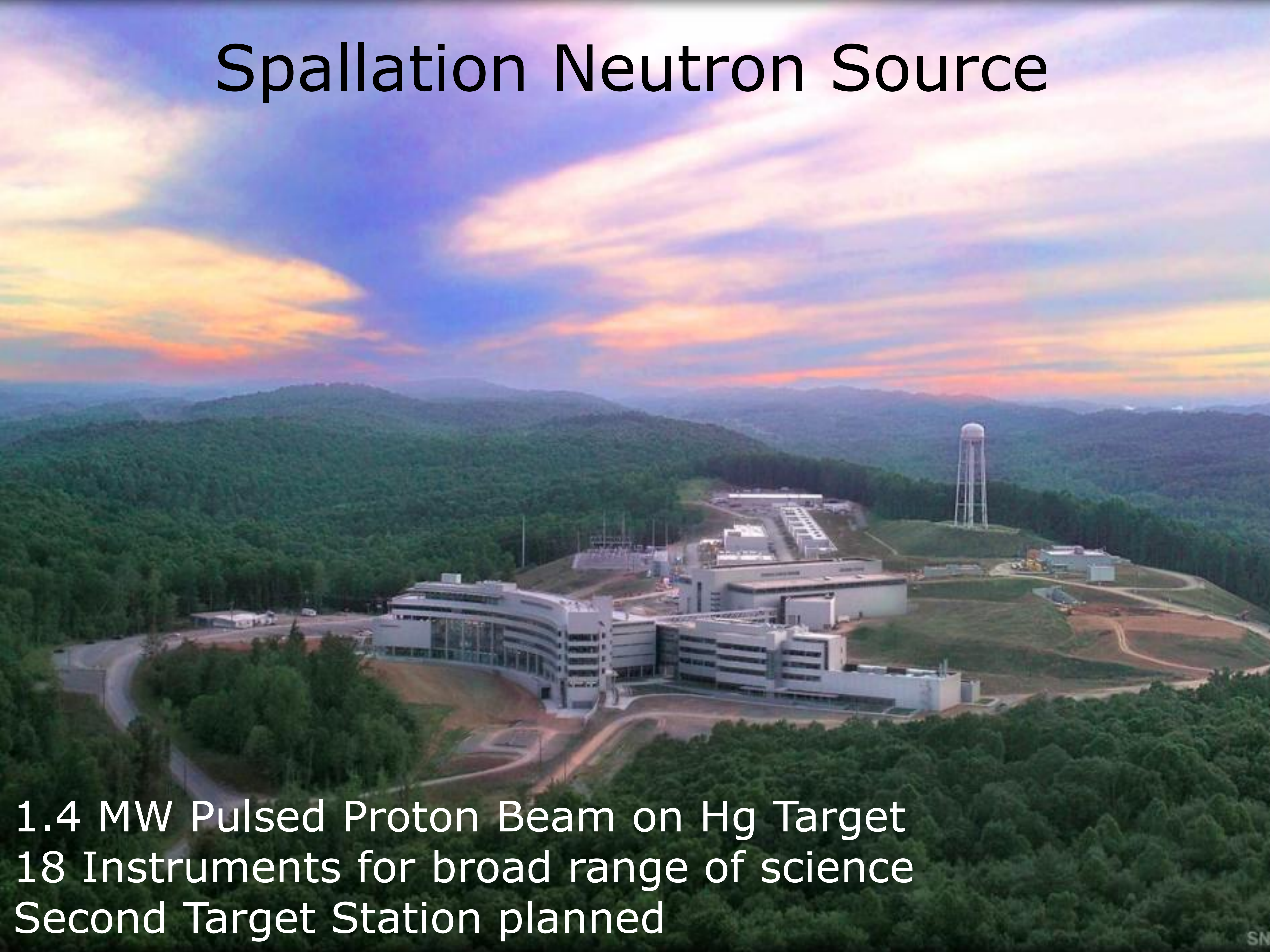
"…magnetic excitations from a novel, presumably singlet local bound state, resulting from the hybridization of the atomic f-electron wavefunctions with p and/or d orbitals from the neighbours."

Kinematics of scattering



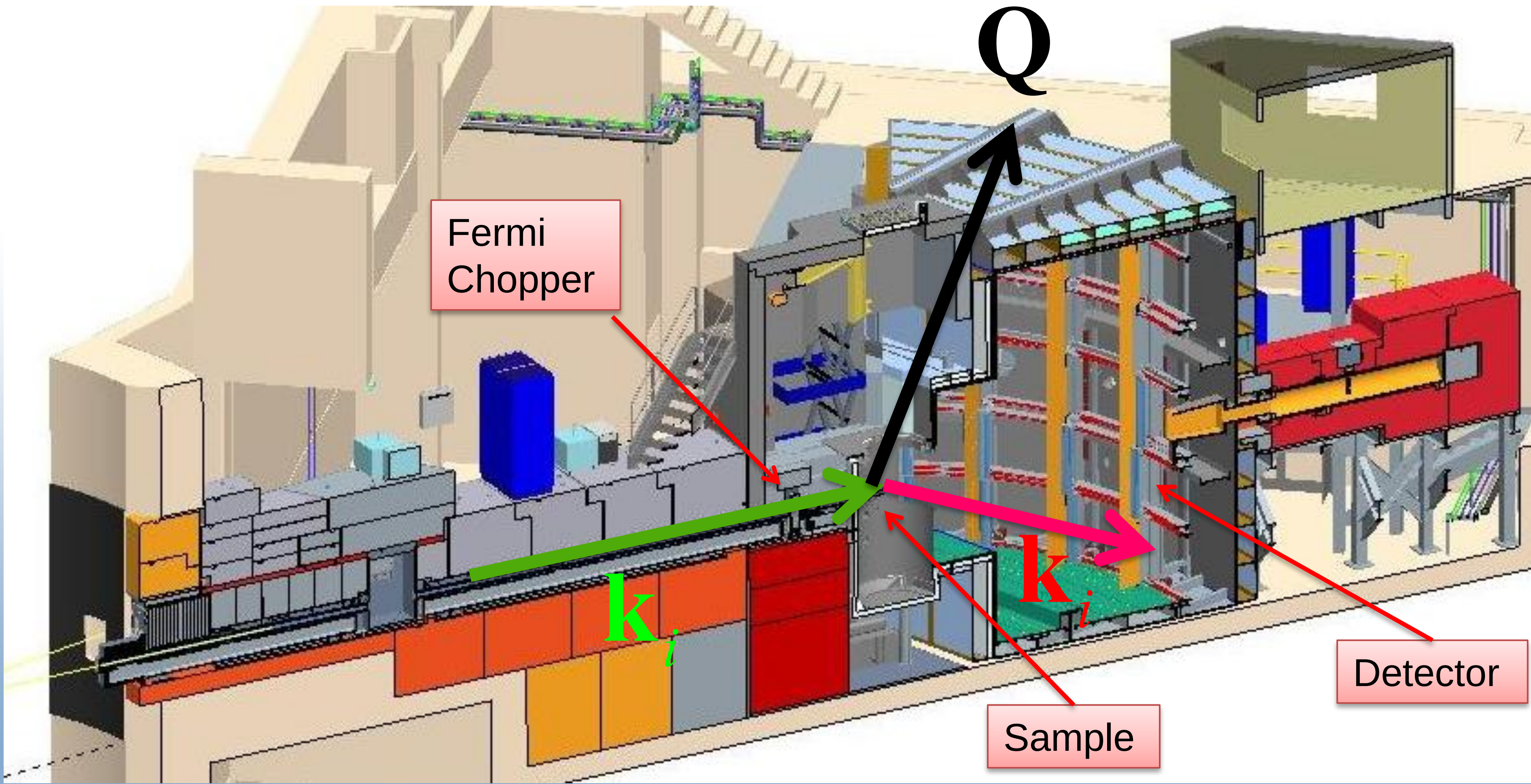


Spallation Neutron Source



1.4 MW Pulsed Proton Beam on Hg Target
18 Instruments for broad range of science
Second Target Station planned

SEQUOIA Time of Flight Spectrometer (ORNL)



$$t_{\text{chopper}} \rightarrow v_i$$

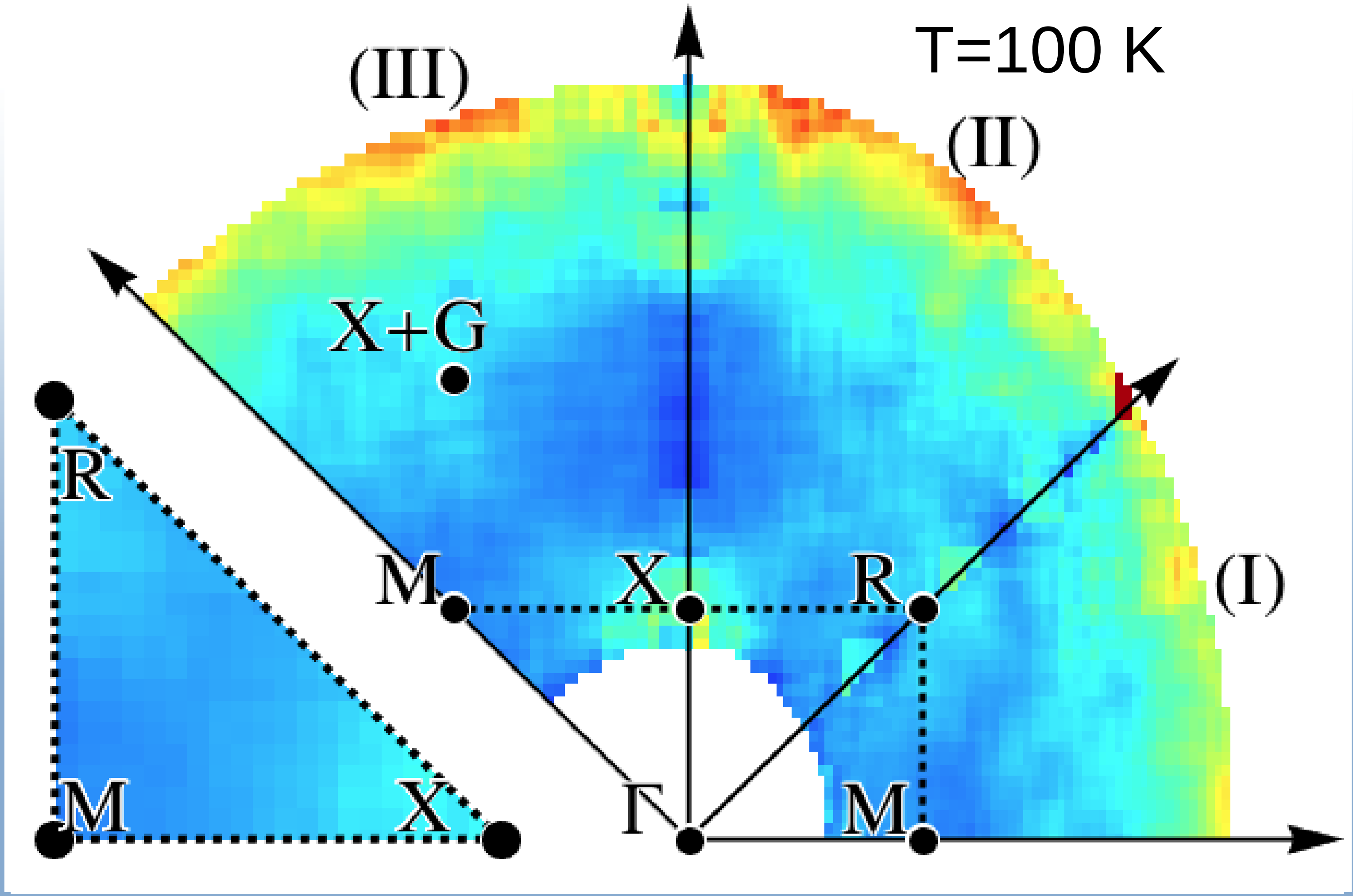
$$t_{\text{detector}} \rightarrow v_f$$

$$\hbar w = \tfrac{1}{2} m \left(v_i^2 - v_f^2 \right)$$

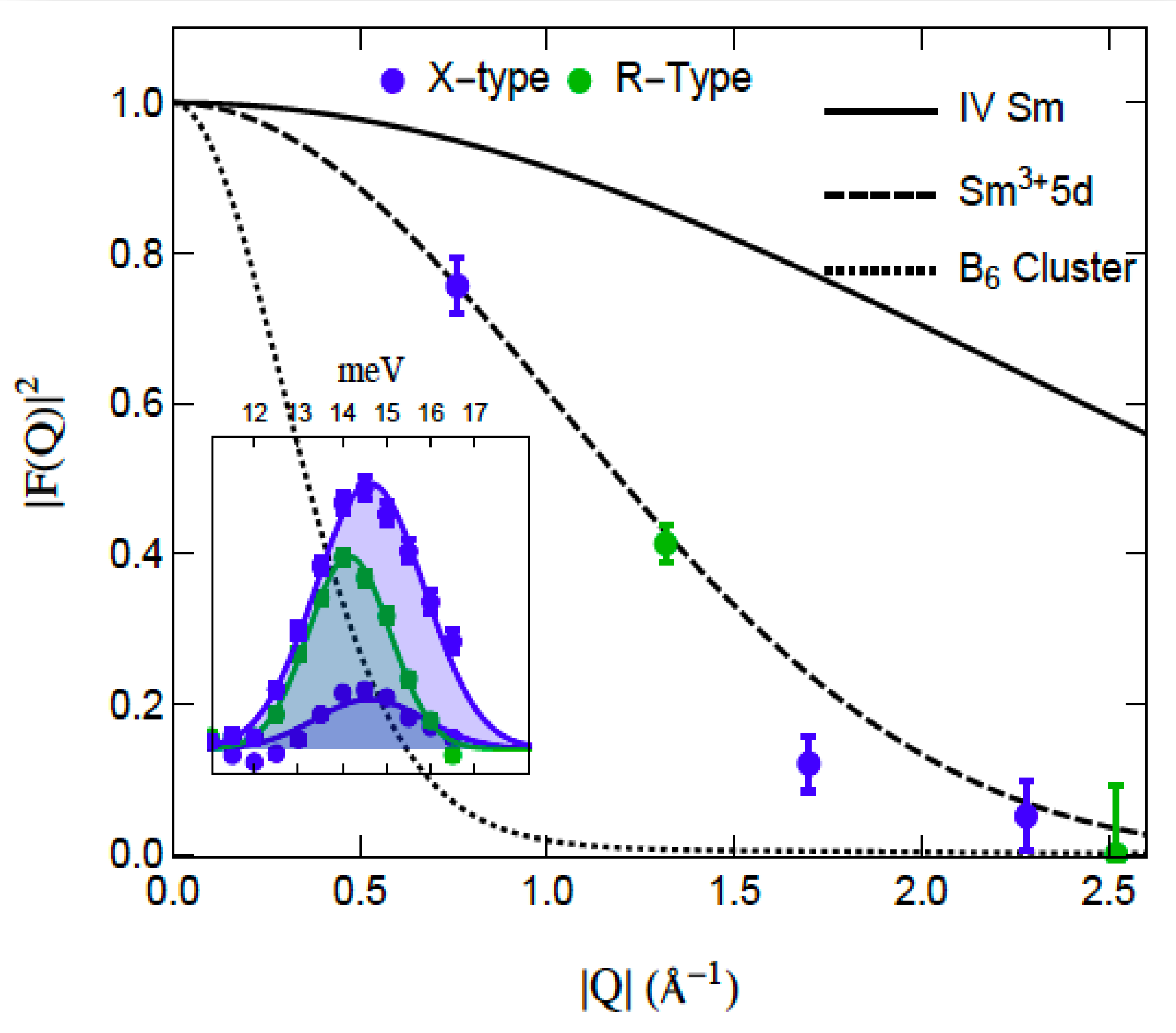
$$\hbar \mathbf{Q} = m \left(\mathbf{v}_i - \mathbf{v}_f \right)$$

Nesting wave vectors for SmB_6

Fuhrman and Leiner et al. PRL (2015)



Exciton form-factor



- Bloch's theorem for simple Bravais lattice:

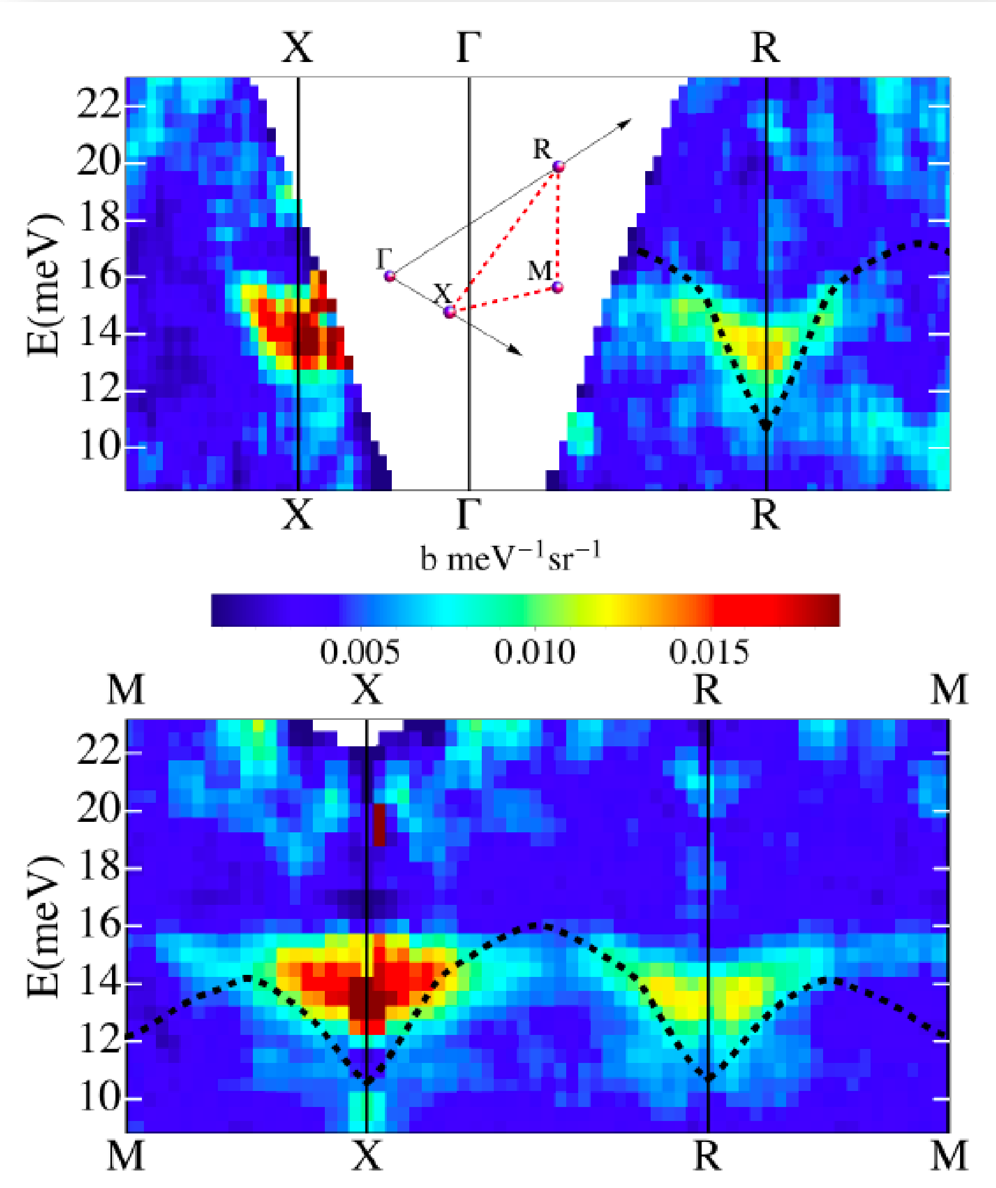
$$\frac{\tilde{I}(\mathbf{Q}+\mathbf{G},\omega)}{\tilde{I}(\mathbf{Q},\omega)} = \left|\frac{F(\mathbf{Q}+\mathbf{G})}{F(\mathbf{Q})}\right|^2$$

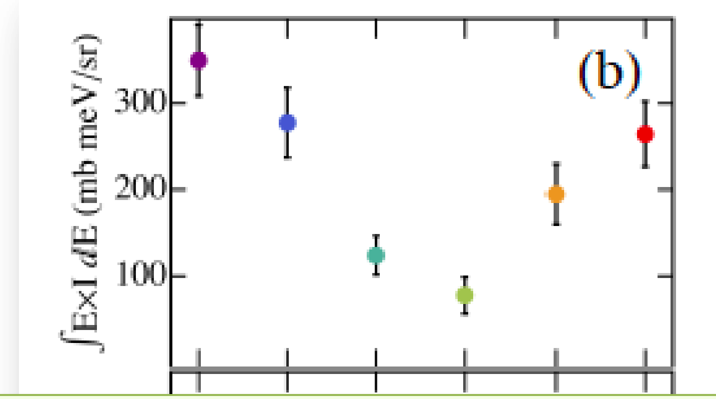
- The Formfactor $F(\mathbf{Q})$ reflects the spatial extent of spin density:

$$F(\mathbf{Q}) = \langle j_0(Qr)\rangle + \left(1 - \frac{2}{g_J}\right)\langle j_2(Qr)\rangle$$

- The data is consistent with 5d wave function
- Surprising given small group velocity

Exciton in insulating SmB_6

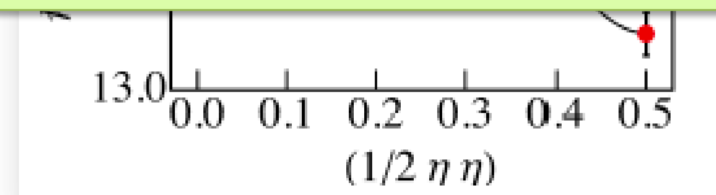




Total moment sum rule:

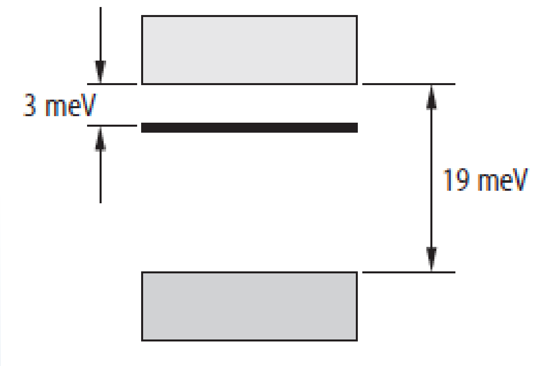
$$\left(\frac{\mu}{\mu_B}\right)^2 = \frac{\iint Tr\{\mathcal{S}(\mathbf{Q}\omega)\} d^3\mathbf{Q}\hbar d\omega}{\int d^3\mathbf{Q}} = 0.29(6)/\mathrm{Sm}$$

This is 40% of the total magnetic scattering from Sm^{3+} and is not dissimilar to the estimates 50% of Sm in the 3+ state

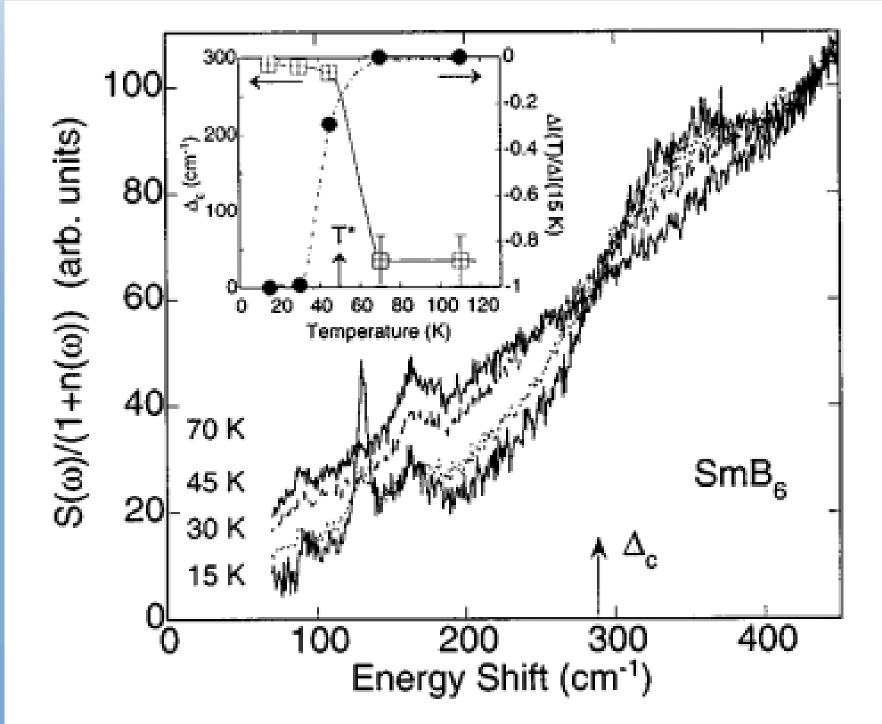


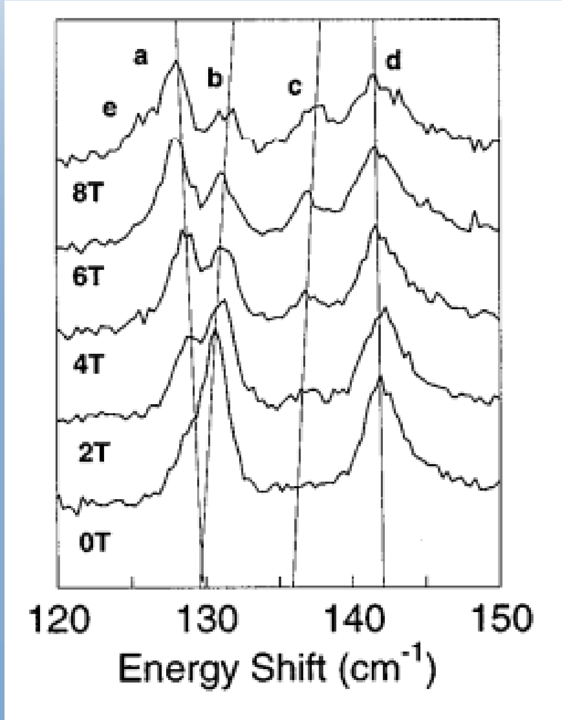
Relation to transport and spectroscopy

- Difference between transport and optical gap
- STM QPI (Hoffman)
- Raman mode

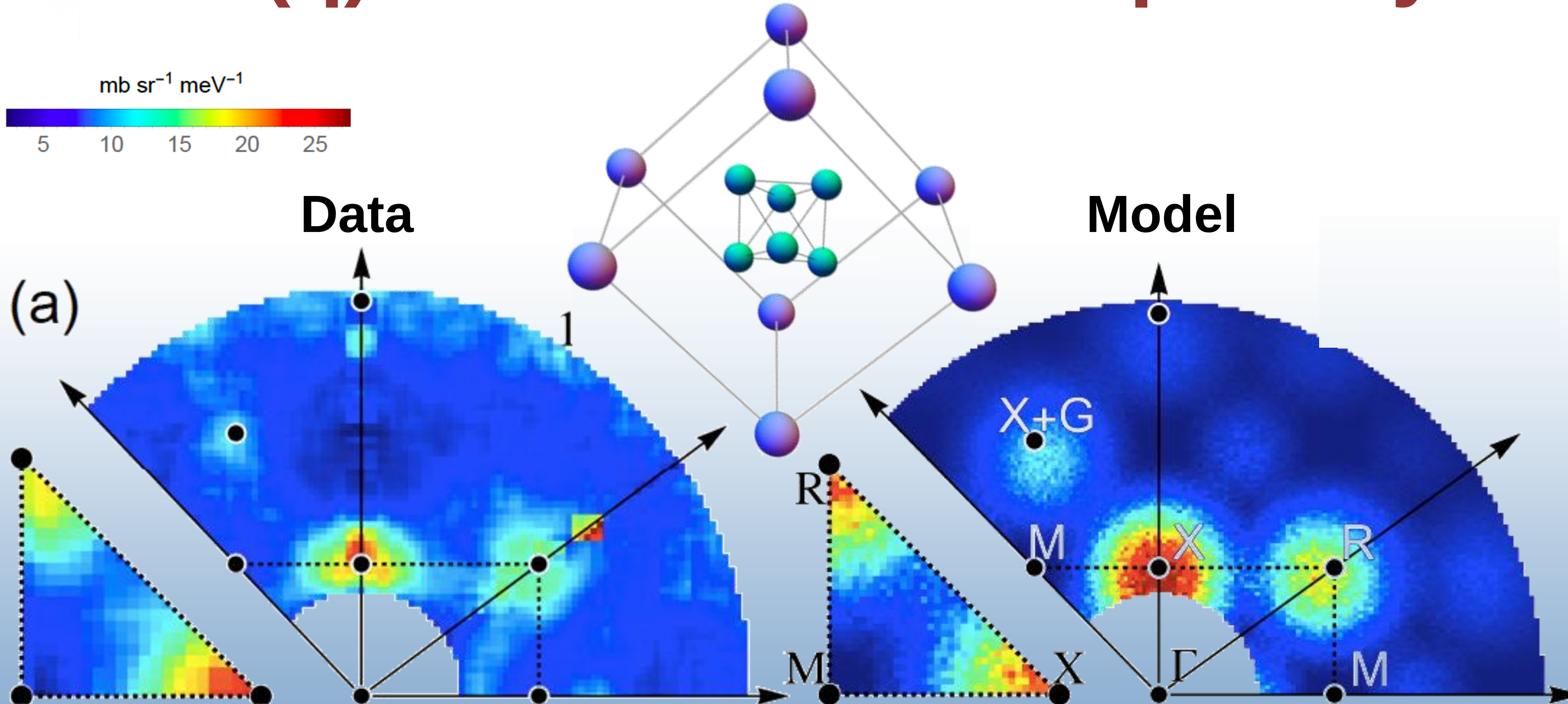


Nyhus st al (1997) and Valentine and Drichko (2015)



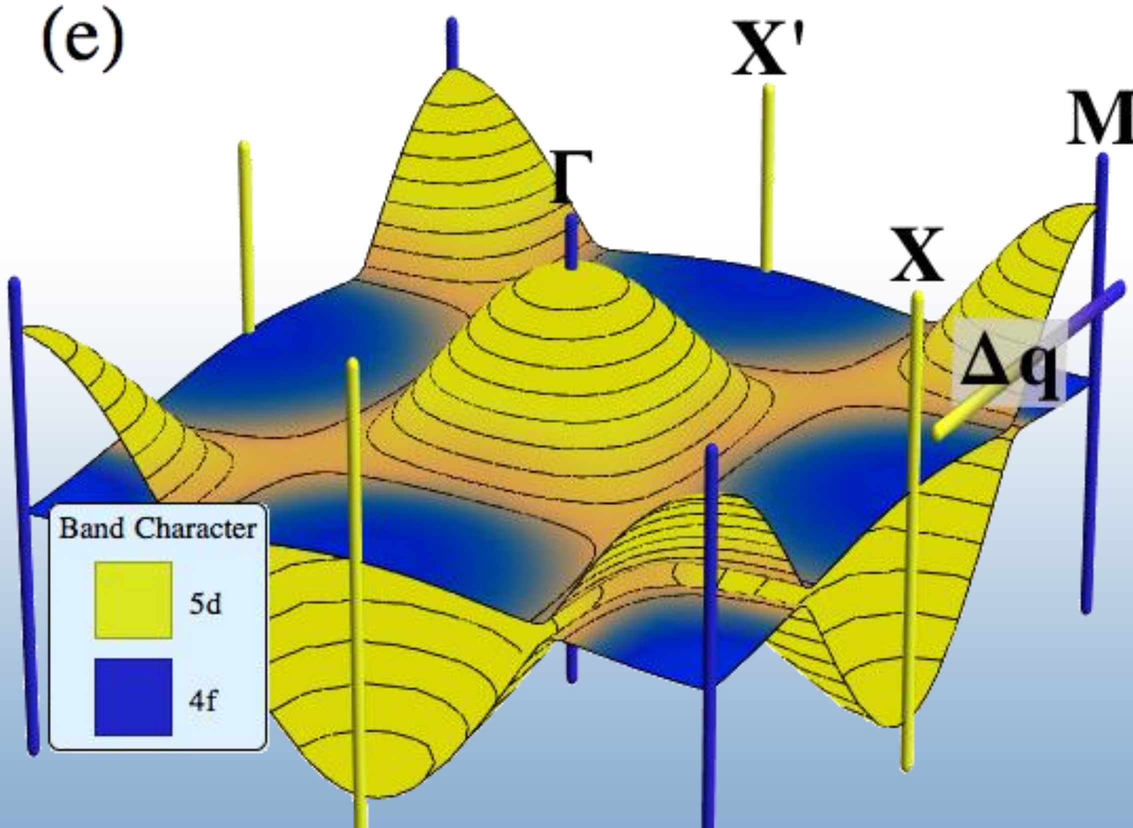


S(q) & Lindhard susceptibility



- A tight binding band structure dominated by body-diagonal hopping through B_6 can account for the intense parts of the magnetic scattering.
- Can use S(q) as a probe of hybridized band structure

A topological band structure

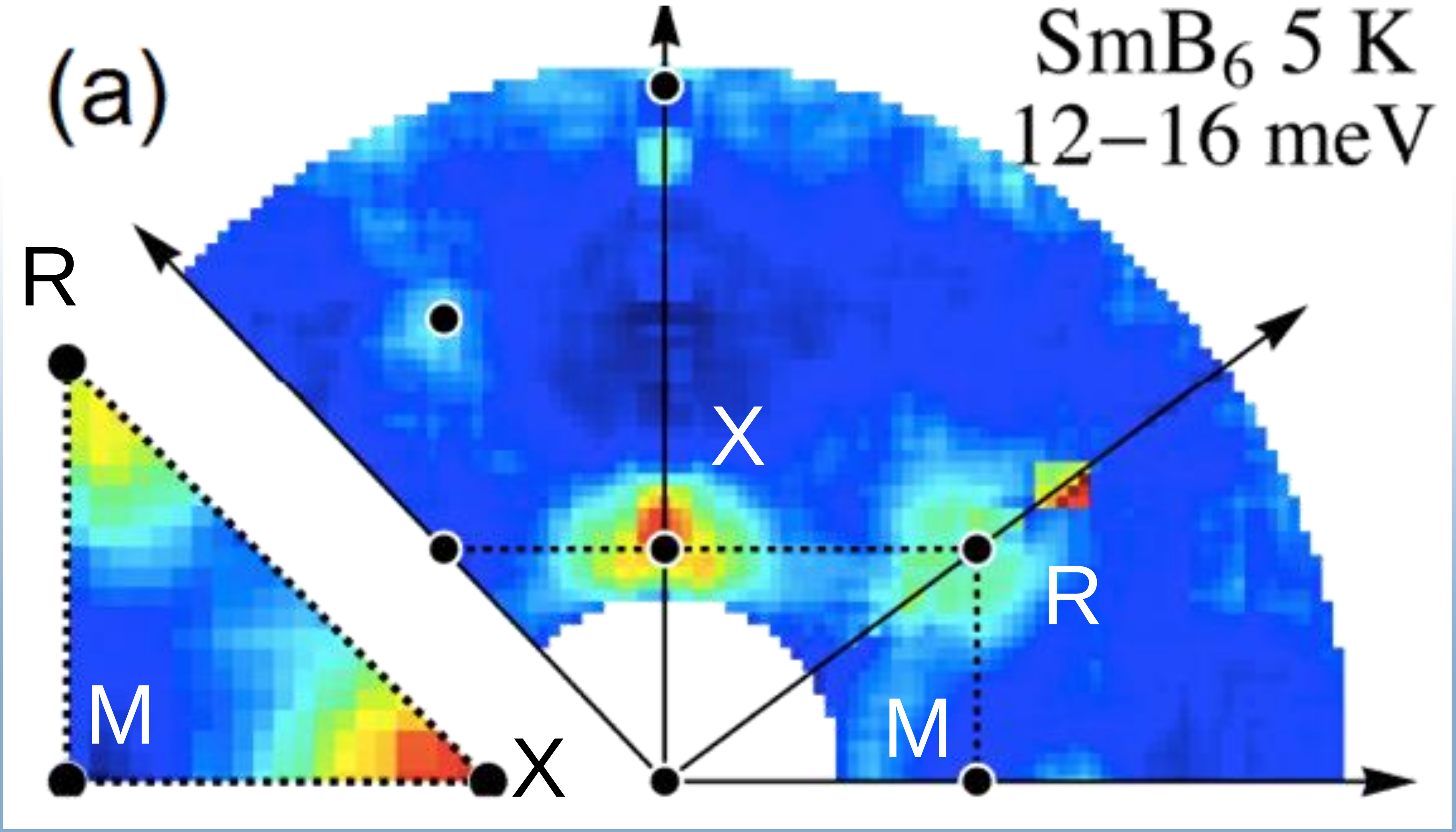


With inversion and time reversal symmetry the topological index is determined by the product of parities of occupied Bloch states at 8 symmetry points of 1 BZ:

$$n = \left(d_X d_M\right)^3 d_G d_R = d_X d_M = -1 \quad \left(d_G = d_R = 1 \text{ in cubic symmetry}\right)$$

Strong topological insulator because X and M have different parity

From Scattering to Z_2 invariant



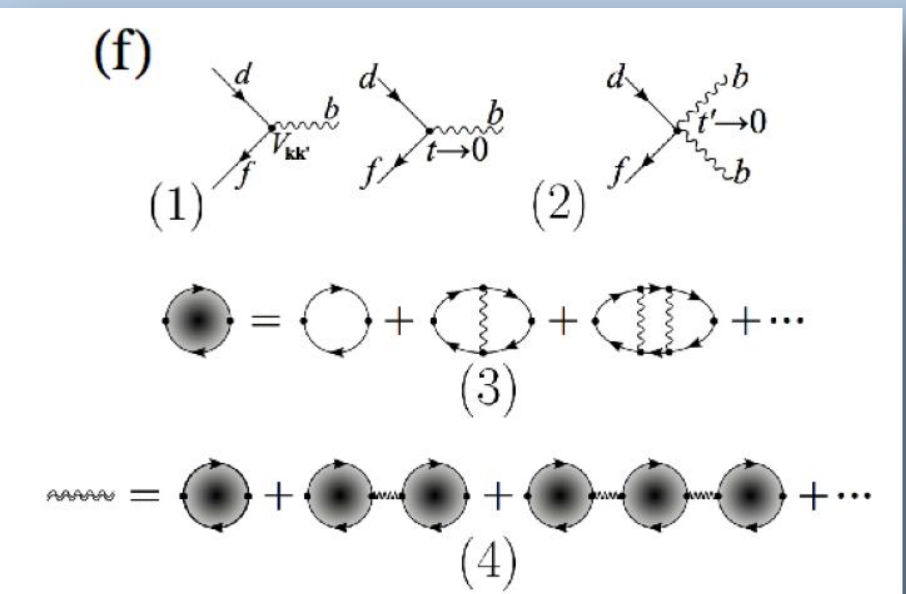
Cubic symmetry: An STI has intensity at the X or the M point. Not at both
Hypothesis: The pattern of scattering reflects topology.

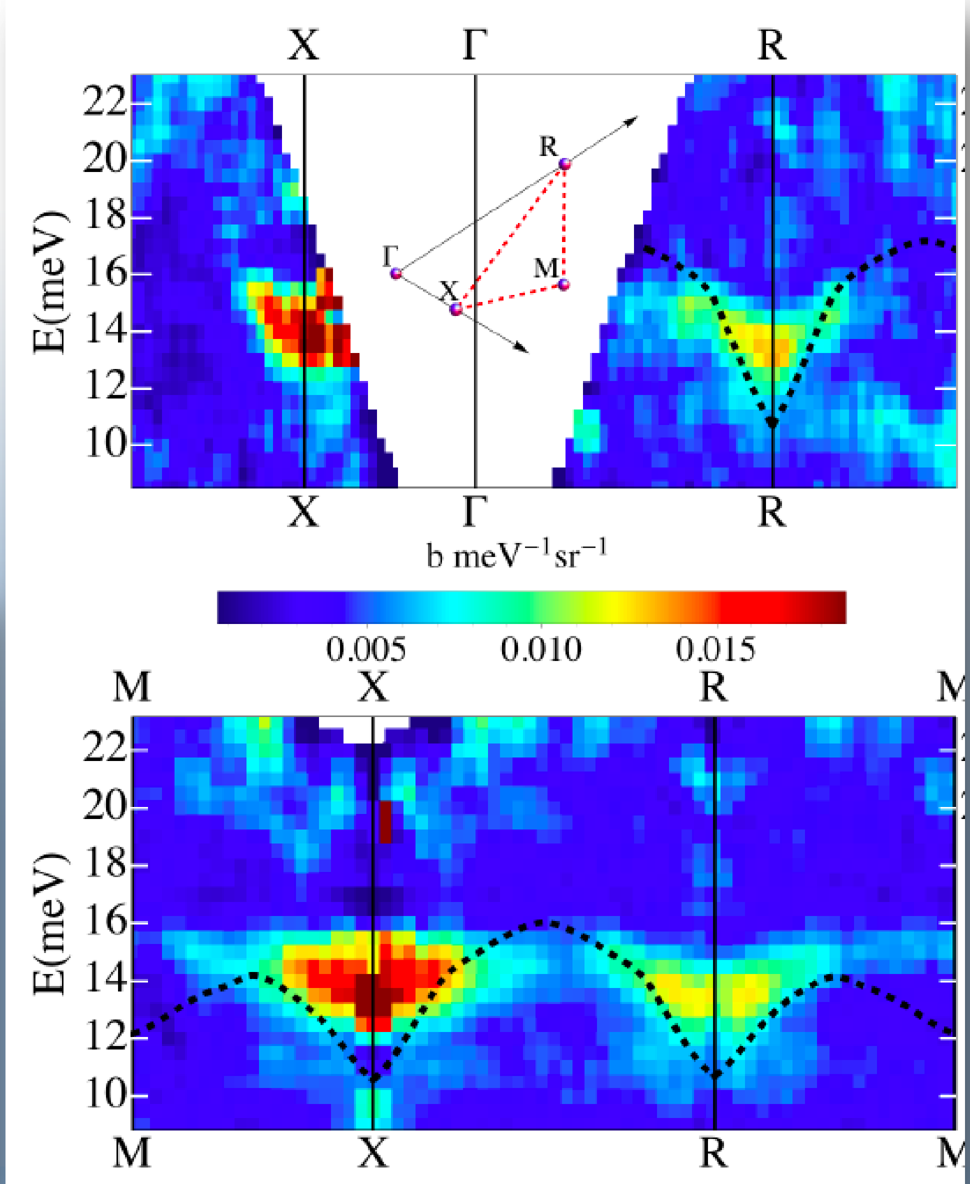
Slave Boson MFT of exciton

Risebrough (1990), Nikolic (2015)

Slave boson fluctuations yield:

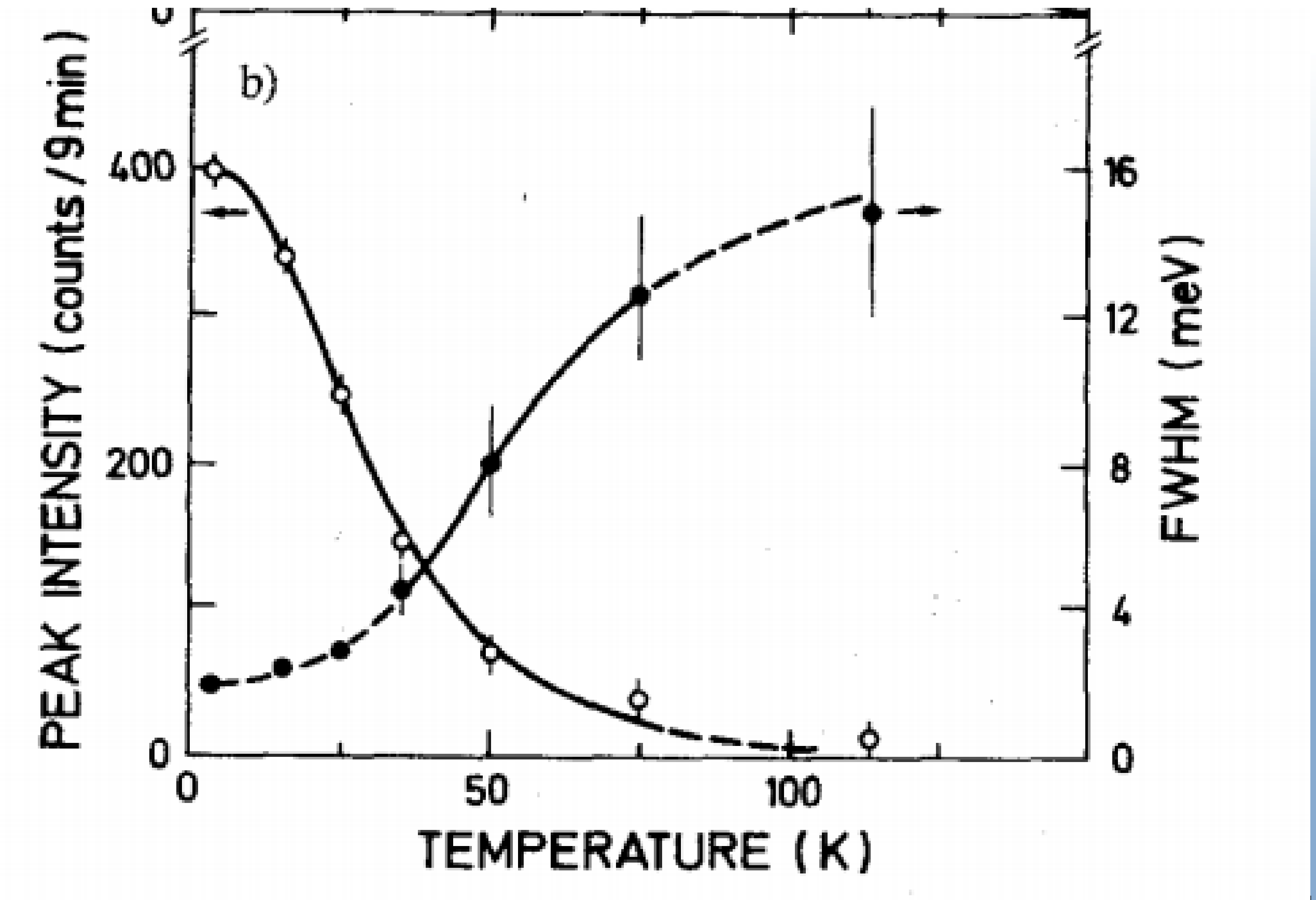
- Renormalized Hybridization gap
- Formation of Exciton bound state
- Exciton dispersion from RPA



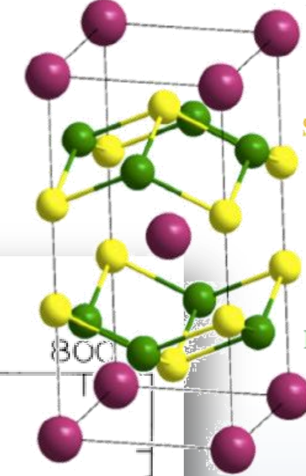


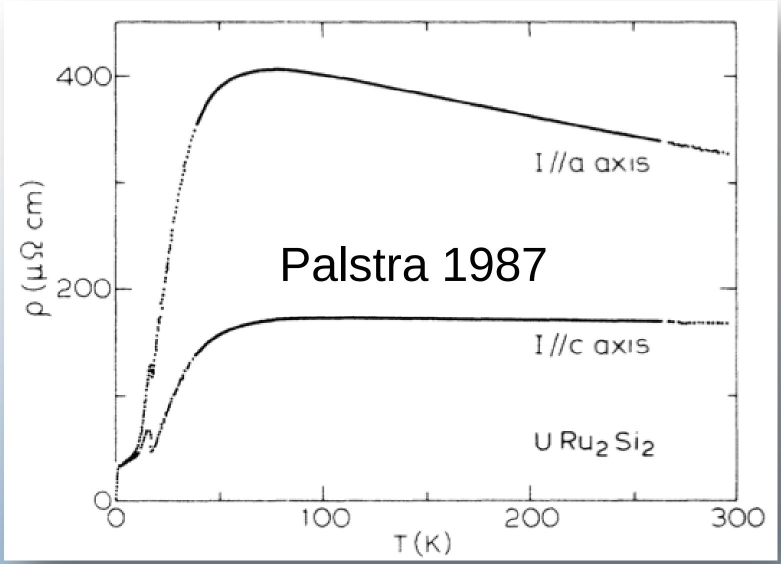
Exciton: appears with the gap

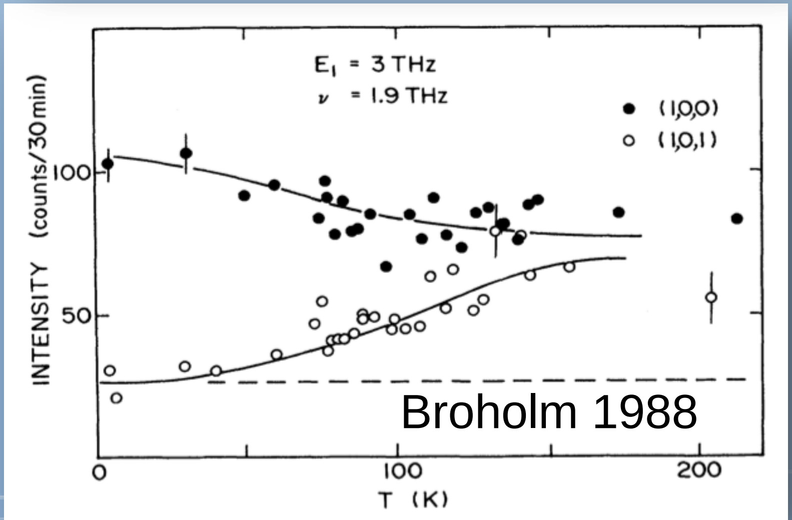
Mignot and Alekseev Physica B (1995)

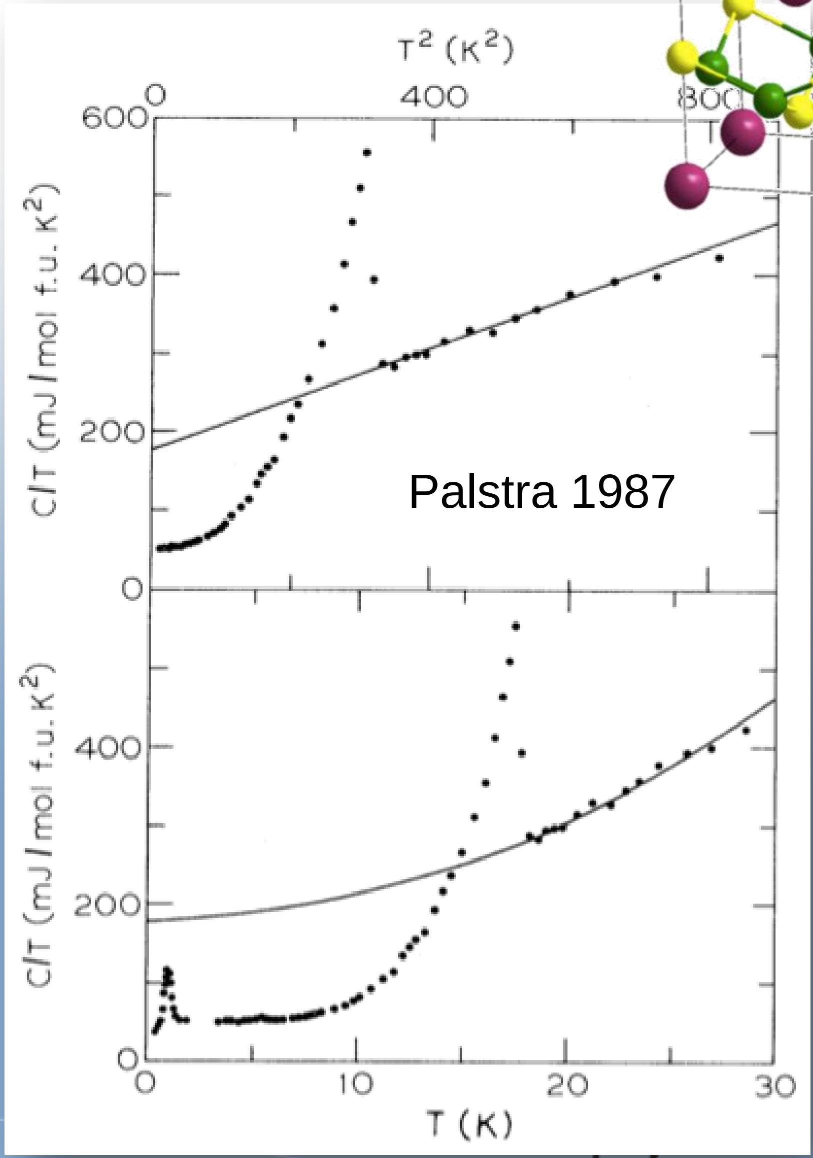


URu_2Si_2 : Coherence & hidden order

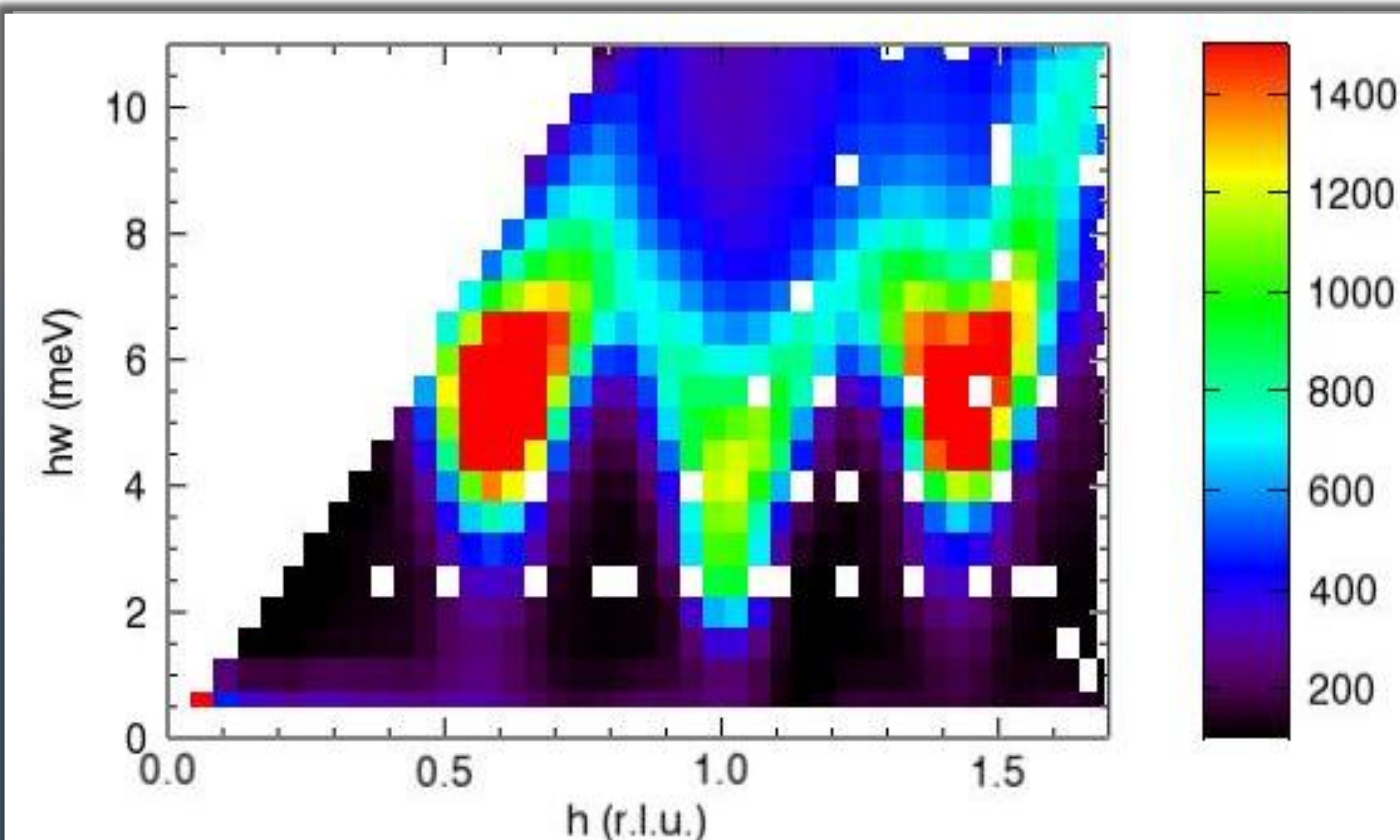




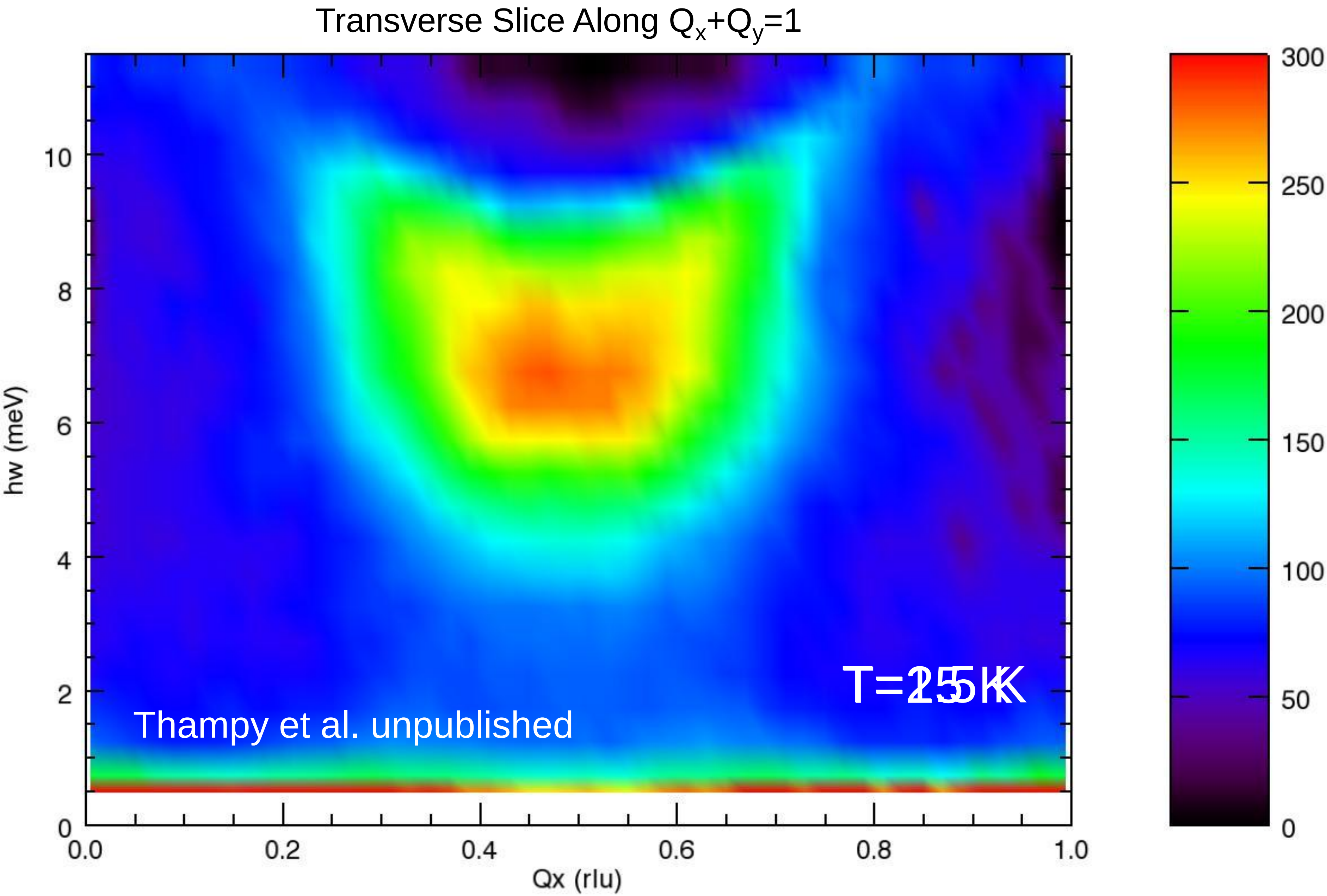




A resonance in URu_2Si_2

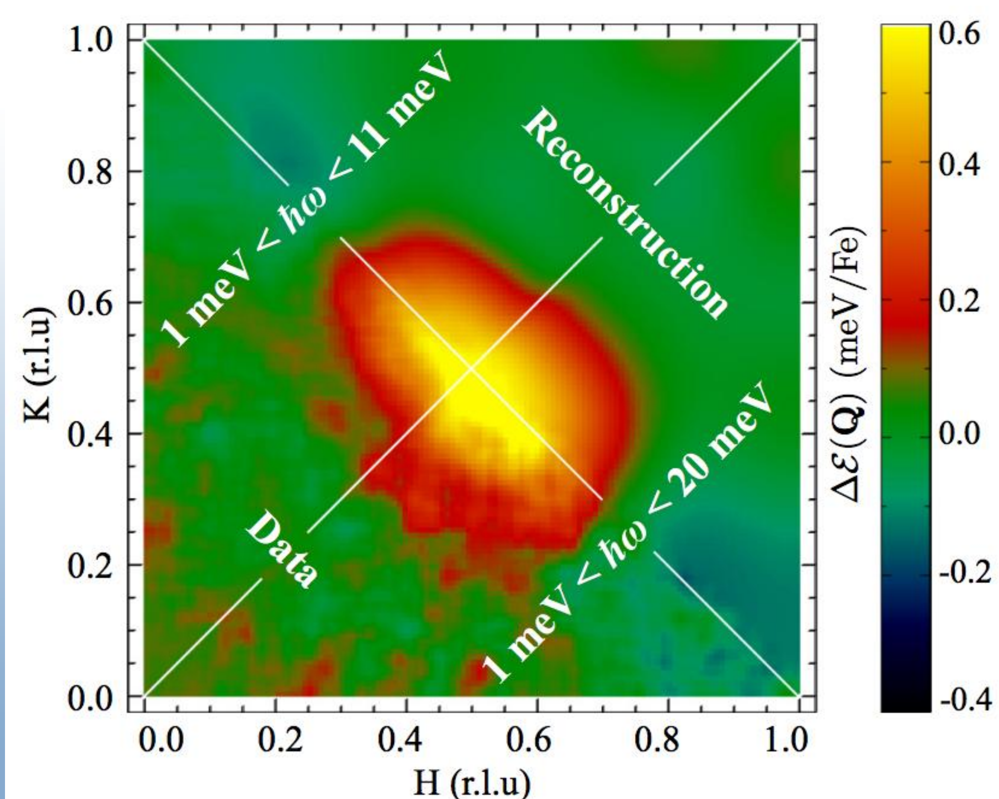


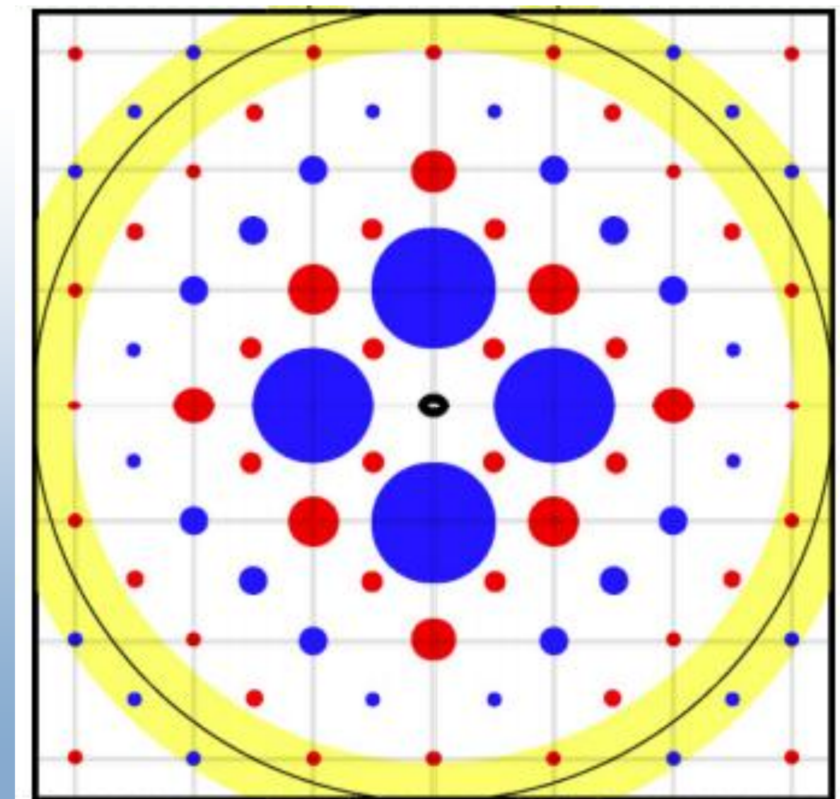
From Critical Fluctuations to Resonance



Spatially resolved magnetic condensation energy

J. Leiner et al., PRB RC (2015)





Magnetic “Potential” Energy: $\Delta\left\langle \mathcal{H}_{\mathrm{mag}} \right\rangle = -0.31(9)\ \mathrm{meV/Fe}$

Increased Kinetic Energy $\mathrm{D}\left\langle E_{\mathrm{kin}} \right\rangle = +0.30(9)\ \mathrm{meV/Fe}$

Net condensation energy [C(T)] $\mathrm{D}E_{SC} = -\ 0.013(1)\ \mathrm{meV/Fe}$

Conclusions & Outlook

- **SmB_6**
  - $c(\mathbf{Q})$ indicates significant body diagonal hopping
  - Coherent mode: Weakly dispersive and long lived
  - Visible in Raman and possibly associated with "Impurity band"
  - d-electron form factor distinct from Q=0 magnetism
  - Is this the soft mode of surface magnetism?
- **General**
  - Hypothesis: Neutron intensity is sensitive to nested band crossings & reflects band topology
  - Exciton condensation energy may be relevant for stabilizing exotic electronic orders
- **Future**
  - Higher resolution & Pressure dependence
  - Probe broader range of correlated insulators STI and WTI
  - Very interested in realistic calculations of scattering