Exciton in the Topological Kondo Insulator SmB$_6$

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Institute for Quantum Matter

• **Synthesis**
  – Bob Cava, (Princeton)
    • Frustrated magnets
  – Tyrel McQueen
    • Topological, superconducting & molecular solids

• **Spectroscopy**
  – Collin Broholm
    • Neutron scattering
  – Peter Armitage
    • THz Spectroscopy

• **Theory**
  – Oleg Tchernyshyov
    • Frustrated magnetism
  – Ari Turner
    • Topological Materials
Frontiers in Hard Condensed Matter

• Quantum Spin liquids
  – Evidence for emergent electrodynamics (artificial light)
  – Hamiltonian + continuum for quantum spin liquid
  – Field driven effective chemical potential

• Correlated Topological materials
  – Neutrons as a probe of renormalized bandstructure
  – Systematics of bound state
  – Surface magnetism

• Linked degrees of freedom
  – Spin waves + phonons
  – Spin waves + orbitons
  – Macroscopic: Link disparate responses

• Quantum Critical itinerant electrons
  – Comprehensive scaling to chart types of criticality
  – Anomalous transport and spin correlations

• Unconventional Superconductivity
  – The magnetism within a $d$-superconductor?
  – Image the cooper pair
Correlated TIs: Why and How

• **2D correlated metal**
  – Interesting (Quantum Hall state)
  – Useful: Electronic devices are surface based

• **Requirements:**
  – Insulating & correlated bulk
  – Time reversal symmetry

• **Possible bulk states**
  – Spin liquid in topologically non-trivial insulator (tall order)
  – Topological Mott insulators
  – Kondo Insulator
Outline

• Introduction
  – Kondo Insulators and SmB$_6$
  – Neutron Scattering

• The SmB$_6$ enigma
  – Transport and thermal properties
  – A resonance with d-form-factor
  – Slave boson MFT + RPA of exciton

• Conclusions
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Topological Kondo Insulators

Maxim Dzero, Kai Sun, Victor Galitski, and Piers Coleman

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

Neuprane et al. (2013)

\[ T < T_H \]

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SmB$_6$: Kondo Insulator or Exotic Metal?

J. C. Cooley, M. C. Aronson, Z. Fisk, and P. C. Canfield
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!
An insulating SmB$_6$ surface?

Options to explain rising low T resistance:
- Surface magnetism breaks time reversal symmetry
- Unprotected Surface states; topologically trivial Kondo ins.
- Both: Topologically trivial insulator with surface magnetism
Lower T resistance in float zone crystals

Surface magnetism from $\text{Sm}^{3+}$
**Aluminum:*** filamentary inclusions observed in diffraction and may account for dHvA

**Carbon:** Produces a plateau. Carbon is “everywhere” but not in IQM floating zone crystals!
SmB$_6$/C–bulk effects

Parametric:
- Field
- carbon

$$\frac{C_p}{T} = \gamma + \beta_3 T^2 + AT^2 \ln \frac{T}{T^*}$$ for all C-doped samples and fields

$$\beta = \beta_3 - A \ln T^*$$ where $T^* = 17$ K and $\theta_D = 230$ K

C-doping & magnetic field shift the chemical potential
• Carbon induced carrier doping populates surface states near the hybridization gap
ARPES view of $\text{SmB}_6$


Odd number of band crossings ➔ Topological Kondo Insulator
Magnetic Neutron Scattering

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

\[ S^{\alpha\beta}(Q,\omega) = \frac{1}{2\pi\hbar} \int dt \ e^{-i\omega t} \frac{1}{N} \sum_{\mathbf{R}\mathbf{R}'} e^{iQ(\mathbf{R}-\mathbf{R}')} < S^\alpha_\mathbf{R}(0) S^\beta_{\mathbf{R}',t} > \]
Spin Fluctuations & Neutrons Scattering

\[ S_{\alpha\beta}(q\omega) = \frac{1}{1 - e^{-\beta h \omega}} \frac{\chi''_{\alpha\beta}(q\omega)}{(g\mu_B)^2 \pi} \]

\[ \chi_0(q) = \sum_k f\left(\frac{\epsilon_{k+q}}{\varepsilon_k}\right) \]

\[ V_{2-y}O_3 \text{ Bao et al. PRL (1993)} \]
Neutron Scattering from SmB$_6$

Double isotope sample $^{154}$Sm$^{11}$B$_6$
From Pavel Alekseev

Reference sample La$^{11}$B$_6$
From Koopayeh/McQueen
SEQUOIA Time of Flight Spectrometer

\[ \hbar \omega = \frac{1}{2} m \left( v_i^2 - v_f^2 \right) \]
\[ \hbar Q = m \left( v_i - v_f \right) \]

- \( t_{\text{chopper}} \rightarrow v_i \)
- \( t_{\text{detector}} \rightarrow v_f \)

Fermi Chopper
Sample
Detector
Nesting wave vectors for SmB$_6$

T=5 K
Exciton form-factor

- Bloch’s theorem for simple Bravais lattice:
  \[
  \frac{\tilde{I}(Q+G,\omega)}{\tilde{I}(Q,\omega)} = \left| \frac{F(Q+G)}{F(Q)} \right|^2
  \]
- The Formfactor \( F(Q) \) reflects the spatial extent of spin density:
  \[
  F(Q) = \langle j_0(Qr) \rangle + \left( 1 - \frac{2}{g_J} \right) \langle j_2(Qr) \rangle
  \]
- The data is consistent with 5d wave function
- Surprising given small group velocity
Exciton in insulating SmB$_6$

Total moment sum rule:

$$\left(\frac{\mu}{\mu_B}\right)^2 = \frac{\int \text{Tr} \{ \mathcal{S}(Q,\omega) \} d^3Q h\omega}{\int d^3Q} = 0.29(6) / \text{Sm}$$

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.
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.

ARPES so far does not provide needed low energy details.
Slave Boson MFT of exciton

\[ H = \int_{1BZ} \frac{d^3k}{(2\pi)^3} \left[ \sum_\sigma \xi_k d_{\sigma k}^\dagger d_{\sigma k} + \sum_\alpha \epsilon_{\alpha k} f_{\alpha k}^\dagger f_{\alpha k} \right] \\
+ \sum_{\alpha \sigma} \left( V_{\sigma \alpha k} d_{\sigma k}^\dagger f_{\alpha k} + h.c. \right) \right] + U \sum_{\alpha \beta R} f_{\alpha R}^\dagger f_{\alpha R} f_{\beta R}^\dagger f_{\beta R}, \]
RPA theory of Exciton (P. Nikolic)

Slave boson fluctuations yield:
- Renormalized Hybridization gap
- Formation of Exciton bound state
- Exciton dispersion from RPA
Conclusions

• The surface of high quality SmB$_6$
  – Can be Insulating
  – Dominated by Sm$^{3+}$
  – Magnetizable

• Strong sensitivity to C doping
  – Surface states near hybridization gap
  – Correlated impurity band is generated

• 14 meV exciton within Kondo insulator
  – Q-dependence associated with body diagonal hopping
  – Weakly dispersive and long lived
  – d-electron form factor

• Theory of the Kondo insulator
  – Slave boson MFT for renormalized band structure
  – RPA treatment of fluctuations accounts for exciton dispersion
  – More work needed to understand mode intensity
Future plans in TKI

• Magnetic fluctuations in Kondo Insulators
  – When is there an exciton and is there a correlation with topological bandstructure
  – On the agenda non-cubic KI: CeRu$_4$Sn$_6$, CeNiSn

• Field effects on the bulk
  – Determine spin degeneracy of exciton by high field experiment on SmB6

• Correlated surface physics of SmB6
  – Neutron reflectometry
  – Circular magnetic dichroism

• An opportunity to put theories to the test!
  – Slave boson MFT and neutron scattering
  – LDA+DMFT