Mixed valence insulators with neutral Fermi surfaces

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D. Chowdhury, I. Sodemann, TS, arXiv:1706.00418

I. Sodemann, D. Chowdhury, TS, arXiv: 1708. 06354

Debanjan Chowdhury

Inti Sodemann

Topological insulating materials (in 3d)

Early: $Bi_{1-x}Sb_x$, Bi_2Se_3, Bi_2Te_3, ...

Many materials by now.

Some interesting current candidates:

SmB_6 (**Samarium** hexaboride), other rare-earth alloys, **Iridium** oxides, ...

(Involve electrons from atomic d or f orbitals: ``strong'' electron interactions).

In this talk, I will focus on the currently most popular candidate material for a correlated topological insulator SmB_6

This poses many interesting theoretical challenges even beyond just topological aspects
- I will answer some of them.

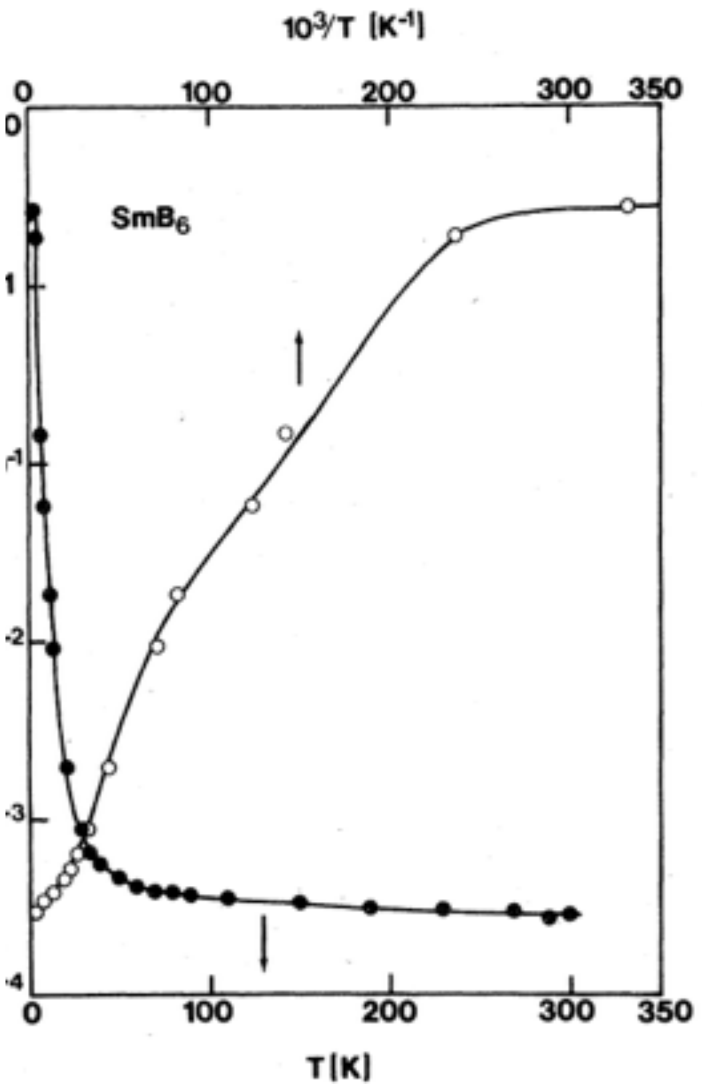
Plan

0. Brief summary of some phenomena in SmB_6 (a mixed valence insulator)

- Correlated topological insulator?…….
- Or something even more exotic (bulk neutral fermi surface??)

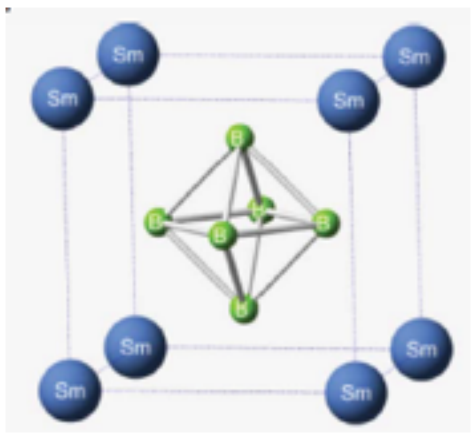
1. A theory of emergent neutral fermi surfaces in a 3d mixed valence insulator

SmB_6 : a classic correlated insulator
(studied since late 1960s)



Allen, Batlogg, Yachter, 79

Bulk electrical insulator but many unusual phenomena.



Strongly correlated Sm f-shell electrons
+ mobile conduction electrons.

Often called a Kondo insulator:

Local f-moments screened by conduction electrons to form an insulator

More precisely, a mixed valence insulator.
Sm valence fluctuates between 2+ and 3+ (average 2.6)
Sm^{2+}: completely filled (crystal field split) J = 5/2 shell
Sm^{3+}: one f-hole + one conduction electron

Topological insulator?

Proposal (Dzero, Sun, Galitski, Coleman 2010):
Topological Kondo insulator

Low energy physics: renormalized band theory
leading to a filled topological band

Low-T: Saturating resistivity - known now to be due to a surface metallic state
(as expected for a topological band insulator)
(Wolgast et al, Zhang et al, 2013)

Topological nature of surface state not entirely settled yet.
(conflicting reports in ARPES, …..).

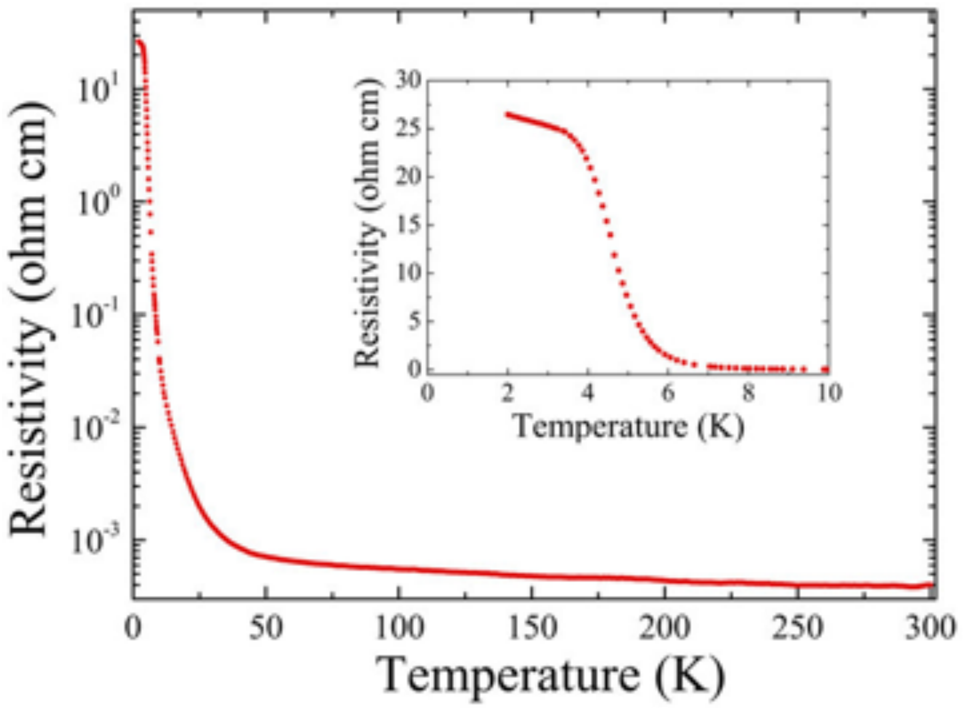
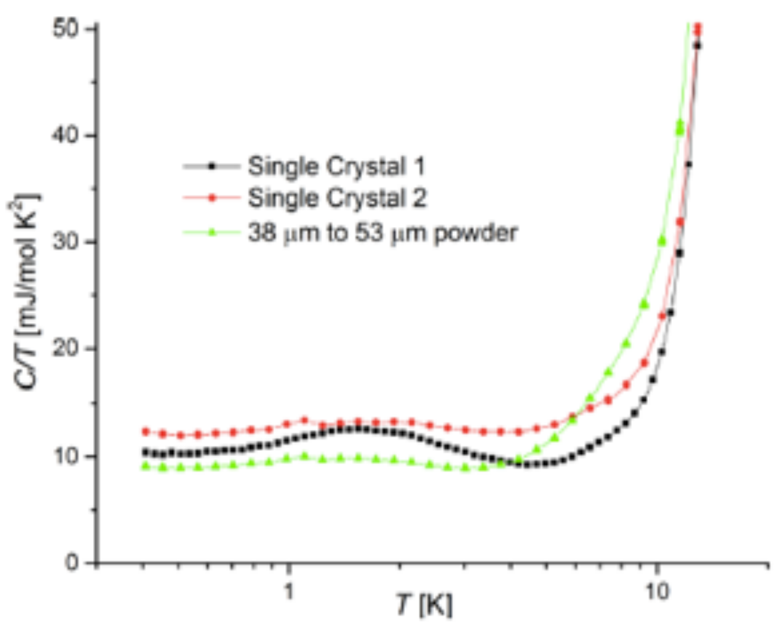


Image credit: M. Ciomaga Hatnean et al,
Scientific Reports, 2013

Other bulk ``complications”: In-gap states

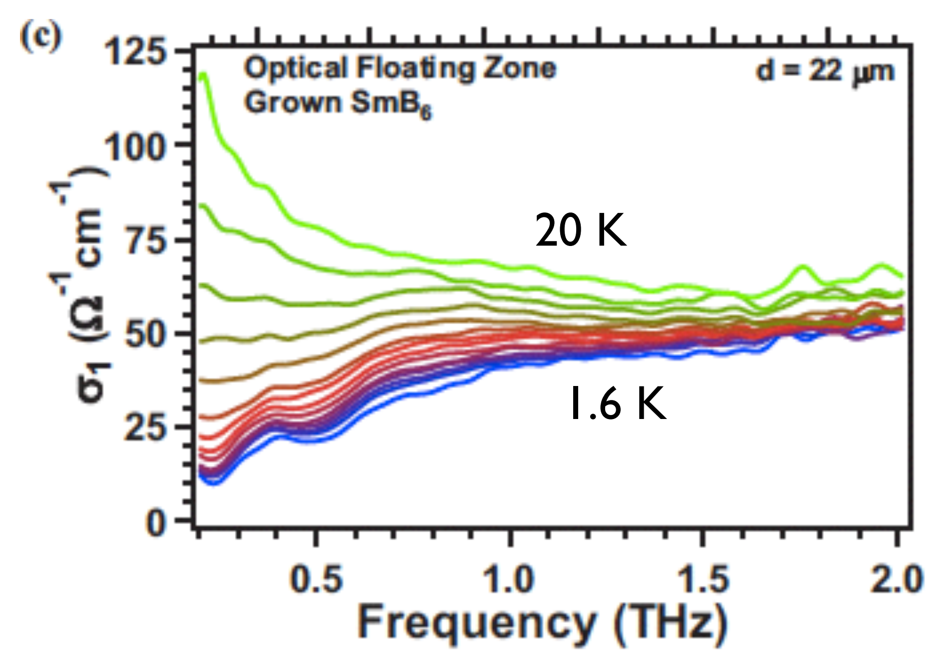
Many low-T anomalies (known for many years)

Linear-T specific heat:
(Eg: Gabani et al, 2002; Phelan, ….Broholm, McQueen et al, 2014)



Data from Wakeham et al, 2016.

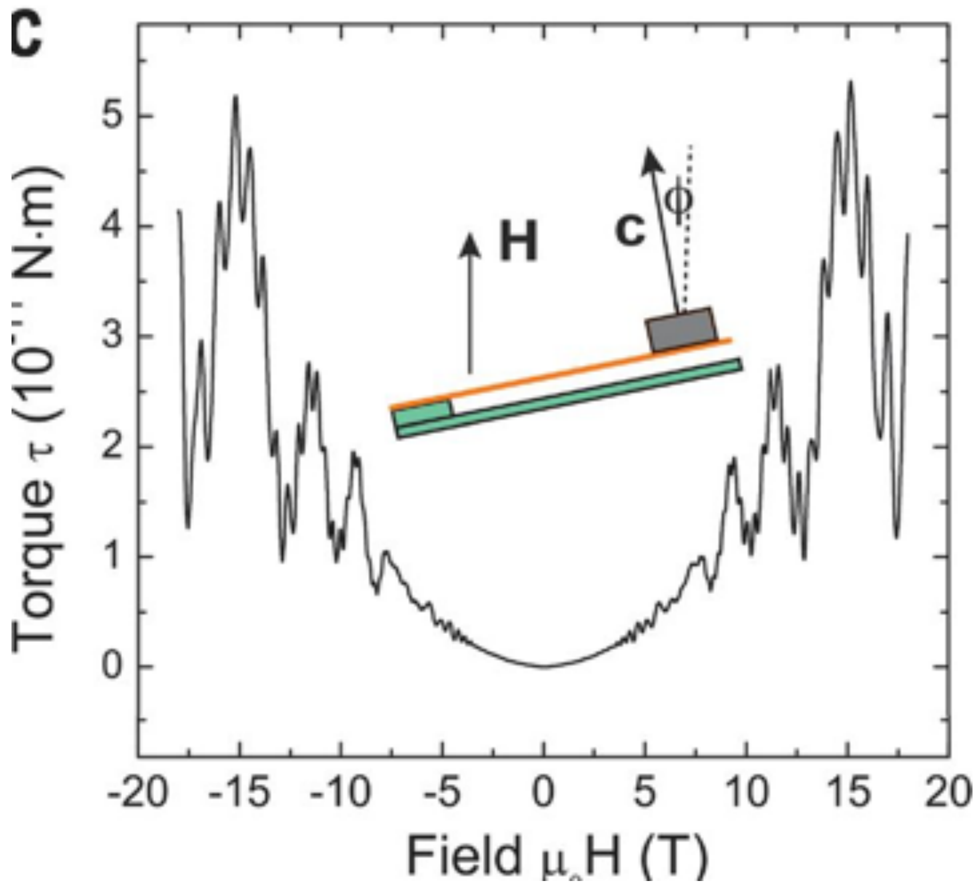
Sub-gap optical absorption:
Laurita et al, 2016

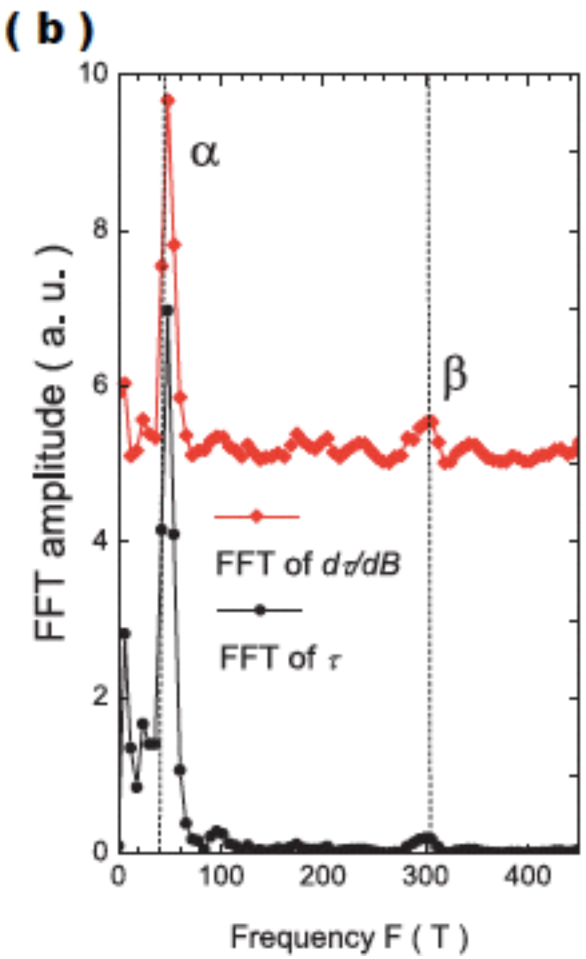


Others: NMR relaxation, conflicting thermal conductivity data on different samples, and by different groups (Li et al 16, Sebastian et al 17, Taillefer et al 17).

Quantum oscillations

G. Li,…..Lu Li, Science 2014





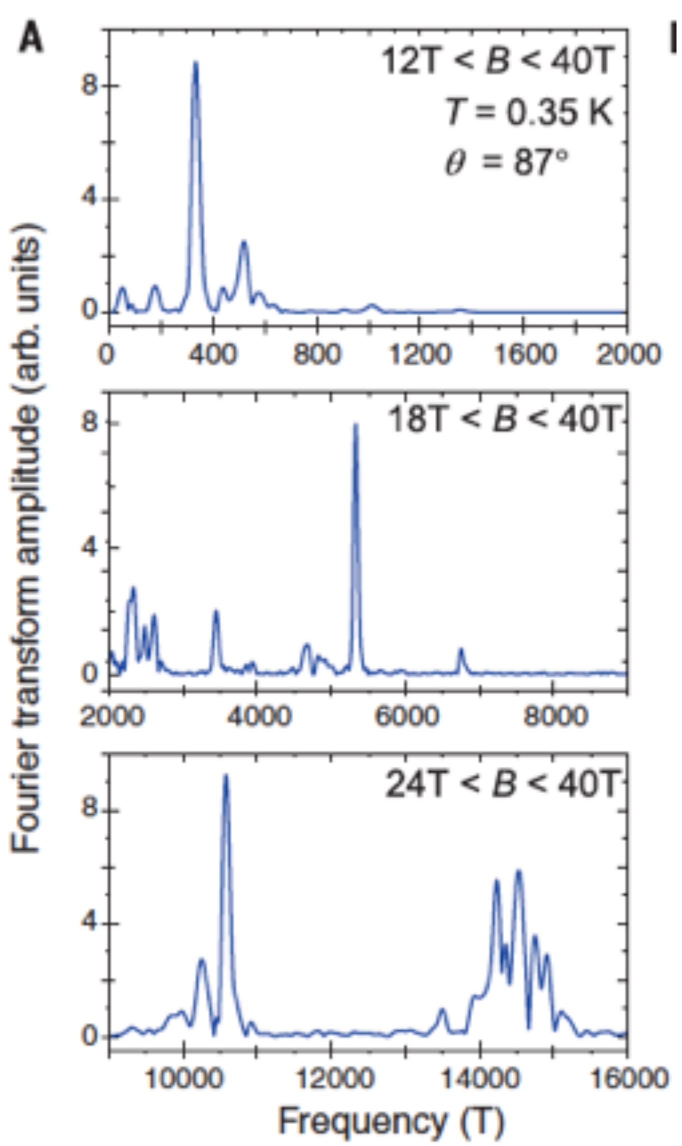
Oscillations attributed to surface state;
no oscillations seen in resistivity.

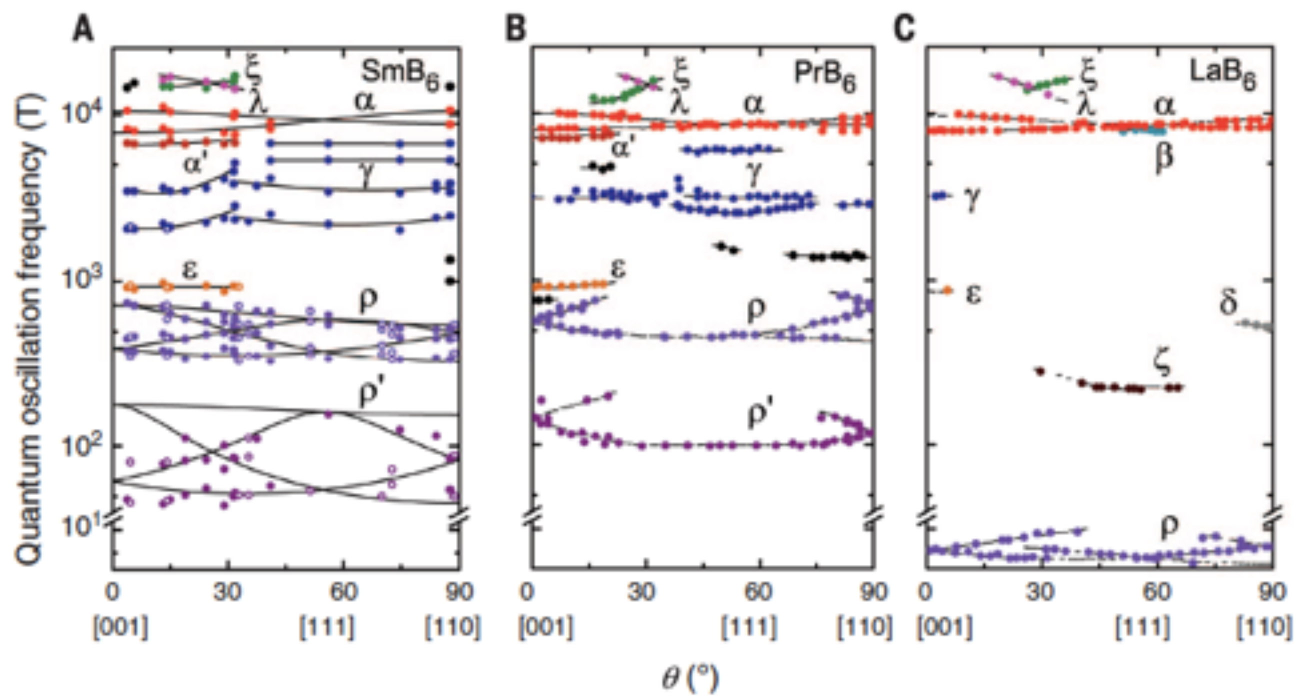
More quantum oscillations

Tan,….., Sebastian et al, Science, 2015

New very high frequency orbits similar to LaB6, PrB6.

Low-T enhancement of amplitude.





Radical proposal: Quantum oscillations are coming from the **bulk in-gap states** and not the metallic surface.

Comments

Interpretation of these quantum oscillations **and** origin of low-T anomalies highly controversial.

Somewhat similar phenomena are being seen in another mixed talent insulator YbB_{12} (Matsuda, Kasahara, Lu Li, … to appear)

I will take seriously the possibility that the quantum oscillations/other anomalies come from neutral quasiparticles in the bulk that form a Fermi surface, and see if it can make theoretical sense.

Other ideas

Knolle, Cooper 1.0: Quantum oscillations in a small gap band insulator (no connection to in-gap states).

Knolle, Cooper 2.0: Bosonic exciton with a small gap and finite-Q dispersion minimum

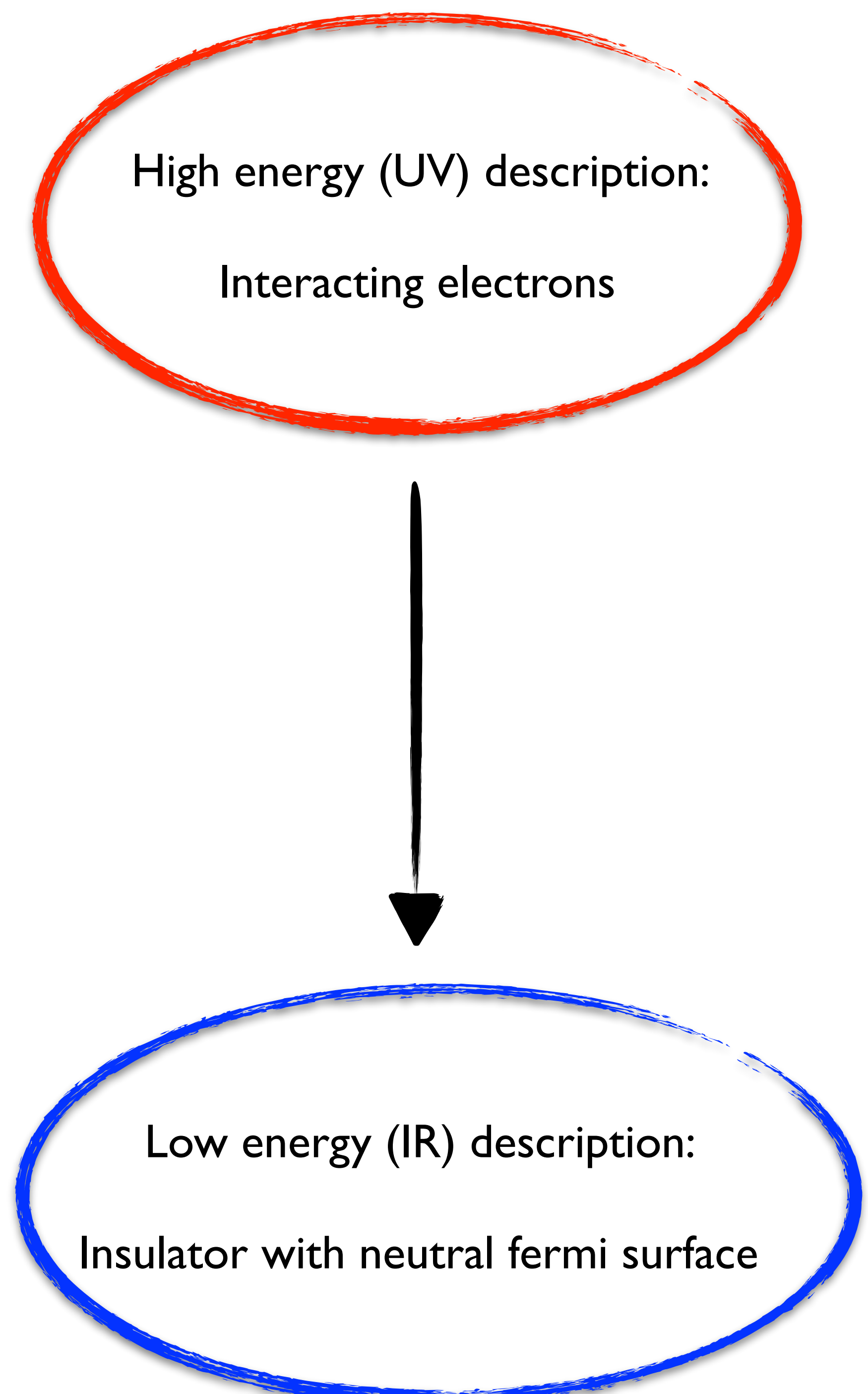
Baskaran: Majorana Fermi surface

Ortun, Chang, Coleman, Tsvelik: ``Skyrme insulator” with Majorana Fermi surface

Bulk neutral Fermi surfaces in insulators

Can they exist? Physical properties?

Mechanism in a mixed valence system?



Some very simple but very powerful observations

Neutral fermions in electronic solids

Two distinct kinds of neutral fermions

(i) Majorana fermions

Coherent superposition of electron and hole

$$\gamma = \frac{c + c^\dagger}{\sqrt{2}}$$

Requires superconducting state

Electrical charge not sharply defined but ***average*** electric charge = 0.

(ii) Neutral fermions in insulators

- emergent excitations with a ***sharp*** electric charge = 0

Microscopic constraint:

All `local' excitations carry integer charge ne (e = electron charge).

n odd: fermion (eg: n = 1 is electron)
n even: boson. (eg: n= 2 is Cooper pair)

Neutral excitations that can be created locally are necessarily bosons.

An emergent neutral fermion cannot be a local object.

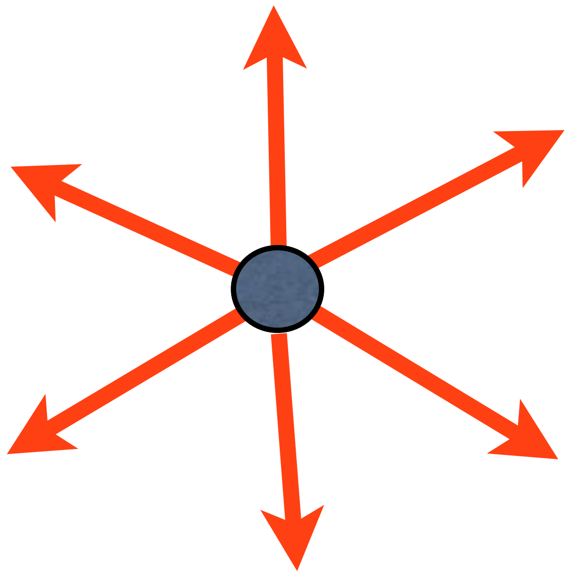
Non-locality of neutral fermion

An emergent neutral fermion in an electronic solid cannot be a local object.

We must ``hide'' it from the UV.

Only ***one known*** route: Couple the neutral fermion to a dynamical emergent gauge field.

To create the neutral fermion must also create associated ``electric'' field lines of the emergent gauge field.



What kind of gauge fields?

Option 1: Discrete gauge field (eg, Z_2)

In 3d these states will have loop-like excitations carrying gauge magnetic flux.

Inevitable consequence: finite-T thermodynamic phase transition associated with proliferation of these loops.

SmB_6 : No evidence of a phase transition down to 1K
(well below temperature at which quantum oscillations/other anomalies are seen).

So we must discard this option.

(Corollary: both proposed versions of Majorana fermi surfaces problematic).

What kind of gauge fields?

Option 2: A continuous gauge field

Simplest and best understood is a U(1) gauge field.

Theories with more complicated non-abelian gauge groups typically have some instability (confinement or a pairing of the fermi surface, etc).

=> Natural possibility:
Neutral fermion Fermi surface + emergent U(1) gauge field in 3d

Many universal properties known from decades of theoretical study.

How to stabilize such a neutral Fermi surface?

Microscopic mechanism

Well known example:
Quantum spin liquids in ``Weak Mott insulators" (eg, in organics)
(Motrunich, 05; Lee and Lee 05)

Mixed valence insulators are microscopically different.
Is there a natural mechanism to stabilize a neutral fermi surface in a mixed valence insulator?

Yes! New ingredient - fermionic excitons.

(Chowdhury, Sodemann, TS, 2017)

Periodic Anderson model

Sm valence fluctuates between Sm^{2+} and Sm^{3+} with average ≈ 2.6.

Sm^{2+}: full filling of a crystal field multiplet

Sm^{3+}: one f-hole + electron in the conduction band

Simplified model:

$$\begin{aligned} H &= \sum_{k\alpha} \epsilon_d(k) d^\dagger_{k\alpha} d_{k\alpha} + \epsilon_f(k) \tilde{f}^\dagger_{k\alpha} \tilde{f}_{k\alpha} \\ &\quad + \sum_r (\epsilon_{\beta\gamma} V_{\alpha\beta} d^\dagger_{r\alpha} \tilde{f}^\dagger_{r\gamma} + H.c.) - U_{df} \sum_r n^{\tilde{f}}_r n^d_r \\ &\quad + U_{ff} \sum_r n^{\tilde{f}_r} (n^{\tilde{f}_r} - 1), \end{aligned}$$

$\tilde{f}$: f-hole (charge +e); d: conduction electron (charge -e)

Average f-hole density = d-electron density

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Largest term:
strong correlation limit

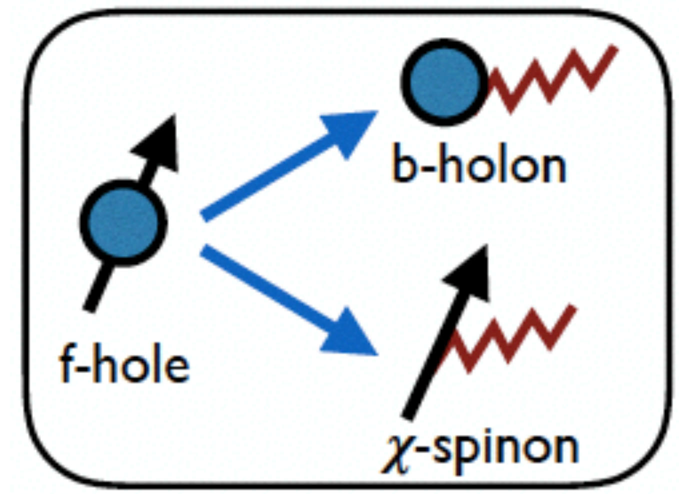
$\tilde{f}$: f-hole (charge +e); d: conduction electron (charge -e)

Average f-hole density = d-electron density

Formation of fermionic exciton

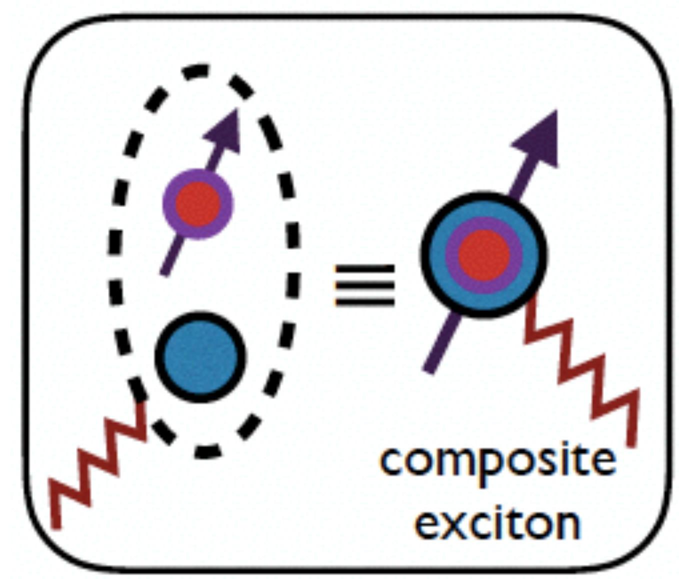
Fractionalize the f-hole:

$$\tilde{f}_{r\alpha} = b_r \chi_{r\alpha}$$



Holon b_r: spin-0 boson with physical charge +e;
Spinon $\chi_{r\alpha}$: spin-1/2 fermion with physical charge 0.

Both b and χ are charged under an internal $U(1)$ gauge field.



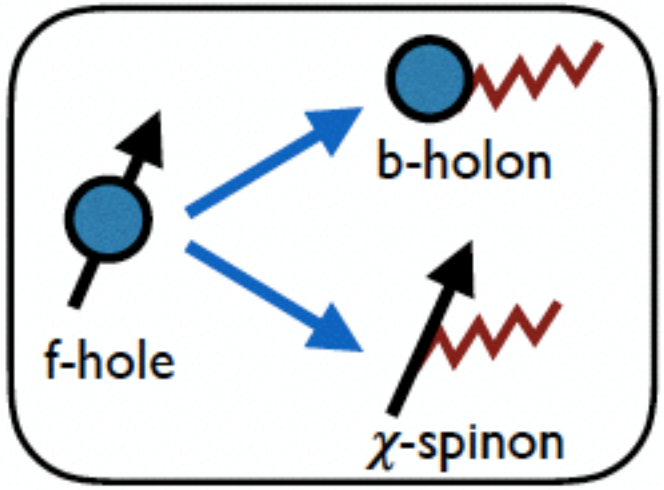
Large U_{df} (but $\ll U_{ff}$): Coulomb attraction between b and d
=>can form a bound electrically neutral **fermionic exciton**

$$\psi_\alpha = b d_\alpha$$

Comments

Average holon density = average microscopic f-hole density = average d-electron density

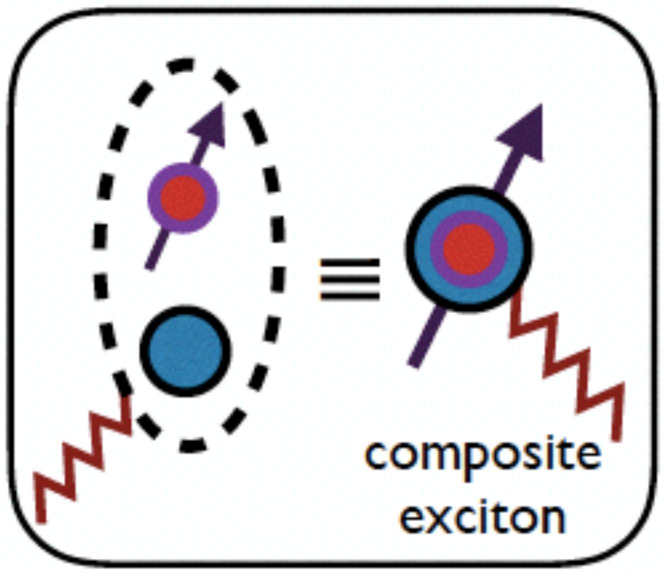
=> There are exactly as many holons as there are d-electrons.



Strong exciton binding limit: b, d gapped to give an electrical insulator.

Low energy degrees of freedom: excitons and spinons (and U(1) gauge field)

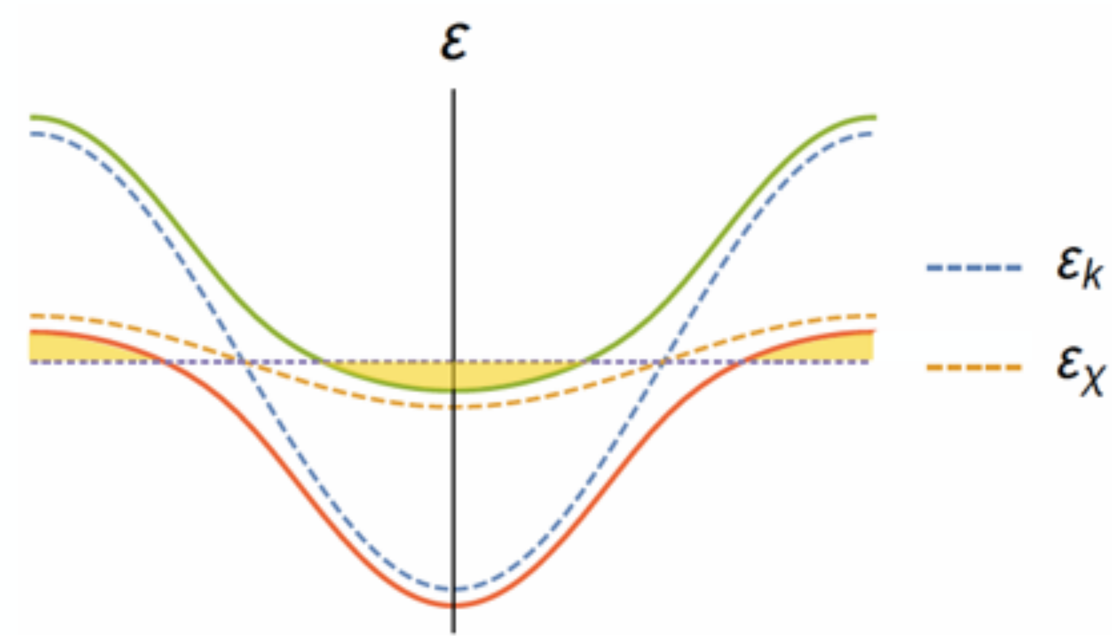
Exciton density = spinon density = original conduction electron density.



Effective model

Hamiltonian

$$H = \sum_{k\alpha} \epsilon_k^{\psi} \psi_{k\alpha}^{\dagger} \psi_{k\alpha} + V \epsilon_{\alpha\beta} \psi_{k\alpha} \chi_{-k,\beta} + h.c + \epsilon_k^{\chi} \chi_{k\alpha}^{\dagger} \chi$$



Possible ground state: **Compensated ``semi-metal'' of electrically neutral fermions**

An electrical insulator with a neutral Fermi surface (+ U(1) gauge field)

Composite Exciton Fermi Liquid

Physical properties

Standard theory of Fermi surface + U(1) gauge field in 3d

1. Heat capacity $C_v \sim T \ln(\frac{1}{T})$
2. Sub-gap optical absorption $\sigma(\omega) \sim \omega^\phi$ ($\phi = 5/3$ or 2 depending on impurity mean free path)
3. NMR relaxation $\frac{1}{T_1} \sim T$
4. Thermal conductivity $\kappa \sim T$

Magnetic field effects

External B-field induces internal b-field that is seen by neutral fermions.

$b = \alpha B$

(B-field couples to holon and its response induces internal b-field.)

Hard to calculate but expected to → 1 near metal-insulator transition

Consequences: Non-zero thermal Hall effect (weak fields), deHaas van Alphen oscillations with frequencies of order conduction electron fermi surface orbits.

Sodemann, Chowdhury, TS, arXiv, Aug 2017.
Refinement of discussion by Motrunich, 07; Katsura, Nagaosa, Lee, 2010

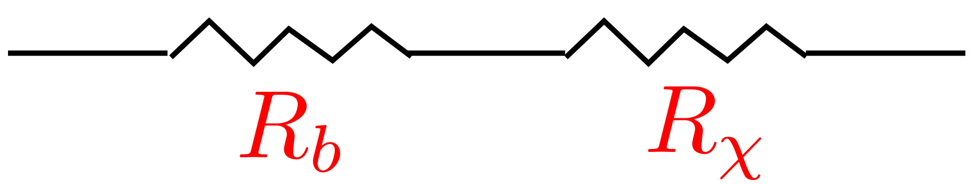
Resistivity oscillations

Total resistivity (ignoring possible surface contribution) determined by well known ``Ioffe-Larkin" rule:

Both charged boson and neutral fermion contribute but in series.

$$\rho = \rho_b + \rho_\chi$$

Boson resistivity   Neutral fermion resistivity



Neutral fermi surface insulator:
b gapped $=>$ ρ_b is large and insulating $(\sim e^{\frac{Delta}{k_B T}})$.

χ metallic $=>$ ρ_χ metallic.

Total resistivity is insulating but a small quantum oscillation from ρ_χ may be observable on top of activated background!

Surface metallic state: how to understand?

A suggestion:

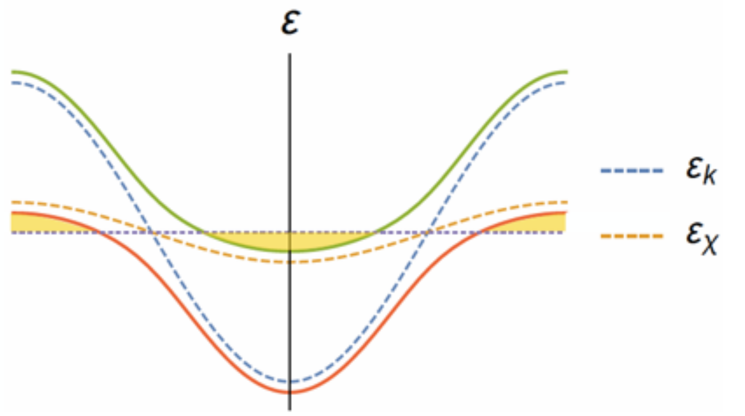
1. Composite fermionic exciton band may itself be topological (but only partially filled)

=> at surface will get (odd number of) Dirac cones of these neutral fermions.

2. The holons may condense at the surface without condensing in the bulk

=> neutral fermions at surface get converted to ordinary electrons

=> get odd number of electronic Dirac cones at surface without a topological bulk.



Summary

Concrete description of a phase of mixed valence insulators with a neutral Fermi surface coupled to a U(1) gauge field.

Phenomenology appealing starting point/framework to interpret experiments in SmB_6, and other similar systems (YbB_{12}, ……).

Proposal of correlated topological Kondo insulators may ultimately have lead to the discovery of a much more exotic state (``beyond topological")!!

In progress: DMRG study of extended periodic Anderson model to look for such a composite exciton Fermi liquid (Zheng Zhu, Donna Sheng, Chowdhury, and TS).