Kondo, Kondo, everywhere, but what is going on in the bulk: Kondo insulators and strong correlations

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Abstract

A class of materials has been found where quasiparticle excitations have an enormous effective mass, known as heavy fermion materials. Examples of such materials are Kondo insulators, in which this behavior is driven by spin-orbit coupling and the presence of localized f orbitals. Coupling between free electrons and localized spins produces interesting physics, namely a large effective mass, through screening and hybridization. In this paper, we discuss a toy model realizing the physics of these materials, the Kondo Lattice Model, and its connection to experiment. Finally, we investigate some of the properties of SmB_6, a potential topological Kondo insulator.

Part I

Introduction and Effective Mass

In the world of strongly correlated problems, where materials' electron-electron interactions are strong and mean field theory can often fail, there exists an emergent behavior where fermions in the material appear to have a mass which is orders of magnitude greater than the normal electron. Such heavy fermion materials generally partially consist of rare earth materials, which have f orbitals and strong spin-orbit coupling. Under a variety of conditions, the f orbitals can localize to the ions, causing a competition between insulating, semiconductor, and even metallic behavior.

While some of this competition is well understood, there remains a rich set of physics to be explored. One heavy fermion material discovered in the 1960s [1], SmB_6, has recently created a flurry of new progress. The material is now believed to be more complex than simply a Kondo insulator but one with topological properties. Materials with such properties, known as topological insulators, generally have surface states that are protected from disorder and surface reconstruction effects . While SmB_6 may have resilient surface states, there are confusing, and at times contradictory, set of experimental observations that produce an exotic story for this insulator.

2 How are Fermions Heavy?

Perhaps the most frequent phrase when dealing with "Kondo physics" is the phrase *heavy fermions*. The term heavy fermions relates to the effective mass of quasiparticles measured in experiments.

The easiest way to think about how one can observe these quasiparticles is to look at Fermi Liquid Theory (FLT). In FLT, problems with strong electronic Coulomb interactions can be connected with a description of free or weakly interacting quasiparticles rather than bare electrons. These quasiparticles have dispersion relations of $\epsilon(k) \sim \hbar^2 k^2/2m^* - \mu$ of a free particle and a mass given by

$$\boxed{\frac{1}{m^*} = \frac{1}{p_F}\left(\frac{\partial \epsilon(k)}{\partial k}\right)_{k=k_F}} \tag{1}$$

While this quantity is unable to be directly observed experimentally, it may be extracted from the specific heat

$$\gamma = \lim_{T\to 0} \frac{C_V}{T} \propto m^* \tag{2}$$

can be measured with good accuracy. Usual metals, *e.g.* pure copper, will have $\gamma \sim 1 - 10$ mJ/K^2mol while heavy fermion compounds have observed this to be $100 - 1600$ mJ/K^2mol[3]. Thus these materials appear to have a effective mass, and thus density of states, several orders of magnitude higher than expected. The large effective mass of heavy fermions is in fact an indication for interesting low temperature physics characterized by universal properties lying beyond the FLT paradigm.

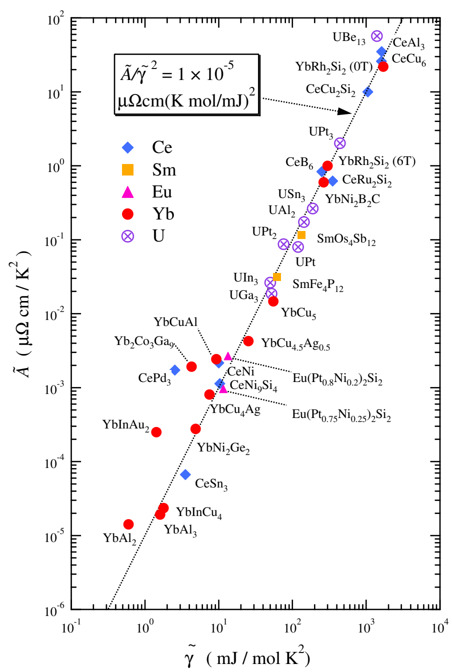


Figure 1: Kadowaki-Woods ratio for many Heavy Fermion materials, normalized for ground state degeneracy [2]

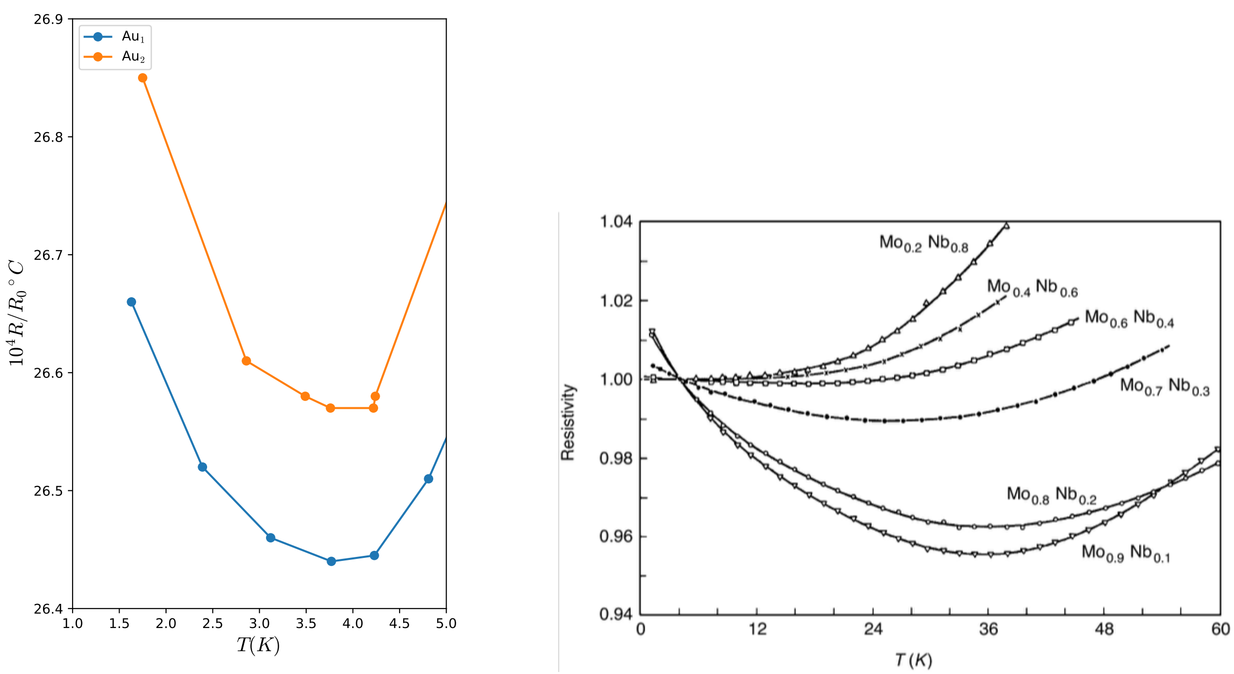
One universal property can be calculated within FLT by considering the resistivity. The resistivity can be calculated as $\rho \sim \rho_0 + AT^2$ where A is some material dependent constant experimentally measured, due to forward scattering. For materials that have this T^2 law and T specific heat, we can define a ratio of A/γ^2, known as the Kadowaki-Woods ratio. As $A \propto m^{*2}$ and $\gamma \propto m^*$ the Kadowaki-Woods ratio should be constant [3]. In Fig. 1 this universality is shown for a multitude of heavy fermion materials.

The remainder of the paper will give the current experimental and theoretical understanding of the materials with large γ or obtain a heavy effective mass not described by FLT. To do so, two models are introduced to explain the wide range of heavy fermion behaviors, differentiating between a single magnetic impurity and a dense lattice of impurities.

Part II

A Single Impurity- the Kondo Problem

3 Experimental Evidence



(a) Resistance data recreated from [4]. The gold samples contained Cu and Ag impurities

(b) Resistance scaling as a function of temperature for MoNb alloys containing 1% of Fe [5]

Figure 2: Experiments showing the rise in resistivity

On the beginning of the path toward the understanding of the materials that were studied in Ref [2], there were a series of experiments that found interesting behaviors in the low temperature resistivity. One of the first, illustrated in Fig. 2a, was a 1934 experiment that found an unexpected rise in resistivity from Gold with a small amount magnetic impurities. Another experiment, shown in Fig. 2b varied the doping of MoNb with a 1% Fe impurity concentration showing a deviation from the $\rho_0 + AT^2$ with the addition of $-\ln T$ behavior, at a transition temperature T_k (the Kondo temperature). The cross over at the temperature T_k is known as the Kondo effect. Connecting the high temperature FLT description and the Kondo temperature transition was known as the Kondo problem.

4 The Kondo Model

To describe the microscopic behavior of these (now more understood) heavy fermion materials, we begin with the Anderson model, which describes a localized magnetic ion[1] interacting with a sea of conduction electrons of dispersion $\epsilon_{\mathbf{k}}$

$$H_{\text{Anderson}} = \sum_{\mathbf{k},\sigma} \underbrace{\boxed{\epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma}}}_{\text{Conduction}} + \underbrace{\boxed{V_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} f_{\sigma} + h.c.}}_{\text{Conduction-Impurity}} + \underbrace{\boxed{E_f n_f + U n_{f\uparrow} n_{f\downarrow}}}_{\text{Impurity}} \tag{3}$$

where $c^{\dagger}_{\mathbf{k}\sigma}$ is a conduction electron creation operator and f_{σ} is an f orbital annihilation operator. Because of the time reversal symmetry and overall spin 1/2 of the impurity, there will be a Kramer's doublet or a double degenerate energy state in the atomic limit of the orbital.

To extract the physics of the Kondo effect, we will look at what happens when we remove the unoccupied and double occupied states of the impurity. With that in mind, we can look at the virtual processes of conduction electrons interacting with the impurity. There are two import processes here, which involve two sets of hops (hopping onto then from the impurity) which changes the spin ($\uparrow \leftrightarrow \downarrow$) of the conduction electron and the impurity spin. This spin flip interaction can be modeled as a spin-spin interaction Hamiltonian, where the conduction electrons spin operator is written as $\sum_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\alpha} \vec{\sigma}_{\alpha\beta} c_{\mathbf{k}'\beta}$ such that the new Hamiltonian is

$$H_{\text{Kondo}} = \sum_{\mathbf{k},\sigma} \underbrace{\boxed{\epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma}}}_{\text{Conduction}} - \sum_{\mathbf{k},\mathbf{k}'} \underbrace{\boxed{J_{\mathbf{k}\mathbf{k}'} \left(c^{\dagger}_{\mathbf{k}\alpha} \vec{\sigma}_{\alpha\beta} c_{\mathbf{k}'\beta} \right) \cdot \vec{S}_f}}_{\text{Conduction-Impurity}} \tag{4}$$

with S_f being the spin of the impurity.

A surprising feature of the spin-spin interaction is the sign of J. Using second order perturbation theory of the conduction-impurity process from the Anderson Hamiltonian we will obtain an effective J as $J_{eff} = -4|V_{\mathbf{k}}|^2/U$ which is inherently negative with $U > 0$. This extra negative sign makes the interaction antiferromagnetic rather than ferromagnetic, a surprise at the time as it was expected to be a ferromagnetic interaction.

Out of this model we find two interesting results. The first is the asymptotic freedom of the impurity. At high temperatures the local magnetic moments are free but upon cooling create a strong coupling to the conduction electrons; this is known as asymptotic freedom, the same physics governing quarks in QCD [3]. Because this is related to scaling and not emergent physics, we will gloss over the scaling details and focus on what happens at the lower temperatures.

Hinted by the Kadowaki-Woods ratio, many of the observables can be written in a universal form [6]. If we let F be some function then both the spin susceptibility, inverse scattering rate, and

[1] which we will take, without loss of generality, to be an f orbital in labeling

specific heat (at strong coupling) can be written as a universal function T/T_K,

$$\chi(T) = \frac{1}{T} F_\chi \left({}^T/_{T_K}\right)$$
$$\frac{1}{\tau(T)} = \frac{1}{\tau_0} F_\tau \left({}^T/_{T_K}\right)$$
$$C_V \propto {}^T/_{T_K}$$

The second result is finding a Kondo resonance, also known as the Abrikosov-Suhl Resonance [3]. Here a singlet between the conduction electrons and magnetic impurity forms at the fermi surface and creates a peak in the spectral function of width proportional to the Kondo temperature T_k. As the temperature is lowered, the impurity is screened by the conduction electrons slowly becoming non-magnetic. Screening of the local magnetic moment is known as the *Kondo effect*. This effect provides evidence of a universal behavior of at low temperatures of the resistance minimum due to magnetic impurities.

Part III
Many Impurities - the Kondo Lattice

5 Experimental Evidence

A key part of the material in Fig. 2b was that it had a *small* amount of magnetic impurities (Fe). If instead there were many magnetic moments in the lattice, as is the case with SmB_6 and other materials, then we might expect new physics to come out. Experimentally this is seen with a high temperature Curie-Weiss susceptibility of $\chi \sim (T+\theta)^{-1}$ from magnetic impurities.

We also see that SmB_6 is a strong insulator when its resistance grows at low temperature as shown in Fig. 3, unlike the change in resistivity seen earlier in Part II. There were also a series of materials like SmB_6, *e.g.* $CeFe_4P_{12}$ or YbB_{12} , that were metallic at high temperatures but insulating at low temperatures known as Kondo Insulators [7]. Some of the physics of Kondo Insulators is now understood, but there are still many open questions, particularly with SmB_6 to be explored in Part IV.

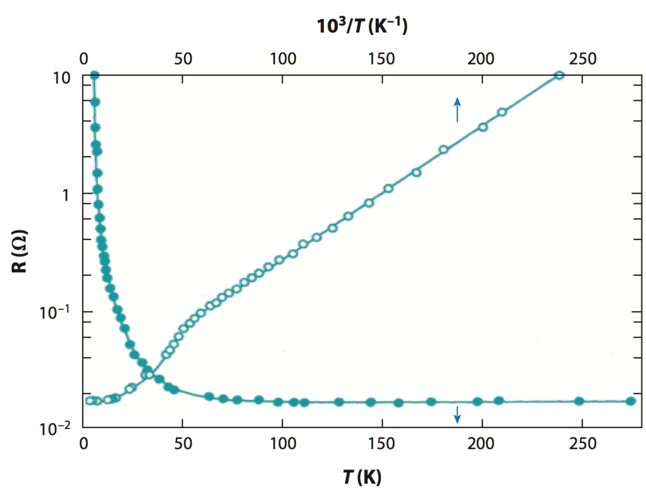


Figure 3: SmB_6 resistance measurement [1, 7]

6 The Kondo Lattice Model

Some of these Kondo insulator experiments lead Doniach [9] to introduce a lattice version of the Kondo model eq. (4) with many magnetic spins (with the double occupied and unoccupied degrees

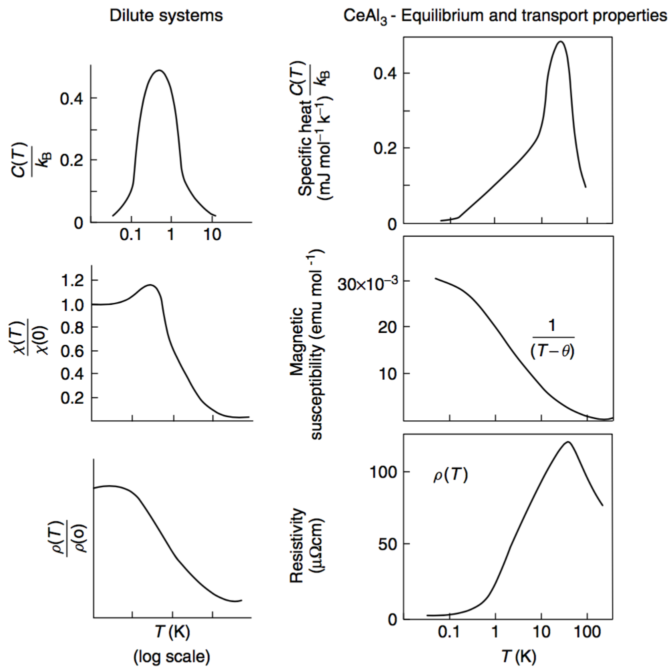


Figure 4: Differences in typical experiments between materials described by the Kondo model (left) and the Kondo lattice model (right) [8]. The specific heat includes the $-\ln T$ component away from Fermi liquid behavior. Note that we focus on Kondo Insulators which have a different low temperature resistivity as seen in Fig 3.

removed) interacting with conduction electrons

$$H_{\text{KLattice}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - J \sum_{j,\alpha\beta} \left(c^{\dagger}_{j\beta} \vec{\sigma}_{\beta\alpha} c_{j\alpha} \right) \cdot \vec{S}_j \tag{5}$$

where usually $J = -|J|$ an antiferromagnetic coupling, and $\vec{S}_j$ is a local spin 1/2 moment [7]. The motivation of this model is to describe a dense lattice of magnetic impurities that match the high temperature behavior of Fig. 4 and explain the many low temperature phenomena observed, such as a metal-insulator transition. Doniach argued that one still found the Kondo temperature, as seen experimentally, but there was another fundamental energy (temperature) scale.

Consider the single impurity Kondo model, but with one extra impurity added, such that we have $\vec{S}_{f_1}$ and $\vec{S}_{f_2}$. One could write out second order perturbation theory in which we consider the two Hamiltonian terms, one from the conduction-spin interaction from impurity 1 and another from impurity 2. Then upon integrating out the conduction electrons the remaining term goes like

$$H_{RKKY} \sim J_{RKKY}(\mathbf{r}) \vec{S}_{f_1} \cdot \vec{S}_{f_2} \quad \text{with} \quad J_{RKKY}(\mathbf{r}) \sim J^2 \rho \frac{\cos 2k_F |\mathbf{r}|}{|\mathbf{r}|^3} \tag{6}$$

with ρ the conduction electron density of states per spin and $\mathbf{r}$ is distance from the impurity. This is called the RKKY interaction after Ruderman, Kittel, Kasuya and Yosida [6]. While that is a straightforward way to derive the effective Hamiltonian, there is an alternative picture of description. Because each local moment acts like an effective magnetic field to the conduction electrons; thus the electrons will want to anti-align to the impurity spins (recall the antiferromagnetic coupling). In-between the two impurities will be governed by some periodic function related to the how the spins are pointed, to maximize the antiferromagnetic interaction but weakened the further from the impurity the electron is.

Doniach noticed this new effective interaction energy scale, and argued that it scaled like $T_{RKKY} \sim J^2\rho$. He concluded that $T_K \ll T_{RKKY}$ the spin-spin interaction will create antiferromagnetic ordering. On the contrary, when $T_K \gg T_{RKKY}$ then a scattering resonance will stabilize the singlet ground state considered from the Kondo model, along with heavy fermions. Unlike the Kondo model, which created a rise in resistivity, the coherent resonant scattering of the lattice model produces a drop in resistance as shown on the right in Fig 4. When they are on the same order, something less straightforward must happen. Moreover, for low temperatures, Kondo insulators have a disappearance of the RKKY interaction [3].

Previously we saw that a single impurity underwent screening into a non-magnetic ground state and produced a large peak at the fermi surface, yet the Kondo lattice model can produce an insulator with a charge and spin gap. Following the arguments in Ref. [7], consider the $t/J \to 0$ limit of the Kondo lattice model. This limit reduces to just spin/electron interactions (the J term), forming a singlet ground state

$$|\Psi_0\rangle = \prod_j \frac{1}{\sqrt{2}} \left(|\Uparrow_j \downarrow_j\rangle - |\Downarrow_j \uparrow_j\rangle\right) \tag{7}$$

where $\Uparrow$ / $\Downarrow$ is the localized spin and $\uparrow$ / $\downarrow$ are the conduction electrons. Consider the excitations of this ground state. To switch a singlet to a triplet we'd gain an energy of $2|J|$, which means this model is spin gapped. We can then add or remove an electron to site i, which we will take to be $\uparrow_i$

$$\begin{aligned}
\sqrt{2}c_{i\uparrow}^{\dagger} |\Psi_0\rangle &= \Uparrow_i (\uparrow_i \downarrow_i) \prod_{i \neq j} \frac{1}{\sqrt{2}} \left(|\Uparrow_j \downarrow_j\rangle - |\Downarrow_j \uparrow_j\rangle\right) \\
\sqrt{2}c_{i\uparrow} |\Psi_0\rangle &= \Uparrow_i \prod_{i \neq j} \frac{1}{\sqrt{2}} \left(|\Uparrow_j \downarrow_j\rangle - |\Downarrow_j \uparrow_j\rangle\right)
\end{aligned}$$

For both wave functions we've created have extra energy of $3|J|/2$ and thus separated by $3|J|$. Therefore the Kondo lattice model at strong coupling gives a ground state that's a Kondo insulator with spin gap $2|J|$ and charge gap $3|J|$.

Lastly, there is a hybridization picture of obtaining a gap. Using mean field theory on the Kondo lattice model, a flat band of localized f electrons can hybridize with the free conduction electrons. The hybridization opens a gap, which if the chemical potential lies within the gap the material is insulating. The conduction band is then heavy fermion holes, with a positive charge unlike the high temperature phase. Mean field theory however is not enough to explain many of the properties of the Kondo insulator SmB_6, for example.

Additionally, heavy fermion superconductivity can emerge from magnetic impurity interactions [3, 7, 10]. Like a Cooper pair, the localized spin and high energy electrons form a "composite" fermion (rather than boson), leading to new phenomena. Those effects won't be covered here but is interesting modern emergent behavior that is being studied.

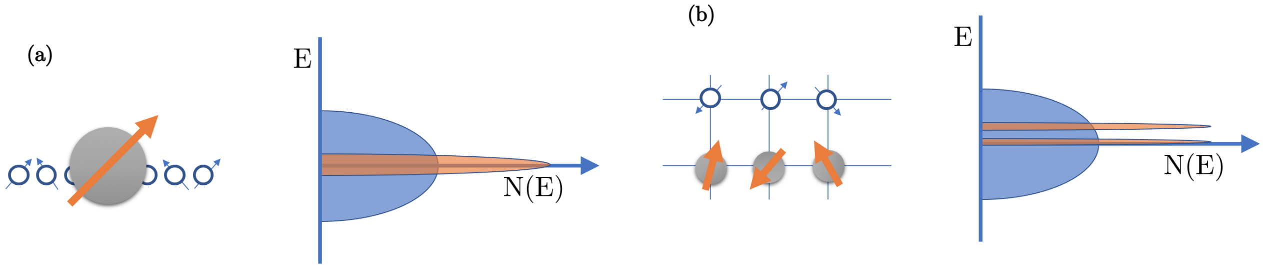


Figure 5: The difference between the Kondo model and the Kondo Lattice model. (a) depicts a single impurity interacting with conduction electrons which opens up the Kondo resonance while (b) shows a dense lattice of impurities interacting with conduction electrons which can create a hybridization gap of the Kondo insulator. Adapted from [6].

Part IV

More open questions - SmB_6

7 What Makes SmB_6 Different?

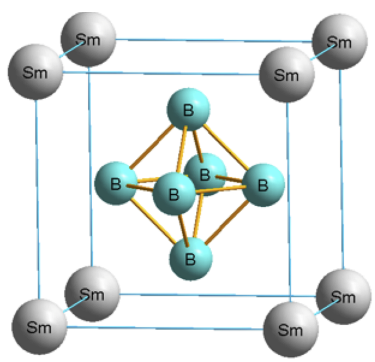


Figure 6: Crystal Structure of SmB_6 [11]

While SmB_6 was a prototypical example of a Kondo insulator, even now there are many puzzling questions about its properties. The first is the resistance saturation somewhere below 4K. At high temperatures the material behaves as a metal, and at low temperatures it becomes insulating as a hallmark Kondo insulator but the $-\ln T$ behavior does not extend to $T \to 0$. This is, however, in line with what one would expect from a topological Kondo insulator (TKI).

Different groups set out to measure the surface conductivity compared with the bulk. One group, Wolgast et al. [12], constructed an elaborate way to verify bulk vs surface conduction. In their paper[2], it was found that below 4K there was indeed a change from bulk to surface conductance, with many signs pointing to being a TKI. However the experiment was sensitive to sample preparation (etching the surface for example) and could not definitely conclude another source of surface conduction.

Why would surface conductance be exciting? Because conducting surface states are sensitive to disorder or other surface effects (they tend to favor localization under disorder, for example) and can be difficult to observe in experiments, except when protected by an interplay of symmetry and topology. Topological order, however, cannot exist in 3D only in 2D, but surface states can be protected with gapless topologically distinct surface states creating a 3D topological insulator. (TI) These states are called Dirac surface states [7](For more information see the references within [7]).

Soon after Wolgast et al., Kim et al. [13, 7] measured Hall voltages on a wedge shaped sample to determine the dependence on thickness. At $\gg 4K$ temperatures the Hall resistance[3] was found to be inversely proportional to the sample's thickness indicating bulk conductivity. Below 4K, the

[2]Originally titled *Discovery of the First Topological Kondo Insulator: SmB_6* but then renamed to *Low-temperature surface conduction in the Kondo insulator SmB_6*

[3]resistance taken by measuring the resistance perpendicular to an applied current

Hall resistance became thickness independent indicating surface conduction.

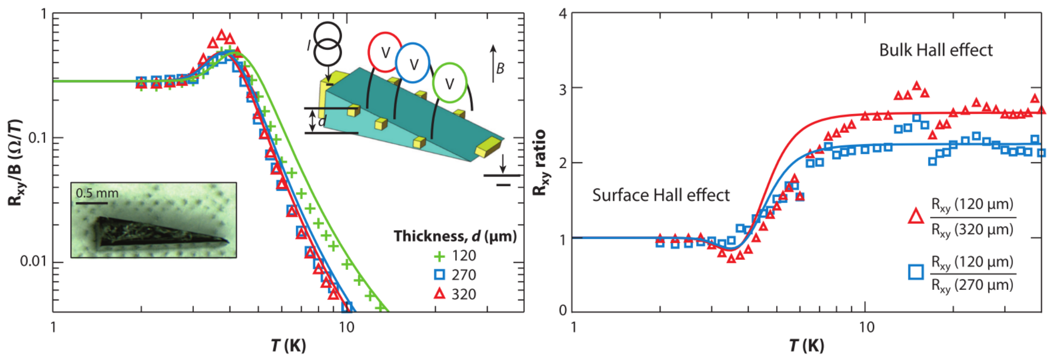


Figure 7: Kim et al. Hall measurements on a wedge shaped sample [13, 7]

Still these experiments only showed that SmB_6 *has* resilient surface states, not that they are topologically protected. An experiment that was used to verify 2D TIs, spin-resolved Angle Resolved PhotoEmission Spectroscopy (ARPES), has not been successful with this material because of the small energy gap in the bulk. That isn't to say there aren't results for this experiment, but they are conflicting with other observations, with one group even appears to have found signs of a trivial insulator rather than a TI from the presence of Rashba-splitting [7].

Even with ARPES out of reach, by applying a magnetic field time reversal symmetry can be broken. Using weak-antilocalization (WAL) effects, more results have pointed toward a topological nature of the surface state, but can still be related back to spin-orbit coupling. Measuring a non-trivial Berry phase using quantum oscillation experiments, a phase of π in particular, would further the TKI theory and more experiments have shown this to be a case, except a baffling quasiparticle effective mass measurement of $\sim 0.1 m_e$ [7].

While there are further experiments shedding more and more light on its properties, each new turn comes with further questions. Theoretically it has been suggested recently that SmB_6 may be in fact a Skyrme insulator [14] or that the bulk is a Majorana Fermi liquid [15]. The bulk behaving as a Fermi liquid is backed up by measurements where the linear specific heat was measured after the sample was ground up into a powder, such that the surface area drastically increased [16].

8 A Model for Topological Kondo Insulators

Instead of focusing on an effective model describing the microscopic mechanisms of SmB_6, Dzero et al. has provided a theoretical model for a general topological Kondo Insulator [17]. A more complex approach can be used using the Anderson lattice model, however we will present an effective Hamiltonian they have introduced instead. A simple TKI Hamiltonian on a cubic lattice consists of hybridizing conduction electrons (with dispersion $\epsilon_c(\mathbf{k})$) with the localized f electrons (with $\epsilon_f(\mathbf{k})$),

$$H = \sum_{\mathbf{k}} \begin{pmatrix} c^\dagger_{\mathbf{k}c} & c^\dagger_{\mathbf{k}f} \end{pmatrix} \underbrace{\boxed{\begin{pmatrix} \epsilon_c(\mathbf{k}) & V\vec{d}_{\mathbf{k}} \cdot \vec{\sigma} \\ V\vec{d}_{\mathbf{k}} \cdot \vec{\sigma} & \epsilon_f(\mathbf{k}) \end{pmatrix}}}_{\mathcal{H}(\mathbf{k})} \begin{pmatrix} c_{\mathbf{k}c} \\ c_{\mathbf{k}f} \end{pmatrix} \tag{8}$$

where $\vec{d}_{\mathbf{k}} = (\sin k_x, \sin k_y, \sin k_z)$. Notice that near $\mathbf{k} = \mathbf{0}$ $\vec{d}_{\mathbf{k}} \approx \mathbf{k}$. If we define $\epsilon_{\pm}(\mathbf{k}) = (\epsilon_c(\mathbf{k}) \pm \epsilon_f(\mathbf{k}))/2$ the energy of the effective Hamiltonian is

$$E = \epsilon_+(\mathbf{k}) \pm \sqrt{\epsilon_-^2(\mathbf{k}) + V^2|d_{\mathbf{k}}|^2}. \tag{9}$$

To determine the topological properties, one needs to consider the 8 high symmetry points in the Brillouin zone which are invariant under time reversal symmetry. This restricts $\mathcal{H}$ to have the following symmetry properties

$$\mathcal{H}(\mathbf{k}) = \mathcal{P}\mathcal{H}(-\mathbf{k})\mathcal{P}^{-1}$$
$$\mathcal{H}(\mathbf{k}) = \mathcal{T}\mathcal{H}(-\mathbf{k})\mathcal{T}^{-1}$$

where $\mathcal{P}, \mathcal{T}$ are parity and time-reversal operators respectively with the form

$$\mathcal{P} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}; \quad \mathcal{T} = \begin{pmatrix} i\sigma_2 & 0 \\ 0 & i\sigma_2 \end{pmatrix} \tag{10}$$

where σ_2 is the second Pauli matrix. If its assumed that $\vec{d}_{\mathbf{k}} = -\vec{d}_{-\mathbf{k}}$, or that the hybridization form factor is odd, then at any of the time reversal symmetry points it must be 0 (as $\vec{d}_{\mathbf{k}} = \vec{d}_{-\mathbf{k}} = -\vec{d}_{\mathbf{k}}$). The Hamiltonian $\mathcal{H}$ can be written at those points, denoted $\mathbf{k}_m^*$ as

$$\mathcal{H}(\mathbf{k}_m^*) = \epsilon_+\mathbb{1} + \epsilon_-\mathcal{P}. \tag{11}$$

with m as an index for each of the 8 symmetry points.

What determines the topological properties of the insulator are topological indices; here there is one strong index and three weak indices. The indices are made up of products of $\delta_m = \text{sgn}(\epsilon_c - \epsilon_f)|_{\mathbf{k}_m^*}$, and the overall sign can be classified into strong or weak topological insulators or a conventional band insulator. This is known as a Z_2 index as there are two possible descriptors, ± 1. With the right combination of band structure one can create a strong topological Kondo insulator, as well as a weak TI and conventional insulator [7, 17]. With the ability to create a toy model of a TKI provides hope for discovery a 3D TI with perhaps heavy fermion properties, even if SmB_6 is not believed to be described with this particular toy model.

Part V

Conclusion

Magnetic impurities and localized magnetic moments have shown to create an expansive set of emergent phenomena. Much of the related effects create quasiparticles with a large effective electron mass, explained in part by various Kondo or Anderson models. Such massive particles are indicative of interesting emergent phenomena, mostly at low temperatures. In particular, low temperature resistivity measurement was of particular importance to understanding the underlying mechanisms, albeit not all low temperature behaviors have been explained.

We focused on SmB_6, a Kondo insulator that is strongly believed to be a 3D topological Kondo insulator. While there are many open questions to explain the experimental observation, a plethora of theories are being created to better understand and test the behavioral mechanisms.

There were two further topics to be explored beyond the scope of this paper. The first, renormalization and the scaling of the Kondo model, provide clearer pictures as to the connections of various toy models to effective models. The second, heavy fermion superconductivity, provides more questions and another set of emergent physics to be studied.

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