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Kondo Breakdown and Quantum Oscillations in SmB_6

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Recent quantum oscillation experiments on SmB_6 pose a paradox, for while the angular dependence of the oscillation frequencies suggest a 3D bulk Fermi surface, SmB_6 remains robustly insulating to very high magnetic fields. Moreover, a sudden low temperature upturn in the amplitude of the oscillations raises the possibility of quantum criticality. Here we discuss recently proposed mechanisms for this effect, contrasting bulk and surface scenarios. We argue that topological surface states permit us to reconcile the various data with bulk transport and spectroscopy measurements, interpreting the low temperature upturn in the quantum oscillation amplitudes as a result of surface Kondo breakdown and the high frequency oscillations as large topologically protected orbits around the X point. We discuss various predictions that can be used to test this theory.

SmB_6 , discovered 50 years ago[1, 2], has attracted recent interest due to its unusual surface transport properties: while its insulating gap develops around $T_K \simeq 50\text{K}$, the resistivity saturates below a few Kelvin[3]. The renewed interest derives in part from the possibility that SmB_6 is a topological Kondo insulator, developing topologically protected surface states at low temperatures [4–7]. Experiments[8–10] have confirmed that the plateau conductivity derives from surface states, and these states have been resolved by angle-resolved photoemission spectroscopy (ARPES)[11–14]. Furthermore, spin-ARPES experiments have revealed the spin-momentum locking of the surface quasiparticles expected from topologically protected Dirac cones[15].

Yet despite this progress, some important experimental results are unresolved. In particular, quantum oscillation experiments on SmB_6 have given rise to two dramatically different interpretations[16, 17]. Ref [16] observes low frequency (small Fermi surface) oscillations with the characteristic $1/\cos(\phi)$ dependence on field orientation expected from 2D topological surface states. On the other hand Ref [17] detects a wide range of frequencies (both high and low frequency oscillations) which have been interpreted in terms of angularly isotropic three dimensional quasiparticle orbits, resembling a metallic hexaboride without a hybridization gap (such as LaB_6). A striking aspect of these measurements, is that the oscillations strongly deviate from a classic Lifshitz-Kosevich formula below $\sim 1\text{K}$. Two recent theoretical proposals have been advanced to account for this bulk behavior, as a consequence of magnetic breakdown[18], of the formation of non-conducting Fermi surfaces[19].

Another aspect of recent measurements, is the wide disparity in the reported effective masses of the carriers. The effective mass observed in both quantum oscillation experiments, $m^*/m \sim 0.1 - 0.2$ is an order of magnitude smaller than effective mass observed in ARPES[11–14], $m^*/m \sim 1$ and two orders of magnitude smaller than those extracted from magnetothermoelectric transport experiments,[20] $m^*/m \sim 10 - 100$. Moreover the Fermi

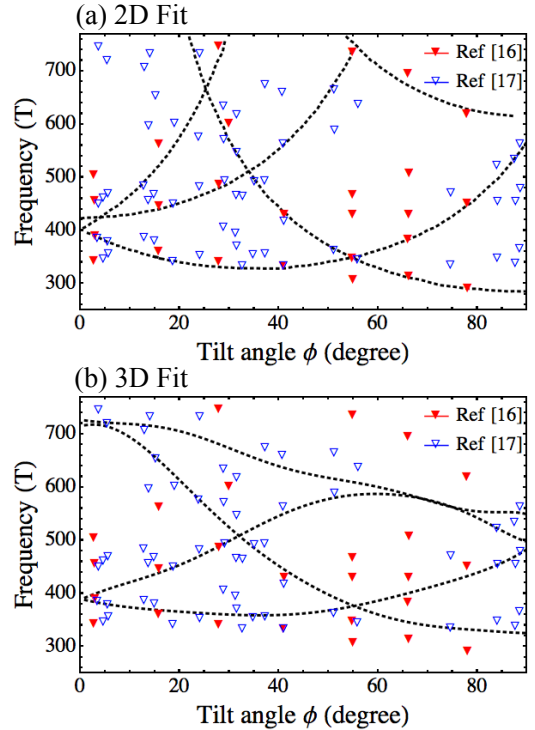


FIG. 1: Low frequency oscillations extracted and replotted from Ref[16] (red, filled symbols) and Ref[17] (blue, open symbols). Lines are model fits based on (a) two dimensional surface states[16], (b) three dimensional bulk bands[17]. Error bars are the size of symbols which include both experimental errorbars and also errors from extracting data from a logarithmic plot. Given the error bars, there is a good agreement between two experiments for low frequencies and it is not possible to distinguish if a 2D or a 3D model fits better *a priori*.

surface areas are also drastically different in these sets of different experiments.

The goal of this paper, is to discuss and contrast the quantum oscillation data that has inspired these alternative interpretations, seeking an interpretation that can be reconciled with the robust insulating behavior and sur-

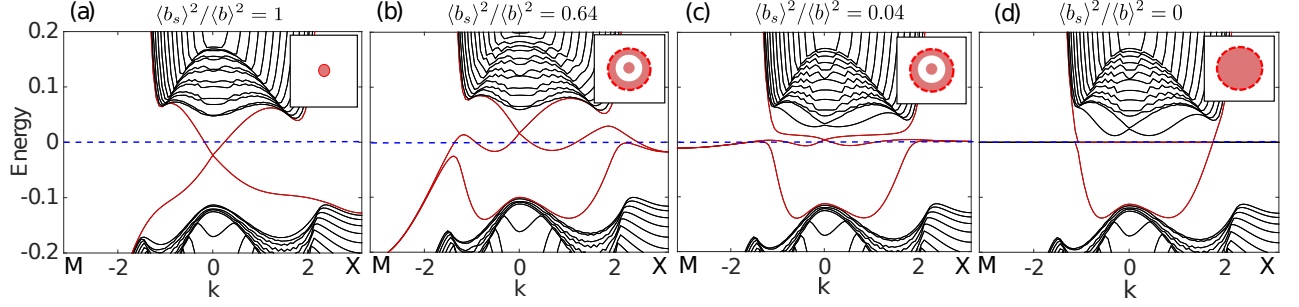


FIG. 2: Kondo breakdown and onset of surface Kondo effect. 3D strip calculations are done for varying $\langle b_{(s)} \rangle^2 / \langle b \rangle^2$ where $\langle b_{(s)} \rangle^2$ is the bulk (surface) slave-boson amplitude indicating the amount of hybridization between the local moments on the surface and the topological surface states. For (a), $\langle b_s \rangle^2 / \langle b \rangle^2 = 1$, the hybridization on the surface is the same as the bulk, leading to heavy surface quasiparticles with a small Fermi surface. As $\langle b_s \rangle^2 / \langle b \rangle^2$ gets smaller in (b) and (c), the Fermi surface area increases as a result of Luttinger's sum rule and a new larger Fermi surface orbit appears. For $\langle b_s \rangle^2 / \langle b \rangle^2 = 0$ (d), local moments decouple from the surface, giving rise to a large Fermi surface with light quasiparticles. Insets show the Fermi surfaces for each figure.

face conductivity of this Kondo insulator. As shown in Fig. 1, in the low frequency range where the two sets of experiments overlap, the data are in agreement within the error bars, and *a priori* permit either a two, or three dimensional interpretation. Beginning with an examination of possible three dimensional bulk interpretations of the data, we will argue that consistency obliges us to return to a surface interpretation of the quantum oscillations, derived from 2D topological surface states with a $1/\cos(\phi - \phi_0)$ angular dependence off various surface facets that can resemble the isotropy of three dimensional orbits. In our theory, the large orbit quantum oscillations observed in experiment are a consequence of the suppression of the Kondo effect on the surface (see Fig. 2) associated with Kondo breakdown[21]. This effect causes the local moments to decouple from the topological surface states over a wide temperature range, leading to lighter quasiparticles with large Fermi surface orbits that resemble the extremal orbits of an unhybridized bulk, in accordance with ARPES experiments[11–14]. In our proposal, the low temperature upturn in the quantum oscillation amplitudes are most naturally accounted for as an onset of surface, rather than bulk quantum criticality.

SmB₆ provides a unique platform to study the orbital effects of magnetic fields in narrow gap insulators: it has a transport gap of about $T_K = 50\text{K}$ and a direct gap of about 230K (20meV). Other Kondo insulators (e.g YbB₁₂ [22] or Ce₃Bi₄Pt₃ ($T_K \sim 35\text{K}$)[23] are “Pauli limited”, with a gap that closes linearly in a field, closing at a critical field in the range $B_c \sim 20 - 50\text{T}$. By contrast, in SmB₆, the much smaller size of the f-electron g-factor ($g \sim 0.1 - 0.2$) suppresses the Zeeman splitting in favor of an orbital closure of the gap at a critical field in excess of 100T [24, 25].

Bulk quantum oscillations: We begin by revisiting the intriguing suggestion that a narrow gap insulator may sup-

port bulk quantum oscillations. De Haas van Alphen oscillations are a thermodynamic effect, resulting from the Landau quantization of a Fermi surface. The Lifshitz-Kosevitch temperature dependence of dHvA oscillations is a result of the discretized sampling of the density of states.

One interesting possibility is that the observed quantum oscillations are a magnetic breakdown effect resulting from the small hybridization gap. Magnetic breakdown[26–28] is a result of the breakdown of the quasi-classical approximation, where the electrons orbiting around the Fermi surface can tunnel among different Fermi surfaces giving rise to larger orbits. Such processes preserve energy but not crystal momentum. However, in the case of small gap systems, magnetic breakdown leads to tunneling through the gap, as a magnetic analog of the Zener breakdown[29]. Such effects are known to occur in type-II superconductors and Knolle and as Cooper[18] point out, may be also be a feature of narrow gap Kondo insulators, independently of whether they are topological. It would be interesting to test this idea in other small gap Kondo insulators like YbB₁₂ and Ce₄Bi₃Pt₄. Here, the basic idea is that if the cyclotron energy $\hbar\omega_c$ is at least comparable with the direct hybridization gap V , $\hbar\omega_c \geq V$ Landau quantization develops, producing a kind of quantum Hall insulator. The authors also point out that the oscillation amplitude in this case can deviate from standard Lifshitz-Kosevich formula if the chemical potential is close to the valence or conduction bands. On the other hand, if cyclotron frequency is much smaller than the direct gap, $\hbar\omega_c \ll V$, the oscillation amplitude is damped exponentially, $R \sim R_0 \exp(-V/\hbar\omega_c)$.

However, the field range used to observe quantum oscillations SmB₆ lies in the small gap limit $\hbar\omega_c \ll V$: to see this, note that at $B = 10\text{T}$, the cyclotron frequency is $\hbar\omega_c \simeq 1 - 2 \text{ meV}$ [41], while the direct gap measured

by ARPES[11–14] and optics[30] is an order of magnitude larger, around $V = 20\text{meV}$, which would lead to an exponential suppression of the amplitude relative to the Lifshitz-Kosevich formula. There is a well-known discrepancy between the direct gap measured in ARPES and optics and the much smaller transport gap of about 50K ($\sim 4.3\text{meV}$) measured from the resistivity, which may be associated with an indirect gap. However, it is the direct gap V that controls the presence of Landau quantization, and so long as $\hbar\omega_c \ll V$, magnetic breakdown is unable to account for the observation of Lifshitz Kosevitch behavior over a wide temperature and field range in SmB_6 .

Another intriguing idea, is that a bulk insulator might contain a Fermi surface of non-conducting excitations that can still develop Landau quantization. This is the essence of a recent proposal by Baskaran[19]. Baskaran's work raises the fascinating question of whether a Fermi surface of electrically neutral particles can still experience a Lorentz force. Quasiparticles in Landau orbits circulate in quasi-classical orbits, which for SmB_6 can be as large as 1 micron[17], which sets a minimum size for the regions of gapless excitations in the bulk, or on the surface. Landau quasiparticles lead to diamagnetism and hence carry circulating currents, which in turn implies the quasiparticles must couple to the current operator \mathbf{j} . The problem is that a diamagnetic coupling inevitably implies a coupling to the electric field \mathbf{E} .

To demonstrate this point, consider a thought experiment in which the magnetic field \mathbf{B} on Landau-quantized quasiparticles is adiabatically increased, raising the energy of each Landau level as required to produce quantum oscillations. The energy of the single particle states in the n -th level increases by an amount of order $n\hbar\Delta\omega_c$ as a result of the change in the magnetic field. Microscopically, the coupling of the Hamiltonian occurs via the vector potential, so the change in energy is given by:

$$\begin{aligned} n\hbar\Delta\omega_c &= \int \langle \psi_H^{(n)} | \frac{\partial H}{\partial t} | \psi_H^{(n)} \rangle dt \\ &= \int \langle \psi_H^{(n)} | -\frac{\delta H}{\delta \mathbf{A}(x)} | \psi_H^{(n)} \rangle \cdot \left(-\frac{\partial \mathbf{A}(x)}{\partial t} \right) d^3x dt \end{aligned}$$

where $|\psi_H^{(n)}\rangle$ is the one-particle wave function of a quasiparticle in the n^{th} Landau level, written in the Heisenberg representation. But the derivative of the vector potential can be identified with the electric field $\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t}$, while $-\frac{\delta H}{\delta \mathbf{A}(x)} = \mathbf{j}(x)$ is the current operator, so that

$$n\hbar\Delta\omega_c = \int \langle \psi_H^{(n)} | \mathbf{j}(x) | \psi_H^{(n)} \rangle \cdot \mathbf{E}(x) d^3x dt \quad (1)$$

From this argument, we see that the energy deposited into quasiparticles due to ramping up the field derives from the electric field associated with a changing vector potential, i.e Faraday's law. Moreover, in order that the field increase the particles energy, the current oper-

ator of the quasiparticles must be finite. Gauge invariance tells us that since $\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}$, the quasiparticles must couple equally to an electric field induced by Faraday's effect or a gradient of the potential, i.e they must be charged and will be conducting. Baskaran proposes[19] that a non-conducting Fermi surface of Majorana fermions can Landau quantize. However, propagating Majorana fermions carry a equal weight of electrons and holes moving in the same direction, so their current matrix elements vanish and they are fully electrically neutral. Thus, as far as we can see, a single band of Majorana fermions can not Landau quantize and will not give rise to Quantum oscillations.

Surface quantum oscillations: The difficulties encountered in a bulk interpretation of the quantum oscillations in insulating, SmB_6 thus lead us to re-examine the possibility that these signals are a topological surface effect. At first sight, such a proposal should be ruled out because the Fermi surface area of the topological surface states are unrelated to the bulk Fermi surface of the conduction electrons in simple model theories for topological insulators. Indeed, the surface Fermi surface area can be vanishingly small if the chemical potential is close to (or at) the Dirac point. Nonetheless, SmB_6 offers us some empirical support for a surface interpretation of the oscillations, for ARPES measurements[11–14] show that the Dirac point is sunk into the valance band and regardless of where the surface chemical potential is, the Fermi surface area of the topological surface states are quite close to bulk Fermi surface area[31]. Moreover, as shown Fig. 1, the low frequency oscillations of both experiments agree within the errorbars, indicating that, at least for these modes, the 2D surface states interpretation deserves further consideration.

The empirical observation that the Dirac point of the surface states is sunk in the valence band suggests a strong particle-hole asymmetry. One mechanism for this asymmetry is through the destruction of Kondo singlets at the surface[21]. The different parity of the localized f-electrons and mobile d-electrons in SmB_6 , causes Kondo screening to develop by coupling to nearest neighbor sites. The reduction of nearest neighbor sites on the surface causes the surface Kondo temperature to be suppressed, so that the screening of local moments at the surface is either develops at much lower temperatures, or fails completely due to the intervention of surface magnetic order or quantum criticality. Such *Kondo breakdown* liberates conduction electrons which were bound in Kondo singlets, which dopes the topological surface states and pushes the Dirac point to the valence band. The resulting surface states have a considerably larger Fermi surface given by

$$\frac{\mathcal{A}_{\text{FS}}}{(2\pi)^2} = \Delta n_f \quad (2)$$

in accordance with Luttinger's sum rule where Δn_f is the

change of the Samarium nominal valence on the surface due to the re-localization of the f-electrons. Note that the nominal valence, a concept introduced by Anderson[32], is different than real valence measured by photoemission. In the Kondo insulating state, the nominal valence of Sm is +2 whereas the real valence is +2.6. Kondo breakdown also leads to much lighter quasiparticles (see Fig 2(d)), giving rise to a Fermi velocity and a large 2D Fermi surface area which are in agreement with ARPES experiments[11–14]. Indeed, Kondo breakdown gives rise to topological surface states which mirror the extremal orbits of the bulk d-states. This leads us to propose that the quantum oscillations observed in both experiments are a consequence of Kondo breakdown extending down to involve to about 1K, following the Lifshitz-Kosevich formula for a large, light Fermi surface.

Next we consider the case when a Kondo effect starts to develop at the surface. The low energy Hamiltonian of the surface moments interacting with topological surface states is given by a chiral Kondo or Anderson model[21]. We use the large N description of chiral Anderson model:

$$\begin{aligned}
H_{CAM} = & \sum_{\mathbf{k}} (v_F \mathbf{k} \cdot \boldsymbol{\sigma}_{\alpha\beta} - \mu) c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\beta} \\
& + \sum_{\mathbf{k}} (\epsilon_f(\mathbf{k}) b_s^2 + \lambda) f_{\mathbf{k}\alpha}^\dagger f_{\mathbf{k}\alpha} \\
& + \sum_{\mathbf{k}} (V_z \sigma_{\alpha\beta}^z + V_\perp \mathbf{k} \cdot \boldsymbol{\sigma}_{\alpha\beta}) b_s f_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\beta} \\
& + \lambda \sum_i (1 + b_s^2 - n_f)
\end{aligned} \tag{3}$$

where c and f are fermionic operators for the topological surface states and f-electrons. The momentum, \mathbf{k} is defined in the two dimensional surface Brillouin zone, here it is in xy plane. v_F and b_s are the Fermi velocity of the conduction electrons and the slave-boson surface amplitude. $\epsilon_f(\mathbf{k})$ and λ are the dispersion and the effective chemical potential of the f band. The explicit form of $\epsilon_f(\mathbf{k})$ is not important yet nearest neighbor hopping gives $\epsilon_f(\mathbf{k}) = 2t_f(\cos k_x + \cos k_y)$ where t_f is the bare f hopping amplitude. $\epsilon_f(\mathbf{k})$, which is usually ignored in simple Kondo models is crucial in this case to open up an indirect gap. Since the inversion symmetry is broken along z direction, previously forbidden on-site hybridization is now allowed. This model provides a minimal description of the surface Kondo effect between the spin-orbital polarized surface states and doubly degenerate surface f-states. In its limiting forms, the ground-state of the chiral Anderson model will be either magnetically ordered state or a heavy fermion liquid, but intermediate states involving quantum criticality, fractalized spin-liquids[33] and superconductivity might form. However, at this stage our simple mean-field theory merely predicts a reduced surface Kondo temperature.

Indications of a revival of surface Kondo effect at low temperatures have been observed around few Kelvin in

magnetothermoelectric transport experiments[20] where the surface states become much heavier. As shown in Fig. 2 (a-d), theory predicts that as the Kondo effect develops at the surface, the doubly degenerate f -band hybridizes with the light, spin-orbital polarized surface states. As a result, only one component of the f -band can hybridize and the other, unhybridized band cuts remains gapless, forming a new Dirac point at the high symmetry point. During this process part of the Fermi surface turns hole-like from electron-like (Fig. 2 (a-d) insets), to account for the change of the total carrier density. Nevertheless, the large Fermi surface orbit is preserved up to large values of b_s^2 . The moment Kondo effect turns on $b_s \rightarrow 0_+$, the effective mass diverges and becomes negative for the large Fermi surface for $b_s^2 \neq 0$. The observation of these new multiple Fermi surface orbits at intermediate temperatures is an important test of the theory.

Discussion: One likely explanation for the upward deviation in the temperature dependence of the quantum oscillations from the Lifshitz-Kosevich formula is the development of *surface* quantum criticality. On both experimental[34, 35] and theoretical grounds[36], the suppression of the Kondo effect by magnetism is known to dramatically enhance quasiparticle masses. Moreover [17] reports that the oscillation amplitudes fits well with theories of quantum critical metals. Another possibility for the deviation from the Lifshitz-Kosevich formula might be surface magnetic break-down. The hybridization gap at the surface is significantly smaller than the bulk gap $V_s \sim 0.1 - 1$ meV. In this situation, the Knolle-Cooper[18] magnetic break-down mechanism is expected to become active, since $\hbar\omega_c > V_s$. In this situation, the Landau quantized orbits are not affected by the small gap and are expected to give rise to quantum oscillations with a deviation from the Lifshitz-Kosevich formula[18].

One of the issues that our discussion is unable to address, is the long-standing issue of a linear temperature dependence in the specific heat, where a conservative estimate of the linear specific heat $C_V/T = \gamma = 2\text{mJ/mol/K}^2$ is at least twice that of bulk metallic LaB_6 . One interpretation of this specific heat might ascribe it to a neutral Fermi surface, even though as we have discussed, such quasiparticles can not exhibit Landau quantization. Although past thermal transport experiments[37] reported a T^3 rather than a T -linear thermal conductivity, the recent developments surely warrant repeating these measurements on higher quality samples. Another possibility for the linear specific heat is inhomogenous metallic bubbles which could be probed by neutrons and muon-spin resonance experiments.

Conclusion: We have contrasted the SmB_6 quantum oscillation data that has inspired different interpretations. After discussing the proposed three-dimensional, bulk interpretations of the oscillations, we have been led to propose an alternative topological surface interpretation, modified by the effects of Kondo breakdown. In this pic-

ture the deviation from Lifshitz-Kosevich formula at low temperatures may either be a result of surface quantum criticality, or the suppressed low-temperature onset of the surface Kondo effect. Since the temperature dependence of the high frequency data is qualitatively the same as the low frequency[38], it is tempting to also ascribe the high frequency oscillations to topological surface states, most likely the 2D Fermi surfaces located around the X point. A more careful angle dependence of the oscillation amplitude is required to test this hypothesis. Lastly, we note that if the surface Kondo effect does indeed set in at low temperatures, a set of new, high mass frequencies should develop at low fields and low temperatures.

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Note added: We have recently became aware of another calculation[40] that uses magnetic breakdown mechanism similar to Knolle and Cooper[18].

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 - [41] $\hbar\omega_c(B = 10T) \simeq 1 - 2$ meV is estimated from fitting the tight binding model to a parabolic band. We have taken the band width of the tight binding model to be 4 eV in accordance with electronic structure calculations[7]. Moreover for a LaB₆[39], which has a similar conduction band without the local moments, the effective smallest effective mass $m^* = 0.2m_0$ which gives $\hbar\omega_c(B = 10T) \simeq 0.5$ meV.