The Mystery of SmB₆ : Topological or Strange Insulator?

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II. Low-temperature conducting state in two candidate topological Kondo insulators: SmB₆ and Ce₃Bi₄Pt₃, N. Wakeham, P. FS. Rosa, Y. Q. Wang, M. Kang, Z. Fisk. F. Ronning and J. D. Thompson. Phys. Rev. B 94, 0351275 (2016).

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Recommended with a commentary by Piers Coleman, Rutgers, USA

Recent experimental developments in the study of the narrow-gap insulator SmB_6 have raised the paradoxical possibility that this candidate topological insulator hides a Fermi surface of neutral quasiparticles within its bulk. In this article I discuss the experimental case for and against this interpretation and the intriguing challenge it may give rise to.

Samarium Hexaboride SmB_6 was discovered more than 50 years ago. Whereas Lanthanum Hexaboride LaB_6 is a traditional d-band metal, SmB_6 contains additional f bands which hybridize with the d-electrons to produce a narrow-gap insulator, often called a "Kondo insulator". The conventional wisdom is that $\text{Sm}B_6$ is highly renormalized bandinsulator - "renormalized silicon".

Yet SmB₆ has two unusual properties that don't fit into the simplest hybridization picture: first, the exponential rise in resistivity at low temperatures behavior inevitably levels out into a low temperature resistivity plateau; second, it develops a linear specific heat $C_V = \gamma T$ at low temperatures, a feature normally associated with a gapless, metallic Fermi surface; remarkably, the specific heat coefficient of this insulator $\gamma \sim 10 \text{ mJ/mol/K}^2$ is about 10 times larger than metallic LaB₆(see Fig. 2a). In 2008, the discovery of topological insulators, led to the new proposal that SmB_6 is a highly correlated topological band insulator[1, 2]. In this picture, an odd-number of band-crossings between the f- and d- bands leads to an interacting topological insulator. Subsequent transport measurements[3–5] and angle-resolved photoemission spectroscopy(ARPES)[6–10] on SmB_6 seem to support the topological interpretation of SmB_6 , providing convincing evidence of metallic surface states with an insulating bulk. This explains the low temperature resistivity plateau, but can the topological surface states also account for the large linear specific heat?

The problem with SmB₆, is that unlike conventional topological band insualators, the narrow band nature of the excitations are practically impossible to precisely resolve using ARPES spectroscopy. This difficulty inspired two groups to attempt detection of the quantum oscillations produced by topological surface states in SmB₆ [11, 12]. Both groups succeeded in detecting dHvA oscillations in the magnetization, but their interpretations differ radically. Li et al. [11] found that the the observed dHvA frequencies could be fit to a $F \propto 1/\cos(\theta - \theta_0)$ angular dependence, naturally interpreted as the signal of two dimensional electron orbits on crystal facets angled at an angle θ_0 . However, Tan et al.[12] found that the angular dependence of the observed signals was consistent with a three dimensional Fermi surface derived from the bulk. In their experiments, they also observed a high frequency quantum oscillation resembling that produced by large d-Fermi surfaces seen in metallic LaB₆. Tan et al. interpreted their results in terms of a Fermi surface of neutral excitations within the bulk insulator, formed they argued, because interactions had driven the topological insulator into a new quantum state.

The four papers I recommend, shed contrasting light on the dichotomy between these two high-profile measurements. Whereas [I] by Denlinger et al. leads one in no doubt that the two-dimensional scenario is sound, papers [II], [III] and [IV] provide strong counter-evidence for intrinsic low energy excitations. In [I], Denlinger et al carry out a comparison between the dHvA data from SmB₆ [11, 12] and Angle-Resolved Photoemission Spectra (ARPES), concluding rather forcefully that the ARPES signals are consistent with two dimensional surface states (Fig. 1). Perhaps most significantly, they argue that the high frequency signal observed by Tan et al. can be understood without hypothesizing a large d-band Fermi surface, by attributing them to crystal facets in which the small angle $\theta - \theta_0$ causes a near divergence in the dHvA frequencies.



FIG. 1. A) Quantum oscillations in magnetic torque are visible against a quadratic background in SmB_6 with amplitude that is between 10-20% of the bulk torque, after [12]. ARPES measurements of cleaved SmB6(001) at T=6K after I (B) M-X-M near-EF spectrum showing in-gap states. (C) Wider spectrum showing the full bulk d-band electron pocket with comparison to LaB6 DFT band structure. (D) Comparison of angular-dependence of the dominant amplitude dHvA frequencies in the 200-1000T range from two separate studies [11, 12] after I, with fits to 2D and 3D models. Dashed lines are a fit to $\langle 110 \rangle$ facet 2D cylindrical orbits [11] while solid lines correspond to the anisotropic $\langle 110 \rangle$ -oriented 3D ellipsoid fit [12] to the diagonal plane data highlighting regions where a significant discrepency with the 3D model is observed.

At first sight, the paper by Denlinger significantly strengthens the direct topological scenario, avoiding the need to address the paradox of Landau quantization in an insulator. Yet even here, there are manifest difficulties with the interpretation. First, it is difficult to understand how the surface scenario can account for the magnitudes of the observed dHvA oscillations. The largest magnitude dHvA oscillations can be resolved with the naked eye in the torque measurements, at something like 5-20% of the background bulk torque (Fig. 1A), a huge effect if the signal derives just from surface states. Moreover, as Tan et observe, the masses of the excitations seen in the dHvA are far too small to account for the observed linear specific heat, unless the oscillations derive from a bulk Fermi surface.

I now to turn to three recent papers that support the presence of intrinsic bulk Fermi surface excitations in SmB_6 . Paper [II] by Wakeham et al, is an intriguingly simple experiment designed to check whether the linear specific heat is a bulk or a surface effect. In this experiment, the authors measure the specific heat of a crystal of SmB_6 . They then

grind the crystal into a dust of micron-size particles, and remeasure it. Intriguingly, the linear specific heat is unaltered, despite a ten fold increase in surface area (Fig. 2). This experiment definitively establishes the bulk origin of the linear specific heat. One might be tempted to associate the linear specific heat with impurity states, or perhaps two-level tunneling excitations, yet the magnitude of $\gamma \sim 10 \text{mJ}/mol/K^2$ is one to three orders of magnitude larger than that seen in semiconductor impurity bands or amorphous glasses. It is difficult to escape the conclusion that the linear specific heat is intrinsic to SmB₆.



FIG. 2. (a) Specific heat capacity of LaB_6 and SmB_6 after [13]. In this measurement, the low temperature linear specific heat of insulating SmB_6 is more than 10 times larger than the d-band metal LaB_6 . (b) Linear specific heat of SmB_6 for single crystals and finely ground powder after [II]. The specific heat capacity is unchanged, despite the tenfold increase in surface to volume ratio, demonstrating that the linear specific heat in SmB_6 is a bulk effect.

Paper [III] by Laurita et al, uses Terahertz radiation to probe the optical conductivity of SmB_6 , measuring the optical conductivity from time-domain transmission experiments. These are the first optical absorption measurements on SmB_6 that directly measure the full complex conductivity at energies below the hybridization gap. The authors find that in a wide variety of crystals, prepared by both Aluminium flux growth and by floating zone methods, there is a consistent bulk optical ac conductivity below the (direct) hybridization gap(Fig. 3), with a conductivity that is approximately linearly dependent on frequency and much higher than the DC bulk insulating behavior.



FIG. 3. Real part of the optical conductivity $\sigma_1(\omega, T)$ obtained from transmission measurements through a floating zone and Al-flux grown samples of SmB₆ after III.

Paper [IV] by Biswas et al reports the presence of slow fluctuating magnetic fields of about 1.8mT fluctuating on a slow time-scale of about 60ns. These fluctuations are seen to *decrease* within 50nm of the surface. The authors suggest that these fluctuations might be associated with some kind of "excitonic" state.

These persuasive experiments bring us back to the radical conclusion proposed by Tan et al, that SmB_6 contains a neutral Fermi surface in the bulk which is diamagnetic, yet insulating. If we take this idea seriously, what are the implications for theory?

Tan et al report a conventional Lifschitz Kosevitch temperature dependence of their quantum oscillations from about 15K to about 0.5K. We know that dHvA oscillations result from a discretization of a quasiparticle density of state into discrete Landau levels,

$$N(\epsilon) \to N(\epsilon_F) \sum_{n} \delta[\epsilon - (n + \frac{1}{2})\hbar\omega]$$
 (1)

The convolution of this discretized density of states with the Fermi-Dirac function is responsible for the observed Lifschitz-Kosevitch temperature dependence of the magnetization oscillations. But such energy discretization also results from the semiclassical quantization of the motion of particles under the influence of the Lorentz force. Can we imagine particles that respond exclusively to a Lorentz force, while at the same time being unresponsive to an electric field? The main difficulty is that gauge invariance requires that particles interact with the vector potential, via the minimal coupling $p \rightarrow p - eA$, and if a particle responds to a magnetic field, which is a spatial gradient $B = \nabla \times \vec{A}$ of the vector potential, then it must also respond to a time-dependence of the vector potential, or electric field $\vec{E} = -\partial \vec{A}/\partial t$. In this way, gauge invariance prevents a selective response to the Lorentz force. It might seem that we have hit a dead end, unless somehow, gauge invariance is locally broken. From this perspective, SmB₆ might be regarded as a kind of "failed superconductor", in which the break-down of phase coherence at long distances leads to a diamagnetic insulator. To read more about investigations along this line, see[14–16].

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