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Authors
Park, Wan Kyu
Sun, Lunan
Noddings, Alexander
et al.

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Topological surface states interacting with bulk excitations in the Kondo insulator SmB$_6$ revealed via planar tunneling spectroscopy

Wan Kyu Park$^a$, Lunan Sun$^a$, Alexander Noddings$^a$, Dae-Jeong Kim$^b$, Zachary Fisk$^b$, and Laura H. Greene$^{a,1}$

$^a$Department of Physics and Materials Research Laboratory, University of Illinois at Urbana–Champaign, Urbana, IL 61801; and $^b$Department of Physics and Astronomy, University of California, Irvine, CA 92697

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Topological insulators are an emerging class of quantum matter in which the nontrivial topology of the bulk band structure naturally gives rise to topologically protected, i.e., robust, surface states (1, 2). Several dozens of such materials have been discovered but most of them, including Bi$_2$Se$_3$, are weakly correlated band insulators. A recent theoretical proposal (3) that certain Kondo insulators (4), which are insulating in the bulk due to strong electron correlations, could also be topological has stimulated vigorous research in the field. In particular, samarium hexaboride (SmB$_6$) has drawn great attention owing to its telltale resistivity behavior saturating below 4 K (5). Various experiments have been implemented to investigate this possibility (6–24), establishing the robustness of the surface states and the Kondo hybridization leading to a formation of the bulk gap, but their topological origin and nature has not been unambiguously confirmed. Factors contributing to this situation include their inherently complex nature due to strong correlations, nontrivial surface chemistry, and insufficient energy resolution. A recent report of quantum oscillations in magnetic torque supports the topological origin of the surface states (22), but conflicting results have also been reported (23).

Planar tunneling spectroscopy, inherently surface sensitive with high energy resolution and momentum selectivity, is ideally suited for the study of surface states, particularly so in SmB$_6$ where the bulk hybridization gap is much smaller than the band gap in Bi$_2$Se$_3$. Lead (Pb) is chosen as the counter electrode in this study because the quality of its measured superconducting density of states (DOS) is an important junction diagnostic and, as we will show, this choice is of crucial importance in unveiling the nature of the surface states. As shown in Fig. 1A, the sharpness of Pb superconducting features in the differential conductance, $dI/dV$, confirms the high quality of the junctions. Spectroscopic properties of SmB$_6$ are revealed more clearly when the Pb is driven normal by temperature or applied magnetic field. The $dI/dV$ curves from both (001) and (011) surfaces show a peak at $\pm 21$ mV, arising from the bulk hybridization gap, in agreement with angle-resolved photoemission spectroscopy (ARPES) results (13). Note, in particular, both surfaces exhibit linear conductance at low bias with a V shape around a minimum slightly below zero bias, as expected for Dirac fermion DOS. Quite notably, the linearity ends at $\sim 4$ mV, well below the bulk gap edge. As detailed below, a careful analysis of this behavior, taken with that when the Pb is superconducting, leads to the unraveling of the intriguing topological nature of the surface states in SmB$_6$.

Bulk SmB$_6$ is insulating because the chemical potential falls within the gap arising from Kondo hybridization of the itinerant 5$d$ bands with the localized 4$f$ bands. The resulting hybridization gap is substantially reduced due to the inherent strong correlations (4). Colored-contour maps of the normalized conductance over the temperature range of 1.72–100 K (Fig. 1B and C) show that there are several distinct stages in the temperature evolution; also clearly shown in the normalized conductance curves taken at fixed bias voltages (Fig. 1D). As the temperature is lowered, the hybridization begins to appear at 70–80 K but evolves slowly due to thermal broadening and valence fluctuations (25). Below 48–53 K, signatures for gap formation appear, which have also been reported (23).

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$^a$To whom correspondence may be addressed. Email: wkpark@illinois.edu or lhgreene@magnet.fsu.edu.

$^b$Present address: National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, FL 32310.

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Significance

Topological insulators are an emerging class of quantum matter in which the nontrivial bulk band structure gives rise to topologically protected surface states. Most are weakly correlated band insulators such as Bi$_2$Se$_3$. Despite numerous investigations on the strongly correlated bulk Kondo insulator samarium hexaboride (SmB$_6$), the topological nature of its surface states remained a mystery. Planar tunneling spectroscopy adopted in this work not only reveals spectroscopic signatures for the Dirac fermion surface states, but also reveals that their topological protection is not as robust as in weakly correlated systems due to interaction with collective bulk spin excitations. This finding suggests important implications on generic topological materials whose ground states are governed by strong correlations.

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including a distinct peak at $-21$ mV and a rapid suppression around zero bias. Theoretically, topological surface states should exist concomitantly with the bulk gap opening. But here, no clear evidence of the surface states is detected down to 25–30 K. Below this, the conductance taken at $+4$ mV decreases more slowly due to some contribution from the surface states and below 15–20 K.

**Fig. 1.** Planar tunneling spectroscopy of SmB$_6$. (A) Typical g(V) curves for the (001) and (011) surfaces taken at 1.72 K when the Pb is in the superconducting ($H = 0.0$ T) and normal states ($H = 0.1$ and 9.0 T). Although high-bias features such as a peak at $-21$ mV overlap, large deviations are seen in the low-bias region due to the superconducting gap opening in Pb. The overall conductance shape when the Pb is in the normal state, particularly the linearity at low bias, is essentially invariant under magnetic field up to 9 T. (B, C) Colored-contour maps of the conductance based on 23 curves taken from 1.72 to 100 K for each junction with the Pb kept in the normal state. Each g(V,T) curve is normalized by dividing it out with the g(V,100 K) curve. The y axis is in log scale for clear view. (D) Temperature dependence of g(V) at a fixed bias of V = $-21$ mV and $+4$ mV, normalized by g($-50$ mV). The x axis is in log scale for clear view. From the inflection points in the g($-21$ mV) curves, the bulk gap is inferred to open at 48–53 K (upward arrows). The deviation of the g($+4$ mV) curves from logarithmic dependence at 25–30 K (downward arrows) signifies the contribution from the metallic surface states.
the conductance increases, indicative of a stronger surface state contribution. Note this behavior corresponds with the resistivity data, which shows a hump in the logarithmic plots and subsequent decrease of the slope (SI Appendix, section 2). Furthermore, below 5–6 K, the conductance at fixed bias exhibits an abrupt increase followed by saturation in both orientations, although weaker on the (011) surface. This is in accord with the resistivity saturating below 4 K due to the dominance of the surface states. Being sensitive to surface DOS, tunneling spectroscopy offers more detailed information on their temperature evolution.

The V-shaped DOS expected for surface Dirac fermions is manifested as linear conductance at low bias (Fig. 2A). A noticeable difference between the two surfaces is that the (001) surface exhibits two distinct slopes and only one is seen in the (011) surface. We point out that if the origin of the surface states in SmB$_6$ were trivial (16), e.g., arising from impurities (26), the tunneling conductance would show a peak at the corresponding impurity band energy, but no such features are seen in our data. The DOS of Dirac fermions is inversely proportional to the Fermi velocity squared (SI Appendix, section 8). Considering the discrepancy in the Fermi velocities reported from different measurements (10, 13, 14, 22), it would be valuable to extract Fermi velocities from tunneling data, e.g., conductance oscillations due to Landau level quantization under magnetic field. But, as seen in Fig. 1A, such oscillations are not observed up to 9 T. And, because the tunneling matrix element that appears in the coefficient of the conductance formula is not known, it is not possible to extract an absolute value of the Fermi velocity by simply taking the conductance slope. However, we can compare the slopes to obtain the ratio of the Fermi velocities for different Dirac fermions residing on a given surface (SI Appendix, section 8). Thus, we decompose the linear conductance region into contributions from one (or two) Dirac cone(s) (Fig. 2B). In turn, the two Dirac bands on the (001) surface are identified as the $\alpha$ and $\gamma$ bands by comparing the slopes of the decomposed linear conductance with the reported Fermi velocities (22). Likewise, the linear conductance on the (011) surface originates from the single ($\beta$) Dirac band. Theories (3, 27–30) predict that topological surface states exist around the projected X points in the surface Brillouin zone. They correspond to the $\Gamma$ and X points on the (001) surface and Y point on the (011) surface. Thus, as summarized in Fig. 2C, the association of the topological surface states as described above is in good agreement with theory; and also with results from quantum oscillations (22) and ARPES measurements (13, 14, 18). The two Dirac points on the (001) surface are at $-0.4$ meV ($\alpha$ band, electronlike) and $+2.3$ meV ($\gamma$ band, holelike). The Dirac point on the (011) surface is at $-0.2$ meV ($\beta$ band, electronlike). These small values indicate that the Dirac points are located close to the chemical potential, i.e., well inside the bulk gap region, in contrast with some ARPES results (14). This discrepancy may result from the chemical potential being sensitive to the surface chemistry. More specifically, while the cleaved surfaces measured by ARPES are likely to be electrically nonneutral due to dangling bonds, as shown experimentally (16, 20, 21), we argue that they are pacified in our junctions via the surface oxidation process to form a tunnel barrier (SI Appendix, section 2). That the surface states are still detected after the harsh process of polishing and oxidation attests to their robustness and thus, their topological origin. Also, that these states are moved to beneath the tunnel barrier oxide layer we form is consistent with recent ion damage experiments (9).

As noted earlier, the linearity in conductance ends at a relatively low bias, where $g(V)$ shows a kink near $+4$ mV or a broad hump around $-4$ mV. Here, we show how this behavior points to the nontrivial nature of the topological surface states. First, a detailed scrutiny of the kink–hump structure shows that the characteristic voltages are nearly temperature independent (SI Appendix, section 4). Second, the 4-mV kink appearing when the Pb is in the normal state becomes a pronounced peak as the Pb becomes superconducting and moves to a higher bias with decreasing temperature (Fig. 3A), suggesting that understanding the features in the superconducting state may hold the key. For a detailed analysis, conductance curves in the superconducting state are normalized against those obtained when the Pb is driven normal by the applied magnetic field of 0.1 T (Fig. 3B). With Pb in the superconducting state at the lowest temperature, the two DOS coherence peaks (indicated as V– and V+) are clearly visible. But, their temperature evolution is quite unusual: With increasing temperature, the conductance at the negative bias coherence peak (V–) becomes larger than the positive bias counterpart (V+). There is also an additional peak outside the gap, which appears only in the positive bias branch at $V_1(2)$ on

Fig. 2. Topological surface states in SmB$_6$. (A) $g(V)/g(\sim-50$ mV) curves are linear at low bias, as depicted by the dashed lines, reflecting the V-shaped DOS for Dirac fermions. At the end of the linear region, they show a kink ($\omega_{\parallel} \approx 4$ meV) and a broad hump (around $-4$ mV). The linear region for the (001) surface consists of two parts with different slopes, whereas the (011) surface exhibits only one slope. (B) For the (001) surface, added contributions from two Dirac cones with distinct Dirac points ($\omega_D$) can reproduce the double linear conductance. For the (011) surface, the linear conductance arises from only one Dirac cone. Analysis of the slopes enables assigning them to corresponding surface bands ($\alpha$, $\beta$, and $\gamma$) in agreement with the literature (22). (C) Illustration of the surface Brillouin zone for each crystal surface and Fermi surfaces where the topological surface states are predicted to reside, in agreement with our results and other measurements in the literature.

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Each surface. Although the $V_{1(2)}$ peak energy is close to that of the phonons in Pb ($\omega_{ph}$), its phononic origin can be ruled out for two reasons (SI Appendix, section 5). First, the Pb phonon features are seen in the tunneling conductance because they are embedded in the superconducting DOS via strong electron-phonon coupling (bulk physics) (31), and thus appear symmetrically in bias. Second, the peaky conductance shape at $V_{1(2)}$ is different from the hump–dip shape of the phonon features; The phonons only appear as peaks in second harmonic measurements (31). The asymmetric appearance of such a pronounced peak and the asymmetric temperature evolution of the coherence peaks rule out the phonons in the Pb as the origin. Inelastic tunneling processes through sources that are extrinsic to the two electrodes and exist in or near the tunnel barrier would appear as kinks (not peaks) in the conductance at symmetric bias voltages, so are also ruled out (SI Appendix, section 11). The $V_{1(2)}$ peak changes to a kink when the Pb is driven normal either by temperature ($T_c = 7.2$ K; $H = 0$ T) or by applied magnetic field ($1.72$ K; $0.1$ T), as seen in Figs. 3A and 4A, respectively. These observations indicate that the peak at $V_{1(2)}$ and the kink at $\omega_{ph}$ have the same origin. In Fig. 3C, we show the temperature evolution of the peaks at $V^+$ and $V_{1(2)}$ quantitatively. On the left, we plot the central positions of the kinks plus superconducting gap values, $(\Delta + \omega_{ph})/e$, along with the peak positions, $V_{1(2)}$. Note their temperature dependences track closely below $T_c$, indicating their connection to the superconducting DOS. On the right, we plot the relative peak heights of the negative bias coherence peak ($V^-$) and the $V_{1(2)}$ peak with respect to the positive bias coherence peak ($V^+$). Both peaks' heights increase with increasing temperature quite rapidly.

To explain these exotic features, we invoke an inelastic tunneling model (SI Appendix, section 11) involving bosonic excitations of energy $\omega = \omega_{ph} (= \omega_1$ or $\omega_2$) in the SmB$_6$. Fig. 3D depicts two particular bias configurations. First, consider the left panel. When $eV = \Delta + \omega_{ph}$, the tunneling probability is enhanced due to additional channels opened via emission of such bosons. This inelastic tunneling through emission of bosons requires the electrons tunneling from the Pb to have a minimum excess energy ($\epsilon$). The absorption process contributes most greatly at $V = -\Delta/e$ around which the empty DOS in Pb shows a peak.
energy of \( \omega_0 \) when arriving at the SmB\(_6\), which is dissipated in the emission process. Its contribution shows up as a pronounced peak at \( V_{1(2)} \) where the tunneling electrons originate from the peaky DOS of Pb (i.e., the coherence peak at \( -\Delta \)). This also naturally explains why the \( V_{1(2)} \) peak position follows \( (\Delta + \omega_{0(2)})/e \) with temperature and then changes to a kink at \( \omega_{0(2)}/e \) when the Pb is driven normal (flat DOS and \( \Delta = 0 \)). Furthermore, this is consistent with the relative height of the \( V_{1(2)} \) peak growing with temperature. With increasing temperature, the Pb superconducting gap closes and thermal population effects broaden the coherence peaks. Such broadening effects are less severe in the inelastic tunneling at \( V_{1(2)} \) because the associated energy has a constant value \( (\omega_{0(2)} \sim 4\) meV\) that is much larger than the energy corresponding to the \( V^+ \) peak, namely, \( \Delta(T) \), which has a maximum value of 1.4 meV and decreases with increasing temperature. Now, consider Fig. 3D, Right. When the SmB\(_6\) is biased negatively, inelastic tunneling involves only absorption of bosons. Surface state electrons at deep energy levels can pop up into the chemical potential by absorbing bosons and thus can participate in the tunneling. Unlike in the emission process, the conductance contribution from this absorption process depends on the population of bosons \( (n_{\omega}) \) in the SmB\(_6\), and that follows the Bose–Einstein distribution, \( \omega_{0} = 1/\exp(\omega_{0}/k_{\text{B}}T) - 1 \). This contribution is maximized when \( \omega_{0} = \Delta \) because of the large and peaked empty DOS of the superconducting Pb into which the electrons from the SmB\(_6\) tunnel at this bias. As the bias is moved away from this coherence peak, the inelastic tunneling is concomitantly suppressed, so its contribution is not as pronounced as at \( \omega_{0} = \Delta \). This explains why it is noticeable only at \( V^- \) in the conductance data. The inelastic contribution at this bias follows from the Bose–Einstein statistics. Because there is an exponential increase in \( n_{\omega} \) with increasing temperature, the relative height of the \( V^- \) peak must increase rapidly with increasing temperature, as seen in Fig. 3C. As described above, because the inelastic processes in the SmB\(_6\) occur asymmetrically with respect to the bias voltage, the asymmetric features observed in the tunneling conductance are consistently explained. The same processes but involving bosonic excitations (phonons) in the Pb instead of the SmB\(_6\) should occur at reversed biases and they cannot explain the experimental features (SI Appendix, section 11).

We have shown how inelastic tunneling via emission and absorption of bosonic excitations in SmB\(_6\) can explain all of the features observed when the counter electrode is in the superconducting or normal state. Low-energy phonon modes in SmB\(_6\) are detected at 2.6 and 11.6 meV (32), well separated from the \( \omega_{0(2)} \) (4–meV) value detected in our tunneling spectroscopy, so they can be ruled out as the responsible excitations. Recent inelastic neutron scattering measurements (24) reported a strong resonance mode at 14 meV identified as spin excitation excitations in the bulk, implying that SmB\(_6\) is not too far from an antiferromagnetic quantum critical point. Building on this finding, a recent theory (33) proposed that the topological protection of the surface states in SmB\(_6\) is incomplete due to their strong interaction with the bulk spin excitations. The features due to such interaction are then detected in usual elastic tunneling because they are embedded in the spectral density of the surface states via self-energy corrections due to emission and absorption of virtual spin excitations, similarly to the case of Pb phonon features observed in the tunneling conductance when Pb is superconducting. In our tunneling conductance spectra, they show up as a kink and a hump at \( \pm\omega_{0(2)} \), respectively, when the Pb is driven normal. The asymmetric appearance and evolution of the \( V_{1(2)} \) and \( V^- \) peaks are due to additional tunneling channels opened up via inelastic processes and their contributions are more pronounced when the Pb is superconducting due to the sharpened DOS.

Our tunneling model involving the spin excitons in SmB\(_6\) can explain the features in both normal and superconducting states. Based on this result, we argue that the hump slightly below the chemical potential observed in an ARPES study (13) has the same origin as that in our tunneling conductance, that is, absorption of virtual spin excitons by the surface states (SI Appendix, section 10). The spin exciton energy \( (\omega_{0(2)}) \) detected in our measurements is much smaller than the bulk value observed in inelastic neutron scattering measurements (24) because the antiferromagnetic coupling at the surface \( (J) \) is reduced substantially, as is the spin exciton energy (33). The incomplete protection of the surface states in SmB\(_6\) is in strong contrast to the case of weakly correlated topological insulators such as Bi\(_2\)Se\(_3\), in which the surface states span the entire region within the bulk gap. It is noteworthy that the decisive influence of spin excitons on the topological surface states in SmB\(_6\) is rooted on the bulk physics involving strong correlations because they are collective excitations in the bulk, suggesting that similar possibilities should be taken into account in the study of other strongly correlated topological insulators. Processes involving spin excitons interacting with the surface states diminish the protection provided by their topological nature. This, in turn, affects the temperature evolution of the surface states, explaining why the decrease in conductance at 4 mV starts to slow down only below 25–30 K (Fig. 1D) instead of the higher bulk gap opening temperature. The rapid conductance jump below 5–6 K and subsequent saturation indicate that protected (or coherent) low-energy surface states may exist only in this low temperature region as the interaction with spin excitons becomes negligible. Similar abrupt changes in several other experiments (34, 35) could also be understood by following this reasoning. A more in-depth understanding of the tunneling process, particularly regarding the relevant length scales (33, 36) and their temperature evolution (SI Appendix, section 12), is expected to facilitate progress toward a more comprehensive picture of the topological states arising in strongly correlated electron systems.

**Materials and Methods**

High-quality SmB\(_6\) single crystals are grown by a flux method. For tunnel junction fabrication, crystals with well-defined facets are embedded in epoxy molds and polished down to subnanometer roughness. The tunnel barrier is formed by plasma oxidation of the crystal surface in a high vacuum chamber and the counter electrode is thermally evaporated through a shadow mask. Differential conductance is measured using standard four-probe lock-in technique in a Quantum Design PPMS Dynacool system. For further details, see SI Appendix, section 1.

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