Imaging emergent heavy Dirac fermions of a topological Kondo insulator

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The interplay between strong electron interactions and band topology is a new frontier in the search for exotic quantum phases. The Kondo insulator SmB$_6$ has emerged as a promising platform because its correlation-driven bulk gap is predicted to host topological surface modes entangled with $f$ electrons, spawning heavy Dirac fermions. Unlike the conventional surface states of non-interacting topological insulators, heavy Dirac fermions are expected to harbour spontaneously generated quantum anomalous Hall states. Dirac fermions are expected to harbour spontaneously generated quantum anomalous Hall states. Nevertheless, the 3D Kondo lattice is unique in that its correlation-driven bulk gap is predicted to host topological surface modes entangled with $f$ electrons, spawning heavy Dirac fermions. Unlike the conventional surface states of non-interacting topological insulators, heavy Dirac fermions are expected to harbour spontaneously generated quantum anomalous Hall states. Dirac fermions are expected to harbour spontaneously generated quantum anomalous Hall states. Nevertheless, the experimental observation of heavy Dirac fermions in SmB$_6$ presents a new opportunity to study the interplay between strong electron interactions and band topology.
different (polar) surface terminations with relative intensity and chemical potential shifts in their surface states, rendering interpretations difficult\textsuperscript{2,21}. Collectively, these suggestive but controversial experiments have renewed the urgency of discovering topological states arising from strong electronic interactions. Ultimately, observation of strongly correlated topological states in SmB\textsubscript{6} requires measurements on a uniform and ordered surface termination, access to filled and empty states at low temperatures, and meV energy resolution in momentum space to disentangle the shallow dispersions of a bulk KI band structure (Fig. 1b) and surface heavy Dirac fermions (Fig. 1d).

Here we use spectroscopic scanning tunnelling microscopy (STM) to directly map the structure and formation of heavy Dirac states on the (001) surface of SmB\textsubscript{6} in two complementary measurements. First, we resolve the energy (\(E\)) and momentum-space (k) structure of two inequivalent Dirac cones from quasiparticle interference (QPI) patterns around atomic defects by measuring spatially resolved differential conductance, \(g(\mathbf{r}, E) \equiv dI/dV(\mathbf{r}, E = eV)\), where \(I\) is the STM tunneling current, \(V\) is the applied bias, \(\mathbf{r}\) is the tip position and \(e\) is the electron charge. Second, we track the formation of heavy Dirac states from their additional contributions to the low-temperature tunnelling spectroscopy by measuring \(g(E, T)\). We find that their onset is far more abrupt than expected from thermal broadening; instead, it is correlated with the development of the bulk KI. Our measurements corroborate one another by each detecting a consistent Dirac-point energy of \(E_D \approx -5\) meV.

We studied nominally pure, 0.1\% Gd-doped and 0.5\% Fe-doped SmB\textsubscript{6} by cleaving single crystals in a cryogenic ultrahigh vacuum and directly inserting into the STM at 4K (see Methods and Supplementary Section I). We found that adding a small amount of Gd or Fe dopants enhanced quasiparticle scattering, but our observed QPI dispersions were consistent across all samples. We focused on regions where exactly half of the atoms remain on the cleaved surface, resulting in an ordered (2\times2) reconstruction (Fig. 2a\textsuperscript{2,22,23}). We identify this surface as a half-Sm termination because intentional Fe dopants, which substitute for Sm, appeared at the lattice sites. A half-Sm termination is beneficial because it is non-polar, eliminating the possibility of polarity-driven surface states\textsuperscript{24}. Furthermore, the (2\times2) reconstruction increases our sensitivity to one of the X-point Dirac cones by folding it to the \(\Gamma\) point (Fig. 2b), where it has a longer vacuum decay length due to its lower in-plane momentum\textsuperscript{25}.

We detected clear interference patterns in raw \(g(\mathbf{r}, E)\) around defects, caused by the elastic scattering of quasiparticles, as shown in Fig. 2c,d. The energy-dependent wavevector, \(\mathbf{k}(E) = k_x(E) = k(E)\), encodes the momentum transfer between initial (\(\mathbf{k}_i\)) and final (\(\mathbf{k}_f\)) states and tracks the underlying electronic structure\textsuperscript{26,27}. In SmB\textsubscript{6}, QPI patterns are typically short-ranged around defects, as in Fig. 2d, reflecting contributions from localized electrons. Correspondingly, they manifest as fairly broad peaks in the magnitude of the Fourier-transformed differential conductance, \(|\tilde{g}(\mathbf{q}, E)|\), with the highest signal to noise ratio along the \(q_x\) direction (Fig. 2e), primarily due to the anisotropy of the scattering form factor (see Supplementary Section V). We quantified their wavevector by fitting angle-averaged linecuts of \(|\tilde{g}(\mathbf{q}, E)|\) along \(q_x\) with a set of Gaussians (Fig. 2f, details in Supplementary Section IV). The QPI wavevector changes rapidly with energy, as shown in Fig. 3, but can be broadly divided into two energy ranges. For energies within the KI gap \(\Delta\), there are two sets of roughly linear dispersions: one very shallow (green guides in Fig. 3), and one steep (blue guides). For energies outside this range, the set of dispersions can be mapped to the known low-energy KI states of SmB\textsubscript{6} (details in Supplementary Section VIII). None of these dispersions were noticeably affected by magnetic fields up to 9T (Fig. 3a,b), consistent with previous STM spectra\textsuperscript{21} (see Supplementary Section VI). All dispersions were reproducible in six different raw datasets on three distinct samples from two different growers, with distinct STM acquisition parameters, three of which are shown in Fig. 3.
between our measured velocities and Dirac points, and those of ARPES, can be explained by the fact that we access a single, non-polar surface, whereas ARPES experiments typically average over a mixture of terminations.

Intracone backscattering, illustrated in Fig. 2b, is the simplest identifiable process responsible for the observed Dirac-state QPI. In this scenario, the QPI scattering vector is given by 2k(E), and the experimentally derived k is in good agreement with the size of surface state Fermi pockets in electronic structure calculations (see Supplementary Section II). Yet, the observation of backscattering is unusual, because in the simplest model for topological surface states, whereby Dirac cones have an in-plane helical spin structure, neither magnetic nor non-magnetic backscattering leads to a peak in the QPI spectrum. On the other hand, introducing even weak out-of-plane ferromagnetic correlations immediately restores the backscattering peak for magnetic defects, while preserving the Dirac cone structure (see Supplementary Section III). Such ferromagnetic canting can occur due to the Dzyaloshinskii–Moriya interaction, the local spin polarization induced by magnetic defects, or in topological insulators with strong interactions, such as TKIs, where it was shown theoretically that surface states possess an out-of-plane spin polarization. As it turns out, hysteresis associated with surface ferromagnetism was recently observed in SmB6 at low temperature. In addition, we found that a small inclusion of nominally non-magnetic Sm vacancies led to an enhanced magnetic susceptibility at low temperatures, akin to the addition of Kondo holes (see also Supplementary Section III). In fact, the combination of magnetic defects and local ferromagnetic correlations was also proposed as the origin of the backscattering QPI signal recently measured in magnetically doped topological insulators.

To associate the Dirac states detected from QPI with a TKI phase, we also tracked their temperature dependence in tunneling spectra, g(E, T). Unlike trivial surface states, the formation of heavy Dirac fermions at the surface of a TKI is predicated on the coherence of the correlation-driven KI gap. With increasing temperature, incoherent Kondo lattice states spread into this gap as the
hybridization between \( f \) and \( d \) electrons unwinds. Eventually, this process is expected to drive a topological phase transition as band-parity inversion is lost, eliminating the non-trivial surface states. However, theory has not yet succeeded in describing coherent Kondo lattice evolution, much less the concomitant formation of heavy Dirac fermions. Here, we experimentally extract this complex connection by tracking the simultaneous temperature evolution of the KI gap and Dirac surface state contributions to \( g(E) \). In general, \( g(E) \) cannot be directly interpreted as the density of states in multi-orbital Kondo lattice systems due to the quantum interference between electrons co-tunnelling into \( f \) and \( d \) states\(^{2,3}\). We account for this effect by modelling the differential conductance spectrum as

\[
g(r_0, E) \propto \left| t^\dagger \text{Im} G(r - r_0 = 0, E) t \right|, \quad t^\dagger = [t_d \ t_f \ t_{f^*}],
\]

where \( t \) is a vector of the tunnelling probability for each orbital and \( G(r, E) \) is the Fourier transform of \( G(k, E) \), the renormalized KI Green's function describing a tight-binding Hamiltonian that qualitatively reproduces known bulk bands\(^{1} \) (see also Supplementary Section IX). Equation (1) includes contributions only from the underlying KI, but not from emergent topological surface states. Even so, it accurately captures all features in \( g(E) \) at 15 K (Fig. 4a), implying that surface states are negligible at this temperature. Fits to equation (1) can be further decomposed into interference terms and the bulk density of states, \( D(E) \), weighted by the relative tunnelling probabilities (Fig. 4a inset). As temperature is lowered, \( D(E, T) \) exhibits a narrow energy window of diminished spectral weight that onsets below \( \Delta_T \approx 35 \) K and expands to \( \Delta \approx 14 \) meV at 2 K. The deviations of \( g(E) \) from the co-tunnelling model intensify with lowering temperature. They are characteristic of a linear band dispersion with a nodal energy of \( E_D = -5 \) meV, and match our independent raw QPI measurements of Dirac surface states (see Fig. 3). The heavy Dirac surface states in SmB\(_6\) emerge only at low temperatures as the KI gap becomes coherent. They are visible in our measurements of \( g(E) \) at 2 K as an additional contribution within the KI gap that is not captured by equation (1) (see arrow in Fig. 4a). The rapid onset of the Dirac surface states, captured from integrating the fit residuals in c \( (w_{ss}, \text{blue dots}) \), cannot be explained by thermal broadening (thick blue line, see Supplementary Section X). Instead, it is correlated with the development of the bulk KI gap, calculated by integrating \( D(E) \) for energies within \( \Delta \) to find the in-gap spectral weight \( w_{ss} \), demonstrating the direct relationship between the evolving host insulator and its topologically emergent states (see inset).
heavy Dirac surface states (Fig. 3). Similar temperature-dependent features in \( g(E) \) spectra have also been observed on the (1 1 x) boron termination\(^1\). We quantified the emergence of the surface states by integrating \( g_{\text{surf}}(E) \) at each temperature (Fig. 4d). We found that the surface states diminish rapidly with increasing temperature, faster than can be accounted for by thermal broadening alone (blue line in Fig. 4d), and indeed faster even than the filling of the insulating gap at around 35 K where the topology of the bands is inverted (see also Supplementary Section X). One possible explanation for this fast decay is that the surface states are reliant on bulk coherence. Certainly, the evolution of their spectral weight is correlated with the weight of residual states in the KI gap, calculated by integrating \( D(E) \) for energies within \( \Delta \) (Fig. 4e). Alternatively, the unusually fast decay of the surface states may reflect their interactions with magnetic correlations generated by Kondo lattice defects\(^1, 14\).

Our simultaneous imaging of Kondo insulator formation and slow in-gap surface modes is consistent with SmB\(_6\), hosting a correlation-driven topological surface state that harbors the heaviest known Dirac fermions. The optimal positioning of the \( f \)-character surface states at the chemical potential, enforced by Kondo lattice interactions, increases prospects for interface engineering to discover novel forms of topological superconductivity and construct transformative quantum devices. SmB\(_6\) and prospective TKIs may become leading testbeds for fractional and non-Abelian statistics, both of which are essential elements of prospective universal topological quantum computation.

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Methods
STM experiments were carried out on single crystals of pure, 0.1% Gd-doped and 0.5% Fe-doped SmB$_6$ grown using the Al-flux method$^{41}$. Crystals were cleaved in a cryogenic ultrahigh vacuum at ~30 K and immediately inserted into our home-built STM. STM tips were cut from PtIr wire and cleaned by in situ field emission on Au foil. The cryogenic ultrahigh vacuum environment allowed the cleaved surface to stay clean for several months. Data were collected on three different samples and multiple fields of view.

Magnetic susceptibility measurements were performed on single-crystalline samples of SmB$_6$ and Sm$_{0.95}$B$_6$, grown by the Al-flux technique with starting composition Sm:B:Al = 1 - $x$:6:700 ($x$ = 0.0 and 0.05, respectively). The mixture of samarium pieces, boron powder (99.99%) and aluminium shots (99.99%) was placed in an alumina crucible and loaded in a vertical tube furnace with ultrahigh-purity Ar flow. The furnace was heated to 1,723 K for 12 h followed by slow cooling to 1,323 K at 2°C h$^{-1}$. At 1,323 K the furnace was shut down, and the flux was removed at room temperature by etching with a NaOH solution. The atomic structure of the resulting single crystals was verified by X-ray diffraction at room temperature in a Bruker D8 Venture diffractometer using a Mo K$_\alpha$ X-ray source. A Quantum Design superconducting quantum interference device was used to measure the magnetic response of the crystals to a magnetic field of 1 kOe. The magnetic susceptibility curves were normalized to their values at 350 K because of the uncertainty in the determination of the actual number of Sm vacancies.

Data availability
The data that support the findings of this study are available from the corresponding author on reasonable request.

Code availability
The code that supports the findings of this study is available from the corresponding author on reasonable request.

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Author contributions
H.P., Y.L., A.S., P.C., Y.H. and M.M.Y. performed the STM experiments. X.W., J.P., P.F.S.R., D.J.-K. and Z.F. synthesized and characterized the samples. P.F.S.R. performed X-ray measurements. J.D.T. performed magnetic susceptibility measurements. H.P., A.S., Y.H., M.M.Y., M.H.H. and J.E.H. developed and carried out analyses. D.K.M. provided theoretical guidance. M.H.H. and J.E.H. supervised the project. H.P. and M.H.H. wrote the paper with key contributions from D.K.M. and J.E.H. The manuscript reflects the contributions and ideas of all authors.

Competing interests
The authors declare no competing interests.

Additional information
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