Imaging the Nanoscale Band Structure of Topological Sb

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Many promising building blocks of future electronic technology – including non-stoichiometric compounds, strongly correlated oxides, and strained or patterned films – are inhomogeneous on the nanometer length scale. Exploiting the inhomogeneity of such materials to design next-generation nanodevices requires a band structure probe with nanoscale spatial resolution. To address this demand, we report the first simultaneous observation and quantitative reconciliation of two candidate probes – Landau level spectroscopy and quasiparticle interference imaging – which we employ here to reconstruct the multi-component surface state band structure of the topological semimetal antimony (Sb). We thus establish the technique of band structure tunneling microscopy (BSTM), whose unique advantages include nanoscale access to non-rigid band structure deformation, empty state dispersion, and magnetic field dependent states. We use BSTM to elucidate the relationship between bulk conductivity and surface state robustness in topological materials, and to quantify essential metrics for spintronics applications.

A. INTRODUCTION

Driven by novel components and fabrication techniques for modern electronic devices[1, 2], it has become imperative to develop a nanoscale understanding of the electronic band structure – the relationship between the electronic energy and momentum – within a wide variety of materials. The scanning tunneling microscope (STM), best known for its atomic resolution imaging capability, can also provide momentum-resolved (k-space) spectroscopic information through two phenomena – Landau quantization and quasiparticle interference (QPI). First, the application of a magnetic field B can quantize the electronic density of states (DOS) into Landau levels (LLs), resulting in oscillations in the STM conductance (dI/dV) spectra[3]. The LL dispersion can be mapped onto the quasiparticle band structure in the semiclassical limit[4, 5]. Increased disorder limits the formation of LLs, but enables the second technique – QPI imaging[6]. Interference between the initial and final wavevectors, k_i and k_f, of elastically scattered quasiparticles of energy ε, can produce a standing wave pattern with wavevector q = k_f - k_i in the dI/dV map at energy ε = eV, allowing the inversion of q(ε) to find k(ε).

The nanoscale spatial resolution, temperature-limited energy resolution, access to filled and empty states, and utility in magnetic field offered by STM measurements of LLs and QPI make them ideal complements to angle-resolved photoemission spectroscopy (ARPES) as band structure probes. In fact, LL spectroscopy and QPI imaging have been cornerstone techniques for over a decade, used to investigate gap symmetry in superconductors[7–9], backscattering in topological materials[10–12], pseudospin protection in graphene[13, 14] and chemical potential fluctuations in a range of materials[14–17]. Despite their tremendous promise, LLs and QPI have never been simultaneously observed – over the same spatial area and energy range – in any material; therefore the equivalence of these one- and two-particle phenomena has yet to be established. In fact, independent use of these techniques on graphene have reported a 40% discrepancy in Fermi velocity[14, 18]. Such discrepancies have been attributed to collective modes[14], variations in carrier density[19], or tip-induced electric fields[20] – but the two techniques have never been quantitatively reconciled. This problem undermines the widespread use of LL spectroscopy and QPI imaging techniques.

Elemental Sb, of current interest due to its non-trivial topology and intriguing potential for spintronic devices, provides an ideal platform to address this issue. Its negative band gap guarantees sufficient bulk carrier density to screen chemical potential fluctuations[10, 16]
and tip-induced electric fields[20], while its topological nature requires the existence of robust surface states (SSs)[21–26], where LL and QPI phenomena may be observed. The topological surface states derive from two spin-split parabolas which form inner and outer Dirac cones connecting the valence and conduction bands (Fig. 1a). The surface states can be described by a five-parameter phenomenological $k \cdot p$ Hamiltonian[27]

$$H(k) = \varepsilon_D + \frac{k^2}{2m^*} + v_0(1+\alpha k^2)(k_x\sigma_y-k_y\sigma_x)+\frac{\lambda}{2}(k_+^3+k_-^3)\sigma_z$$

(1)

where $\varepsilon_D$ is the Dirac point energy, $m^*$ is the effective mass, $\alpha$ and $\lambda$ control the shapes of the two Dirac cones, and $v_0$ is the Rashba parameter corresponding to the magnitude of spin-orbit coupling. This five-parameter dispersion can serve as a key test case for comparing the LL and QPI phenomena, while $v_0$ in particular is an essential utility metric for spintronics devices.

Here we report the simultaneous observation of LLs and QPI over a 300 meV energy range in Sb. We quantitatively reconcile these techniques and use them in concert to reconstruct the multi-component surface state band structure, thus establishing the technique of **band structure tunneling microscopy** (BSTM). We demonstrate the nanoscale spatial sensitivity of BSTM and use it to quantify several metrics of Sb relevant to spintronics applications. More generally, we clarify the relationship of topological surface states to proximate bulk bands, thereby directing the wider exploration of technologically useful topological materials.

### B. RESULTS

Topographic STM images of the cleaved (111) surface of Sb (Supp. Info. I) show large atomically flat regions (Fig. 1b), free from chemical potential fluctuations except in the immediate vicinity of sparse single atom surface defects and step edges. The $dI/dV$ spectrum (Fig. 1c), proportional to the local DOS, is dominated by cusp-like features associated with extrema ($\varepsilon_S$, $\varepsilon_T$) and a saddle point ($\varepsilon_S$) in the SS band structure (Fig. 1a). The Dirac point is not directly visible due its spectral coincidence with other SSs and bulk bands, however, the conducting bulk confers the aforementioned benefits for momentum-resolved spectroscopic studies.

In applied magnetic field $B$ above 4 T, Landau quantization causes conductance oscillations to appear in the $dI/dV$ spectrum (Fig. 2a-b). We assign empirical indices starting with $N = 1$ to all such $B$-dependent peaks (Fig. 2b, Supp. Info. II). We observe a remarkable 27 LLs – more than reported on any other topological material[5, 12, 20, 28] – despite the presence of bulk bands throughout this energy range (Fig. 1a). The LL peaks are sharpest around the Fermi energy, $\varepsilon_F$ (Fig. 2c), evincing monotonic quasiparticle lifetime broadening away from $\varepsilon_F$, in contrast to other topological materials where collective modes complicate the picture[5, 29]. The measured lifetime at $\varepsilon_F$ corresponds to a long elastic mean free path, $l_\ell \sim 65$ nm.

We use the LLs, which correspond to closed contours of constant energy (CCCs) in momentum space, to obtain part of the SS dispersion on Sb in two energy regimes. First, we note that LLs in other topological materials have been interpreted in the Dirac fermion picture[5, 12, 20, 28], with the energy of the $n^\text{th}$ LL, $\varepsilon_n$, given by

$$\varepsilon_n(B) = \varepsilon_D + v_D \sqrt{2e\hbar nB}$$

(2)

where the Fermi velocity $v_D$ is a constant over the energy range of interest. For Dirac fermions, the semiclassical Bohr-Sommerfeld quantization relation gives the momentum space radius for the $n^\text{th}$ LL orbit, $q_n = \sqrt{2(2e/\hbar)} nB$ [5]. Fig. 2b shows the LL peak energies, $\varepsilon_n$, plotted against the empirical LL momentum, $q_n = \sqrt{NB}$. For energies $\varepsilon < \varepsilon_S$, the dispersions obtained at different magnetic fields collapse on to a single curve – validating the Dirac fermion semiclassical approximation with $n = N$, and demonstrating that the Landau quantization arises from a single Dirac cone in this energy range. From Fig. 1a, we conclude that the LL wavevector $q_N$ corresponds to the radius of the inner cone, and independently gives its velocity, $v_{LL} \equiv v_D = 4.20$ eV·Å (6.34 × 10$^5$ m/s). Second, for energies $\varepsilon \leq \varepsilon_S$, the presence of two spin-split cones requires a different interpretation of the LLs based on the Rashba picture[30, 31], where $\varepsilon_n$ is given by:

$$\varepsilon_n(B) = \begin{cases} 
\varepsilon_0 + \frac{1}{2}(\hbar \omega_c + g\mu_B B), & n = 0 \\
\varepsilon_0 + \hbar \omega_c n \pm \sqrt{\delta^2/4 + (2m^* v_0^2) \cdot n}h\omega_c, & n > 0
\end{cases}$$

(3)
Here, $\varepsilon_0$ is the band offset, $\omega_c = eB/m^*$ is the cyclotron frequency, $\delta = (1 - 1/2 \alpha g^* m^*)/\omega_c$, and $g$ is the electron g-factor[30, 31]. Our measured LLs correspond to the positive sign in Eqn. 3, which derives predominantly from the inner Rashba cone, while the LLs of the outer cone, with their tighter energy spacing, are not visible due to broadening effects. Reconstructing both band structure branches in this low energy ($\varepsilon < \varepsilon_S$) regime therefore requires the combined use of the Rashba LLs and the other momentum-resolved technique – QPI.

Fig. 3 shows the simultaneous observation of QPI over a 300 meV energy range, which allows quantitative reconciliation with LL spectroscopy, and complete reconstruction of the SS band structure of Sb both above and below $\varepsilon_S$. The scattering of SS quasiparticles from single-atom impurities on Sb(111) creates interference patterns in $dI/dV(\vec{r})$ maps, exemplified in Fig. 3a-b. Fourier transformations of these patterns reveal prominent modes along the $\Gamma - M$ and $\Gamma - K$ reciprocal directions (Fig. 3c-d) that disperse roughly linearly with energy over $\sim 350$ meV from the Dirac point (Fig. 3e-f). Fig. 3f, showing the $\Gamma - K$ dispersion, extends previous reports of the $\Gamma - M$ dispersions[32–34]. The scattering of SSs from atomic step edges creates similar interference patterns (Fig. 3g, Supp. Info. IV), allowing the extraction of an additional dispersion along the $\Gamma - M$ direction (Fig. 3h)[33, 34]. In the presence of a magnetic field, no change is observed in the QPI. In particular, our measurements over the same spatial region at magnetic fields of 0 T and 9 T show no additional modes corresponding to LLs[35] or field-induced backscattering (Supp. Info. III), indicating the small magnitude of the SS g-factor.

The $k$-space origin of the QPI modes are indicated on the schematic CCEs in Fig. 4a, which display three qualitatively different shapes over the energy range of interest. Their $q(\varepsilon)$ dispersions are plotted in Fig. 4b. First, across the entire observed energy range, the dominant $\Gamma - M$ QPI mode, $\vec{q}_{\Gamma - M,1}(\varepsilon)$, corresponds to inter-band scattering between parallel spins. Meanwhile, the second $\Gamma - M$ mode, $\vec{q}_{\Gamma - M,2}(\varepsilon)$, involves intra-band scattering across the outer band, which comes into play only for $\varepsilon > \varepsilon_w$, where it is sufficiently warped[33]. Finally, the $\Gamma - K$ QPI mode $\vec{q}_{\Gamma - K}(\varepsilon)$ corresponds to inter-band scattering for $\varepsilon_B < \varepsilon < \varepsilon_S$, where both CCEs are nearly circular, and is therefore identical to $\vec{q}_{\Gamma - M,1}(\varepsilon)$ at these energies. The kink in $\vec{q}_{\Gamma - K}(\varepsilon)$ around $\varepsilon_S$ corresponds to a crossover to scattering between the ‘pocket’-like sections of the outer band for $\varepsilon > \varepsilon_S$.

Having determined the origin of all observed $q$-vectors, we use $\vec{q}_{\Gamma - K}(\varepsilon)$ and $\vec{q}_{\Gamma - M,1}(\varepsilon)$ to extract the dispersions of both cones for $\varepsilon > \varepsilon_S$ (Fig. 4c, details in Supp. Info. V), for direct comparison with the inner cone dispersion extracted from Dirac LLs over the same 200 mV energy range (Fig. 2b). The independently measured inner cone dispersions are consistent to within 3% (Fig. 5a), the sign of the deviation being in agreement with that expected from hexagonal warping effects[27]. Furthermore, both LL and QPI measurements agree with ARPES measurements of filled state dispersion to within 10%, comparable to the variation between independent ARPES measurements[32, 36]. We thus reconcile the techniques of LL spectroscopy and QPI imaging, and establish their quantitative credibility as momentum space probes.

Upon resolving this discrepancy which has limited the combined use of LL and QPI techniques, we proceed to use them in concert, exploiting their complementary sensitivity to different $k \cdot p$ parameters to determine the band structure in the Rashba ($\varepsilon < \varepsilon_S$) regime (Fig. 4c). We find that our $\varepsilon < \varepsilon_S$ data is best reproduced in the $k \cdot p$ description with: $\varepsilon_D = -210$ meV, $m^* = 0.1 m_e$, $\alpha = 110$ Å², $\lambda = 230$ eV Å³, and the crucial spin-orbit coupling, $v_0 = 0.51$ eV Å ($7.7 \times 10^4$ m/s).

We thus present a proof-of-principle demonstration establishing band structure tunneling microscopy (BSTM) – a combination of LL and QPI spectroscopy which is crucial to the nanoscale reconstruction of multi-component band structures of 2D electronic materials. In contrast to previous STM work[37], our QPI patterns extend far beyond individual scatterers (Fig. 3a-b), and are thus independent of impurity models and compatible with the Friedel approximation[38]. In contrast to ARPES, BSTM can probe empty states – without sacrificing energy resolution by populating those states thermally. Crucially, we demonstrate the nanoscale spatial sensitivity of BSTM by showing up to 5% non-rigid band structure changes between atomically flat and terraced regions separated by $\sim 200$ nm (Fig. 5b-c), after ruling out tip-induced artifacts (Supp. Info. V). The step edges must have broken bonds, which may cause charge redistribution as well as structural distortion, either of which may bear responsibility for these non-rigid spatial variations.
C. DISCUSSIONS

Our establishment of BSTM on Sb(111) sheds light on several fundamental and practical issues directing the exploration of topological materials. First, the existence of up to 27 LLs arising from a single, robust cone – despite the presence of proximate surface and bulk bands throughout the energy range – is surprising. It had been speculated that in the Bi₂X₃ class of topological materials, the onset of bulk bands induces surface-bulk scattering, limiting the observed range of LLs[5]. In contrast, our demonstration of robust Landau quantization in a semimetal suggests that even in the presence of proximate bulk bands, closed SS contours exhibit a long lifetime, suggesting that they maintain their topological protection against inelastic scattering, in addition to backscattering. Second, the use of topological materials for spintronics devices will require strong spin-momentum locking, long mean free path  ℓ, and small g-factor – parameters which can be quantified by BSTM. We note the quantitative distinction between the Rashba parameter (  0 = 0.51 eV·Å, extracted from the k · p fit) and the Dirac velocity  D = 4.2 eV·Å (Fig. 5a), and clarify that the former is the spin-momentum locking parameter relevant towards spintronics applications. Meanwhile, LL widths place a lower bound on ℓ, while the absence of field-induced backscattering QPI channels places an upper bound on g. Third, the search for better topological materials has gravitated towards insulating ternary and quaternary materials, tuned off-stoichiometry to enhance the SS contribution in transport measurements[39, 40]. However, our observations suggest that the presence of a bulk continuum suppresses chemical potential fluctuations[40], actually enhancing the mean free path rather than diminishing the lifetime of SS quasiparticles as had previously been speculated[5, 41]. We therefore suggest heterostructures, with the appropriate use of semimetals, as an alternate avenue towards better topological devices with immunity to disorder[34].

Our simultaneous spatial and spectral observation of LLs and QPI, followed by their quantitative reconciliation, establish BSTM as a reliable, self-consistent nanoscale band structure probe. Unique advantages of BSTM include nanoscale sensitivity to band structure deformations, accessibility of empty states, and utility in magnetic field. We therefore underscore the crucial role that BSTM can play in characterizing diverse electronic compounds and growth techniques, as well as developing nanoscale devices using heteroepitaxial van der Waals materials[2]. In particular, we suggest that Sb, with its particularly long-lived surface states, may be an excellent choice for investigating the spatial evolution of topological proximity effects[24, 25].

D. METHODS

Sample Growth. Single crystals of Sb were grown using the following method[42]. High-purity antimony (99.999%, supplied by Alfa Aesar®) in shot form (10.15 g, 6 mm) was sealed in an evacuated quartz tube, and heated in a box furnace to 700 °C for 24 hours. The furnace was cooled slowly (0.1 °C/min) to 500 °C, and subsequently cooled to room temperature.

STM Measurements. Our measurements were performed using a home-built STM at liquid helium temperatures. Single crystals of Sb were cleaved in-situ in cryogenic ultrahigh-vacuum to expose the (111) face, and inserted into the STM. Mechanically cut Pt-Ir tips, cleaned by field emission and characterized on gold, were used for the measurements. Spectroscopy data were acquired using a lock-in technique at 1.115 kHz, and conductance maps were obtained by recording out-of-feedback dI/dV spectra at each spatial location. Three samples were investigated in this work, and their correspondence to the data shown in the manuscript is detailed in Supp. Info. I.

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Figure 1. **STM Topography and Band Structure.** (a) Schematic band structure (from density functional theory) of the semimetal Sb(111) with topological SSs (dark grey) connecting the bulk valence and conduction bands (light grey). The spectral range of the observed LLs and QPI is indicated. (b) STM topograph of Sb(111) showing an atomically flat surface (sample bias, $V_0 = +200 \text{ mV}$; junction resistance, $R_J = 10 \text{ G}$). Inset shows the atomically resolved hexagonal lattice ($V_0 = +200 \text{ mV}$; $R_J = 125 \text{ M}$). (c) Typical $dI/dV$ spectrum on Sb(111), with kinks at $\varepsilon_B$, $\varepsilon_S$, and $\varepsilon_T$, corresponding to extremal features in the surface state band structure shown in (a) ($V_0 = +300 \text{ mV}$; $R_J = 500 \text{ M}$; $V_{\text{rms}} = 3 \text{ mV}$).

Figure 2. **Landau Quantization of Surface States.** (a) Representative $dI/dV$ spectra at several values of the magnetic field $B$, vertically offset for clarity, showing the emergence of LL oscillations. Dashed blue lines are guides to the eye following the first four LLs. Setpoint Parameters: $V_0 = +100 \text{ mV}$; $R_J = 0.1 - 0.2 \text{ G}$; $V_{\text{rms}} = 0.4 \text{ mV}$. (b) Dispersion of LL energies $\varepsilon_N$ vs. momentum $\sqrt{N B}$, based on the semiclassical approximation for Dirac fermions (Eqn. 2). Grey band shows the crossover energy below which the LLs are described by the Rashba formula (Eqn. 3, Supp Info II). Between samples, the chemical potential and dispersion vary by $\sim 15 \text{ mV}$ and $\sim 5\%$ respectively. (c) The LL inverse peak widths, measured using Lorentzian fits (Supp Info II), showing quasiparticle lifetime broadening away from $\varepsilon_F$ (data acquired at 2.2 K).
Figure 3. **Quasiparticle Interference of Surface States.** (a, b) $dI/dV(\vec{r}, V)$ maps at sample bias -80 mV (a) and +20 mV (b), exemplifying standing wave patterns generated by impurities. (c, d) Fourier Transforms (FTs) of (a) and (b), showing distinct conductance peaks along the $\Gamma - M$ and $\Gamma - K$ reciprocal directions. FTs have been six-fold symmetrized to improve signal quality (Supp Info III). (e, f) Conductance linecuts through the FTs along the $\Gamma - M$ (e) and $\Gamma - K$ (f) directions, generated from 190 nm spatial maps. The prominent dispersing modes along each direction are labeled $q_{\Gamma-M,1}$ and $q_{\Gamma-K}$. (g) Conductance linecut ($dI/dV(x, V)$) perpendicular to an atomically sharp step, showing dispersing step edge scattering (Supp Info IV). (h) FT of the conductance in (g), showing two prominent dispersing modes along the $\Gamma - M$ direction, labeled $q_{\Gamma-M,1}$ and $q_{\Gamma-M,2}$. 
Figure 4. **BSTM Band Structure.** (a) Schematic evolution of the surface state contours of constant energy (CCEs), with the in-plane spin polarization (brown), and q-space location of the dispersing modes from LL & QPI (detailed in (b)) overlaid. From the Dirac point (ε_D) up to an energy ε_S, the CCEs correspond to a Rashba-split double ‘cone’ structure. The outer ‘cone’ acquires a warped snowflake shape above an intermediate energy ε_W. Above ε_S, the CCE topology changes, and the outer SS band is no longer a closed contour. (b) A compilation of three ε(q) dispersions recorded over the same atomically flat spatial region (q_{Γ-M,2} is acquired from a nearby step edge) using Landau quantization (Fig. 2b, red) and QPI (Fig. 3e-h, blue, green and cyan). (c) The BSTM dispersion ε(k) of the SS band structure, deduced from (a) and (b). Grey lines correspond to a fit to the data using the k · p model in Eqn. 1[27].
Figure 5. **BSTM: Consistency and Spatial Resolution.** (a) The dispersion of the inner SS cone, measured using LL and QPI techniques over the same spatial region. The sign of the observed $\sim 3\%$ difference between the techniques is consistent with hexagonal warping, which results in a difference in dispersion along the $\Gamma - M$ and $\Gamma - K$ directions. The inset shows schematic SS bands in grey, with the horizontal arrows indicating the measured $k(\varepsilon)$ for each panel. (b-c) Nanoscale spatial sensitivity of BSTM demonstrated by comparing the (b) dispersion of the inner band deduced from LLs and (c) Dispersion of the outer band deduced from QPI ($q_{\Gamma - M,1}$) and LLs. Dispersions were recorded over atomically flat regions (filled points) and terraced regions (hollow points), $\sim 200$ nm away from each other. Both (b) and (c) indicate a *consistent, non-rigid difference* in the band structure between the two regions, demonstrated by the offset and slope change between the two curves.