Möbius Kondo insulators

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Heavy fermion materials have recently attracted attention for their potential to combine topological protection with strongly correlated electron physics. To date, the ideas of topological protection have been restricted to the heavy fermion or ‘Kondo’ insulators with the simplest point-group symmetries. Here we argue that the presence of nonsymmorphic crystal symmetries in many heavy fermion materials opens up a new family of topologically protected heavy electron systems. Re-examination of archival resistivity measurements in the nonsymmorphic heavy fermion insulators Ce\textsubscript{5}Bi\textsubscript{4}Pt\textsubscript{3} and CeNiSn reveals the presence of a low-temperature conductivity plateau, making them candidate members of the new class of material. We illustrate our platform to study the interplay between topological phases and insulators have recently emerged as a particularly promising candidate for a TKI, strongly suggesting that these nonsymmorphic heavy fermion insulators, on which scattering between two surface Dirac cones can open a gap without breaking time-reversal symmetry, the autonomy of these surface states is stabilized by glide reflection and time-reversal symmetry\textsuperscript{28-24}. Moreover, nonsymmorphic symmetries give rise to a momentum-dependent twist that enables the surface states to be detached from the bulk on the glide plane. Following recent studies\textsuperscript{23-27}, we refer to these states as Möbius-twisted surface states. From the bulk–boundary correspondence, we are able to define a \( Z_4 \) topological invariant, and discuss the experimental signatures of such a phase. One of the important effects that sets these topological insulators apart from their weakly interacting counterparts is the possibility of breakdown of the Kondo effect at the surface\textsuperscript{28}. We find that this breakdown has a particularly dramatic effect on the Möbius-twisted surface states, giving rise to quasi-one-dimensional Fermi surfaces.

Hamiltonian and nonsymmorphic symmetries

We begin by constructing a tight-binding Hamiltonian for CeNiSn. CeNiSn has an orthorhombic \( \epsilon \)-TiNiSi structure belonging to nonsymmorphic space group no. 62, \( Pnma \), which contains an inversion \( P \), a screw rotation \( S_j = T_{a(j),0}R_j \), and a glide reflection \( G_j = T_{a(j),b}M_j \), where \( R_j \) denotes a \( \pi \) rotation about the \( j \)-axis, \( M_j \) refers to the mirror operator in the plane perpendicular to the \( j \)-axis, and \( T_{a,b,c(j)} \) is the translation operator along \( ax + by + cz \). There are four equivalent Ce sites in the unit cell, which we label as \( \{1A, 2A, 1B, 2B\} \), as shown in Fig. 1. The Ce sites form zigzag chains in the \( ac \) plane which are stacked along the \( c \) direction. Fig. 1b shows how glide reflection connects inter-chain sites \( G_j \) : (1A, 2A, 1B, 2B) \( \rightarrow \) (2A, 1A, 2B, 1B). These layers are then arranged in an alternating fashion along the \( b \) direction; the alternating layers are related by the screw rotation \( S_j : (1A, 2A, 1B, 2B) \rightarrow (1B, 2B, 1A, 2A) \) as shown in Fig. 1c. In the following discussion, we re-scale the dimensions \( a, b \) and \( c \) of the unit cell to be unity. When applying the glide reflection and the screw rotation symmetries twice, the system is shifted by a lattice translation, but the process also involves a double reflection.
near the chemical potential derive from the Ce 4f electrons and the structure of the Ce atoms. The resulting tight-binding Hamiltonian has the Wannier states of these two sets of orbitals onto the common orbitals hybridizing with Ni 3d electrons. A key ingredient of our model is the hybridization between the f orbitals of these two sets of orbitals. Cebom a p-wave form-factor of the conduction and f-electrons, we project the Wannier states of these two sets of orbitals onto the common sites of the Ce atoms. The resulting tight-binding Hamiltonian has the structure

\[ H(k) = \begin{pmatrix} H^c(k) & V(k) \\ V(k) & H^f(k) \end{pmatrix} \]

where \( V(k) \) is the hybridization matrix, and \( H^c \) and \( H^f \) are the nearest hopping matrices for the conduction and f-electrons, respectively. The detailed structure of this Hamiltonian, which respects the full nonsymmorphic symmetries of the lattice, is provided in the Methods.

**Topological surface states with a Möbius twist**

One symmetry-preserving surface which respects to the glide reflection \( G_x \) is the (010) surface. This surface is perpendicular to the glide plane (xy plane) and is also invariant under lattice translations parallel to the surface. The surface energy dispersion as a function of \((k_x, k_y)\) is computed by diagonalizing the Hamiltonian in a (010) slab geometry. The corresponding surface Brillouin zone (BZ) is shown in Fig. 2a. The glide lines on the surface BZ are the set of glide reflection invariant momenta, which are at \( k_z = 0 \) (path XΓX) and \( k_z = \pi \) (path MZM). Along these lines, the Hamiltonian from equation (4) commutes with \( G_x \), and can be block diagonalized into two sectors with two eigenvalues for \( G_x \), \( g_x(k_z) = \pm e^{ik_z/2} \) along the glide lines.

On the glide lines along XΓX or MZM, a pair of surface Dirac cones is stabilized by the glide reflection and time-reversal symmetry. To demonstrate this state (see Fig. 2b), we focus on path XΓX. At the XG point, the glide eigenvalues are real (±1), which implies that the members of each Kramers pair derive from the same glide sector—that is, the glide eigenvalues for two Kramers pairs are \((\pm 1, \pm 1)\) and \((-1, -1)\). By contrast, at the Γ point, the glide eigenvalues are imaginary (±i), so time reversal inverts the glide eigenvalue, which indicates that the members of each Kramers pair come from opposite glide sectors—that is, the glide eigenvalues for two Kramers pairs are \((\pm 1, \mp 1)\) and \((-1, 1)\). When we connect two Kramers pairs at the Γ point to two Kramers pairs at the XG point we obtain the hourglass structure of this surface state\(^{27}\), which contains two Dirac cones at the Γ point (Fig. 2b). This surface state contains a Möbius twist, for if we follow the arrow from Fig. 2b along the loop XΓX, we need go around the loop twice: once on a red and once on a blue branch, before returning to the origin. Due to this unusual connectivity, the surface state can be detached from the bulk along the loop XΓX. Figure 2a displays the result of a band-calculation on a strip, showing the Möbius-twisted character.
The presence or absence of a Möbius-twisted surface state on the (010) surface defines a $\mathbb{Z}_2$ variable. When we combine this with the additional $\mathbb{Z}_2$ variable associated with the possibility of forming a strong topological insulator, by introducing an additional odd number of Dirac cones on every surface, we see that the combination of time-reversal and nonsymmorphic symmetries gives rise to a $\mathbb{Z}_4$ topological invariant $\chi$, for which we can construct a corresponding $\mathbb{Z}_4$ index (see Supplementary Information and also ref. 23), as shown in Fig. 3a. $\chi = 0$ corresponds to a trivial insulator with no gapless surface states. $\chi = 1$ corresponds to a strong topological insulating phase with one single surface Dirac cone (Fig. 3b). $\chi = 2$ corresponds to a nonsymmorphic topological insulator with a Möbius-twisted surface state along $X\Gamma X$ ($M'ZM$) path (Fig. 3c), while $\chi = 3$ corresponds to a strong topological insulating phase with three surface Dirac cones (Fig. 3d).

In our model calculations, we also observe a double-Dirac-cone-like surface state on (001) surface, where the crossings are located at $(k_x, k_y) = (\pm k_y, 0)$. However at the mirror plane $k_y = 0$, this surface state is gapped and is not protected by mirror symmetry $\mathcal{M}_t$ and time-reversal symmetry $\mathcal{T}$, so this state will probably be absent in the real material.

**Discussion**

We have shown that CeNiSn and Kondo insulators with nonsymmorphic symmetries have the potential to form a new class of topological Kondo insulators with unusual surface states.
CeNiSn is of course a low-carrier-density metal, with a small Fermi surface derived from an indirect band-gap closure or a lightly doped conduction band\(^{22,23}\), but such small bulk Fermi surfaces are readily localized by disorder or substitution. This is the likely explanation of the observation of a resistivity plateau below 10 K in antimony-doped CeNiS\(_n\),\_Sb\(_m\) \cite{ref. 22}, where the observation of a resistivity plateau most likely derives from a metallic topological surface states, as in the case of SmB\(_6\). Moreover, the V-shape density of states deduced from nuclear magnetic resonance experiments and point-contact spectroscopy\(^{24,26}\) can be accounted for as signatures of Dirac cone surface states. The large magnetoresistance for fields perpendicular to the a axis\(^{27}\) may be a consequence of metallic surface in the (010) plane, combined with an insulating surface on the (100) and (001) planes. Although the above discussion has focused on CeNiSn, we note that the nonsymmorphic Kondo insulator Ce,\_Bi,\_Pt, also displays a resistivity plateau. Remarkably, in the presence of pressure, the resistivity plateau persists up to 100 K \cite{ref. 18} (see Supplementary Methods). These early experimental results provide strong circumstantial support for the topological nature of these nonsymmorphic Kondo insulators and provide a strong motivation for further detailed investigation.

The confirmation of these ideas requires a direct probe of Möbius conducting surface states, either by ARPES measurements, or by non-local\(^{16}\) or sample-thickness-dependent transport measurements\(^{28}\). If such measurements can confirm the surface origin of the observed resistance plateau, one of the interesting challenges would be to delineate between the twisted surface states of a Möbius Kondo insulator, with two Dirac cones, from an untwisted topological insulator, with only one Dirac cone. Chiral edge modes around ferromagnetic domain walls on the surface of SmB\(_6\) have been reported with quantized conductance \(\tilde{e}^2/h\) \cite{ref. 38}. If an analogous ferromagnetic order emerges on a nonsymmorphic surface, the doubling of the Dirac cones is expected to give rise to a total edge conductance of \(2\tilde{e}^2/h\), twice that observed in SmB\(_6\). Another way to detect twisted surface states is from Hall bar measurements. In contrast with the usual topological insulators, where the quantum Hall conductivity \(\sigma_{xy}\) switches from \(-\tilde{e}^2/h\) to \(\tilde{e}^2/h\) on gating, the twisted surface state will generate three values of quantized Hall conductivity \(\sigma_{xy} = (-\tilde{e}^2/h, 0, \tilde{e}^2/h)\), depending on whether the voltage-tuned chemical potential is below, between or above the two cones.

The strong electron correlations in Kondo insulators opens up the possibility of many interesting phenomena, absent in their weakly interacting counterparts. Here, a particularly important phenomenon is the possibility of a surface breakdown of the Kondo effect\(^{28}\). Surface Kondo breakdown is based on the observation that the reduced coordination of the rare earth ions at the surface causes a reduction of in the surface Kondo temperature. In principle, competing instabilities such as magnetism can now be activated on the surface. The breakdown of the Kondo singlets at the surface liberates a large number of conduction electrons, which then dope the topological surface states. We have examined the effects of surface Kondo breakdown in Möbius surface states by recomputing the surface spectrum in the absence of the surface \(f\)-states. These calculations show that the Kondo breakdown causes the Dirac points in Möbius surface states to sink into the valence band (as shown in Fig. 4a), which then generates large Fermi surfaces (see Fig. 4b). The detached nature of the Möbius surface state causes the resulting Fermi surfaces to become quasi-one-dimensional along the \(k_x\) direction. The interaction of the partially unscreened surface local moments with these quasi-one-dimensional Fermi surfaces is expected to lead to a wide variety of surface electronic instabilities, including unconventional superconductivity\(^{29}\) and charge or spin density wave instabilities.

Another interesting future direction is the possibility of non-symmorphic topological superconductors. Promising candidates are UCoGe and URhGe, which share the same space group as CeNiSn\(^{10,11}\). These materials exhibit spin-triplet superconductivity in coexistence with ferromagnetism. The topological classification of such superconductors is an intriguing future prospect.

Methods

Methods, including statements of data availability and any associated accession codes and references, are available in the online version of this paper.

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Author contributions
All authors performed the calculations, discussed the results and prepared the manuscript.

Additional information
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Competing financial interests
The authors declare no competing financial interests.
Methods

In the momentum space, the tight-binding Hamiltonian is

$$H = \sum_k \Psi^\dagger(k) \mathcal{H}(k) \Psi(k)$$

where $$\Psi(k)$$ is a sixteen component spinor, $$\Psi(k) = (\Psi_f(k), \Psi_c(k))^T$$ with

$$\Psi_f(k) = (c_{1A}(k), c_{1B}(k), c_{2A}(k), c_{2B}(k), c_{3A}(k), c_{3B}(k), c_{4A}(k), c_{4B}(k))$$

$$\Psi_c(k) = (f_{1A}(k), f_{1B}(k), f_{2A}(k), f_{2B}(k), f_{3A}(k), f_{3B}(k), f_{4A}(k), f_{4B}(k))$$

and

$$\mathcal{H}(k) = \begin{pmatrix} H_f(k) & V(k) \\ V^\dagger(k) & H_c(k) \end{pmatrix}$$

(4)

where $$V(k)$$ is the hybridization matrix, and $$H_f$$ and $$H_c$$ are the nearest hopping matrices for conduction and $$f$$-electrons, respectively. To simplify our calculation, we introduce four sets of Pauli matrices: $$\sigma_i$$ acts on the spin basis; $$\lambda_i$$ acts on the basis of conduction electrons and $$f$$-electrons; $$\tau_i$$ acts on the basis of the atom labels 1 and 2; $$\rho_i$$ acts on the basis of the layer labels A and B.

From equation (4), the hybridization matrix has the form

$$V(k) = \begin{pmatrix} V_a(k) & V_{ab}(k) \\ V_{ba}(k) & V_b(k) \end{pmatrix}$$

where

$$V_a(k) = \begin{pmatrix} 2t_i \sin k_y & t_1 + \sigma_1 \sigma_2 e^{-ik_z} \\ -t_i - \sigma_1 \sigma_2 e^{ik_z} & 2t_i \sin k_y \end{pmatrix} = -V_a(-k)$$

$$V_{ab}(k) = \begin{pmatrix} t_i - \sigma_1 \sigma_2 e^{-ik_z} & t_1 + \sigma_1 \sigma_2 e^{-ik_z} \\ -\sigma_1 \sigma_2 e^{ik_z} & t_i - \sigma_1 \sigma_2 e^{ik_z} \end{pmatrix}$$

$$V_{ba}(k) = \begin{pmatrix} t_i - \sigma_1 \sigma_2 e^{ik_z} & -t_1 - \sigma_1 \sigma_2 e^{ik_z} \\ \sigma_1 \sigma_2 e^{-ik_z} - t_i & t_i - \sigma_1 \sigma_2 e^{-ik_z} \end{pmatrix}$$

with $$t_i = i(\omega \sigma_1 + \beta \sigma_2)$$, $$t_1 = i\nu \sigma_1$$, $$t_2 = i(\omega \sigma_2 + \beta \sigma_3)$$, and $$\xi_i = i(\omega \sigma_1 - \beta \sigma_3)$$.

The nearest hopping matrices for conduction electrons and $$f$$-electrons are

$$H_f(k) = (2t'_c \cos k_z + \mu'_l) + 2t'_c \cos k_z \left( \frac{k_y}{2} \cos \frac{k_y}{2} \sin \frac{k_y}{2} \tau_c \rho_1 + \sin \frac{k_y}{2} \tau_c \rho_2 \right)$$

$$+ 2t'_c \cos \frac{k_y}{2} \left( \frac{k_y}{2} \tau_c \rho_1 + \sin \frac{k_y}{2} \tau_c \rho_2 \right)$$

where $$l = c, f$$, $$t'_l$$ are the hopping amplitudes along the i-direction, and $$\mu'_l$$ are the bare energies of the isolated conduction electrons and $$f$$-electrons. In the Supplementary Information we perform the construction of this tight-binding Hamiltonian in detail.

We write down the matrix representations of symmetries as follows:

- Time-reversal symmetry, $$T^{-1} \mathcal{H}(k) T = \mathcal{H}(-k)$$, where $$T = i\sigma_3 \mathcal{K}$$ with $$\mathcal{K}$$ being the complex conjugation operator.
- Inversion symmetry, $$P^{-1} \mathcal{H}(k) P = \mathcal{H}(-k)$$, where $$P = \lambda_1 \rho_1$$.
- Glide reflection symmetry $$G_{x1} G_{x2}^{-1} \mathcal{H}(k, -k, z) G_{x1} = \mathcal{H}(k, -k, -z)$$, where

$$G_{x1}(k) = -ie^{i\frac{k_y}{2}} \sigma_z \left( \frac{k_y}{2} \tau_1 + \sin \frac{k_y}{2} \tau_1 \rho_1 \right)$$

- Screw rotation symmetry $$S_{y1} S_{y2}^{-1} \mathcal{H}(k, z) S_{y1} = \mathcal{H}(-k, z)$$, where

$$S_{y1}(k) = -ie^{i\frac{k_y}{2}} \sigma_1 \left( \frac{k_y}{2} \rho_1 + \sin \frac{k_y}{2} \rho_1 \right)$$

- Mirror symmetry $$M_{x1} = S_{y1} P, M_{x2} = S_{y1}^{-1} \mathcal{H}(k, z) M_{x2} = \mathcal{H}(k, -z)$$, where

$$M_{x1}(k) = -ie^{i\frac{k_y}{2}} \sigma_x \left( \frac{k_y}{2} \rho_1 + i \sin \frac{k_y}{2} \rho_1 \right)$$

- Mirror symmetry $$M_{x1} = S_{y1} P, M_{x2} = S_{y1}^{-1} \mathcal{H}(k, z) M_{x2} = \mathcal{H}(k, -z)$$, where

$$M_{x1}(k) = -ie^{i\frac{k_y}{2}} \sigma_x \left( \frac{k_y}{2} \rho_1 + i \sin \frac{k_y}{2} \rho_1 \right)$$

In the spin–orbit coupled systems, reflection and $$\pi$$ rotation square to $$-1$$. We have $$G_{x1}(k)^2 = -e^{i\pi}$$, $$S_{y1}(k)^2 = -e^{-i\pi}$$, and $$M_{x1}(k, 0, \pi)^2 = -1$$.

Data availability. The data that support the plots within this paper and other findings of this study are available from the corresponding author upon reasonable request.