Kramers’ doublet ground state in topological Kondo insulators

M. A. Griffith, M. A. Continentino, and T. O. Pueo

1Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, 22290-180, Rio de Janeiro, Brazil
2Beijing Computational Science Research Center, Haidian District, Beijing 100009, China
3CeFEMA, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

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We consider the simplest variant of a Kondo insulator where a doublet of localized f-electrons hybridizes with spin-degenerate conduction electrons. We analyse the symmetries of f-orbitals involved in the hybridization and point out that the effective four-band model of such systems is adiabatically connected with one that possesses chiral symmetry, which provides further descriptions of clean Kondo insulators. We obtain general conditions for the appearance of topological non-trivial states and discuss implications for rare-earth based compounds. As an example, we derive the full phase diagram of tetragonal Kondo insulators. We show that the chiral symmetry leads to a non-trivial topological phase when the band-width of conduction electrons sets the largest energy scale, and a new weak topological phase appears as function of the normalized distance between bands’ centers.

The extra symmetry results from a rotational invariance of the involved orbital wave-functions. For tetragonal Kondo insulators we show that this symmetry is important when the band-width of conduction electrons sets the largest energy scale. On the other hand, when other than the $\Gamma^{J}_{1/2}$-doublet participate in the hybridization, the presence of chiral symmetry may only appear in a low hopping neighbor expansion, i.e., it is broken by higher order neighbor contributions (which depend on both the involved doublet and crystal symmetry). This property, therefore, can only exist in those crystalline lattice structures that allow for a pure $\Gamma^{J}_{1/2}$-doublet in the ground state. We identify the relevant point-group symmetries for Kondo insulators involving doublets from the $J=5/2$- and $7/2$-multiplets, discuss implications for rare-earth based compounds and conclude with an indication of a topological Kondo insulator material of this kind.

Model:— We start out from the simplest variant of a 3D Kondo insulator, where a spin-degenerate wide conduction band hybridizes with a narrow band formed by degenerate doublets $\Gamma^{f}$ (of $J,\pm\varepsilon$) of localized f-electrons,

$$
\hat{H} = \sum_{k} \left( \sum_{\sigma=\uparrow,\downarrow} \varepsilon_{k} c_{k,\sigma}^{\dagger} c_{k,\sigma} + \sum_{s=\pm} \varepsilon_{k}^{f} f_{k,s}^{\dagger} f_{k,s} \right) \\
+ \sum_{k} \sum_{\sigma=\pm} \sum_{s=\pm} \left( V_{k,\sigma,s} c_{k,\sigma}^{\dagger} f_{k,s} + V_{k,\sigma,s}^{*} f_{k,s}^{\dagger} c_{k,\sigma} \right). \tag{1}
$$

Here $\varepsilon_{k}^{f}$ are the energy-dispersions of conduction and f-electrons, respectively, and $V_{k,\sigma,s}$ account for their hybridization (both, $\varepsilon_{k}^{f}$ and $V_{k,\sigma,s}$ are considered as effective parameters that include effects from electron correlations. Treat correlations beyond the mean-field limit is very challenging, particularly in three dimensions. Most of these approaches consider one or two-dimensional systems [16–22]). Throughout this work we always assume a sufficiently large crystal field, which separates a Kramers’ degenerate ground-state from the $5/2$- or $7/2$-multiplet.
While generally $\Gamma^{J}$ is some linear combination of the angular momentum eigenstates $\Gamma^{J}_{m_J} \equiv |J, \pm m_J \rangle$, of specific interest to us are cases in which $\Gamma^{J} = \Gamma^{J}_{1/2}$. Fig. 1 illustrates the crystal field splitting after spin-orbit for the cubic and tetragonal structures, where $\Gamma^{(i)}_{1,2,3}$ follow the notation in Ref. [3]. Indeed the interesting ground state here is $\Gamma^{(i)}_{1} = \Gamma^{5/2}_{1/2}$. Before we go into details, it is convenient to express Eq. (1) in the matrix form

$$H(k) = \sum_{k} \Psi_{k}^{\dagger} H(k) \Psi_{k},$$

where $\Psi_{k} = (c_{k \uparrow}, c_{k \downarrow}, f_{k,1+}, f_{k,1-})$ and

$$H(k) = \sum_{i=0}^{5} h_{i}(k) \gamma_{i},$$

with $h_{0,4}(k) = (\xi_{k}^{\pm} \xi_{k}^{\dagger})/2$ and remaining coefficient functions $h_{i}(k)$ defined by the hybridization elements $V_{k,s}$. Here $\gamma_{0} = \mathbb{1}_{4}$ is the identity matrix and $\gamma_{i} = \sigma_{i} \otimes \tau_{1}$ (for $i = 1, 2, 3$), $\gamma_{4} = \mathbb{1}_{2} \otimes \tau_{3},$ and $\gamma_{5} = \mathbb{1}_{2} \otimes \tau_{2},$ are Dirac matrices satisfying the Clifford algebra $\{ \gamma_{a}, \gamma_{b} \} = 2 \delta_{ab}$, with Pauli-matrices $\sigma_{i}$ and $\tau_{j}$ operating in spin- and orbital-space, respectively. The general form of Eq. (2) is fixed by invariance under inversion, $I = \sigma_{0} \otimes \tau_{3}$, and time-reversal, $T = i\mathbb{1}_{2} \otimes \tau_{0} K$ (with $K$ the complex conjugation) [23]. In some cases, the symmetry of participating $f$-orbitals imposes an additional constraint to Eq. (2) as we are going to discuss next.

The extra symmetry:— To illustrate the point consider the hybridization block $c_{k}^{\dagger} V_{m_{J}}(k) f_{k}$ for one of the Kramers’ doublets $\Gamma^{m_{J}}_{\pm}$. Following previous work [24] the 2 $\times$ 2 hybridization matrix reads

$$V_{n-\frac{1}{2}}(k) = \left( \begin{array}{cc} c_{n} \gamma_{3}^{-n-1}(k) & \bar{c}_{n} \gamma_{3}^{-n}(k) \\ -\bar{c}_{n} \gamma_{3}^{-n}(k) & -c_{n} \gamma_{3}^{-n+1}(k) \end{array} \right),$$

where $c_{n}$ and $\bar{c}_{n}$ are purely real/imaginary numbers for $n$ even/odd (as fixed by time-reversal symmetry) and

$$\gamma_{3}(k) = \sum_{R \neq 0} v(|R|) Y_{3}^{m}(\hat{R}) e^{i\mathbf{k} \cdot \mathbf{R}}.$$  

The sum in (4) runs over all neighbor sites $\mathbf{R}$, $Y_{3}^{m}(\hat{R})$ are the spherical harmonic functions of $f$-orbitals (with $\hat{R}$ a unit vector), and coefficients $v(|R|)$ depend on the neighbor-distance. A similar expression [3] holds for the Kramers’ doublets $\Gamma^{7/2}_{\pm}$ [24] and the following discussion therefore applies to both multiplets $J = 5/2$ and $J = 7/2$.

Recalling that $\gamma_{3}^{-m}(k) = (-1)^{m+1}[\gamma_{3}^{m}(k)]^{\ast}$, it is verified that Eq. (3) involves four independent real-valued functions. This is tantamount to noting that in general the hybridization block [3] requires in the Hamiltonian [2] a linear combination of the four matrices $\gamma_{1,2,3,5}$. A different situation, however, occurs for the Kramers’ doublet $\Gamma^{1/2}_{\downarrow}$ where the hybridization block involves the spherical harmonic $Y_{3}^{0}(\hat{R})$ on its diagonal. Rotational symmetry of the latter implies that $c_{0} Y_{3}^{0}(k)$ is a purely real-valued function and Eqs. (4) and (3) are spanned by only three out of the four independent $\gamma$-matrices, i.e., $\gamma_{1,2,3}$ [26]. As we discuss further on, the remaining matrix $\gamma_{5}$ defines a chiral symmetry of the effective Hamiltonian [2].

Low neighbor expansion:— First, we notice that Eqs. (3) and (5) with only three of the four $\gamma$-matrices may also appear in a low-order neighbor expansion for other than $m_{J} = 1/2$, but in this case it is not a robust constraint. For illustration consider Eqs. (3) and (5) in a cubic environment for the Kramers’ doublets $\Gamma^{7/2}_{\pm}$.

$$V_{3}(k) \propto \left( \begin{array}{ccc} h_{3}(k) - i h_{5}(k) & h_{1}(k) - i h_{2}(k) \\ h_{1}(k) + i h_{2}(k) & -h_{3}(k) - i h_{5}(k) \end{array} \right).$$

While coefficient functions $h_{3}, h_{5}$ are non-vanishing already for nearest neighbors, $h_{1}, h_{2}$ become finite only starting from second and third order neighbors, respectively. This vanishing of $h_{1}, h_{2}$ is here traced back to the specific values of spherical harmonics $Y_{3}^{m}(\mathbf{k})$ at the angles of the near neighbor-directions in the cubic lattice, as illustrated in Fig. 1 [i.e. zero for nearest and purely real for next-nearest neighbors], and also holds for tetragonal or orthorhombic but e.g. not hexagonal lattices. The absence of $h_{5}$ in case of the $\Gamma^{1/2}_{\downarrow}$ doublet discussed above, on the other hand, follows from the rotational symmetry of involved orbital functions and, therefore, applies for all neighbor contributions. Returning then to Kondo insulators involving a $\Gamma^{1/2}_{\downarrow}$-doublet, we next discuss that $\gamma_{5}$ shows up as an additional symmetry of the effective Hamiltonian [2].

Chiral Hamiltonian:— In the translational invariant insulating phase, i.e. clean system, one can always adiabatically remove $h_{0}(k)$ from Eq. (2) without closing the gap. In addition, the topological phase diagram remains unaltered since eigenfunctions are not affected by terms
proportional to identity. However, with the lack of \( \gamma_5 \) in the Hamiltonian, by removing \( h_0(k) \) we are also adding an extra symmetry to the system, the chiral symmetry. Therefore, Kondo insulators involving hybridization with a \( \Gamma_{1/2}^f \) doublet are adiabatically connected to systems with chiral symmetry, e.g.,

\[
\gamma_5 \mathcal{H}_k \gamma_5 = -\mathcal{H}_k. \tag{6}
\]

The relation between these \( Z_2 \) Kondo insulators and their adiabatically connected \( Z \) Hamiltonian in class DIII \([27]\) is discussed further on in this section. Hamiltonians in this class are characterized by the winding number

\[
N = \sum_{k \in h^{-1}(n_0)} \text{sgn} \det (\partial h(k)), \tag{7}
\]

where \( \partial h \) is the matrix with elements \( (\partial h)_{ij} = \partial h_{ij} \), and the sum is over points \( k \) in Brillouin zone which map onto some (arbitrary) point \( n_0 \) on the 3-sphere, \( (h/h)(k) = n_0 \). Notice that the winding counted by \([7]\) cannot be changed as long as the chiral symmetry is preserved. That is, the topological properties are robust against time-reversal symmetry breaking perturbations that do not violate \([6, 30]\).

As we will see, a robust chiral symmetry can only realize in tetragonal and hexagonal lattices, and the former are the most relevant for application of our results to known Kondo insulators. Concentrating then on tetragonal Kondo insulators with a \( \Gamma_{1/2}^f \) doublet in the ground state, one finds (upon using parameters from the nearest-neighbor model \([29]\))

\[
N = \begin{cases} 
2 \text{sgn}(v_\perp \delta), & |\Delta| < |\delta|, \\
-2 \text{sgn}(v_\perp \delta), & 2 - |\delta| < |\Delta| < 2 + |\delta|, \\
0, & \text{otherwise},
\end{cases} \tag{8}
\]

where \( \Delta = (\varepsilon_c - \varepsilon_f)/2(t_{f||} - t_{f\perp}) \) is the normalized distance between centers of the bands (i.e. \( \varepsilon_c - \varepsilon_f \)) and \( v_\perp \) the hybridization intensity perpendicular to the symmetry plane. We also assumed that the anisotropy \( \delta \) affects equally the hopping parameters \( t_{c,f} \) of \( c \)- and \( f \)-electrons within/perpendicular to the symmetry plane, i.e.

\[
\delta = t_{f||}^{-1} t_{f\perp}^{-1} \quad \text{and} \quad t_{f||} = \delta t_{f\perp}. \tag{9}
\]

The resulting phase diagram is shown in Fig. 2 for completely localized \( f \)-electrons, \( t_{f||}^{-1} = t_{f\perp}^{-1} = 0 \). Just below each winding number signalized in the phase diagram we also show the topological indices \( \nu_0; (\nu_1 \nu_2 \nu_3) \) following Fu and Kane notation in Ref. \([31]\). The white regions are trivial phases with 0 in all topological invariants.

**Surface states:** — The topological non-trivial regions in Fig. 2 have the surface states ruled by the Fu and Kane indices, i.e., the indices \( \nu_0 = 1 \) and \( \nu_0 = 0 \) set the strong (gray) and weak (blue) topological phases of Kondo insulators respectively, with surface states in all directions, as discussed in \([3, 5, 9]\). The tetragonal structure pushes further away the strong phase from the most relevant parameter regime and gives rise to an additional topological weak phase 0; (001) (green), with appearing surface states only on those surfaces aligned with \( z \) direction. Notice that increasing the hopping anisotropy \( \delta \to 0 \), e.g. by application of uniaxial pressure, induces a phase transition into the new topological weak phase \( N = 0 \) and indices 0; (001). Transitions between topological phases can also occur through correlation induced renormalization of the \( f \)-electron dispersion \([32]\). The inset shows the phase diagram as a function of \( f \)-electron renormalized bandwidth \( t_{f||}^{-1} = \alpha t_{f\perp}^{-1} \) at fixed \( \delta = 0.7 \) (delimited by the dashed line in the main figure).

A topologically interesting behavior is found in the most relevant parameter regime where the band-width of conduction electrons \( t_{f||}^{-1} \) sets the largest energy scale such that \( |\Delta| \ll 1 \). The chiral symmetry provides \( N \neq 0 \) for this phase 0; (111) (i.e., edge states in all surfaces and \( |N| = 2 \)). Projecting the effective tetragonal Kondo Hamiltonians onto the surface states one finds that the winding number \( N \) in Eq. \([7]\) allows us to infer the spin-texture of surface states \([29]\): specifically it counts the chiralities of the Dirac cones, i.e., a vanishing winding
indicates an even number of Dirac cones with opposite chiralities, and a finite winding to an even number of Dirac cones with the same chiralities. The same properties hold true for the strong topological phases with $|N| = 1$.

Previous discussions of the edge states in the general chiral Hamiltonian Eq. (6) are found in Refs. [39–41]. In particular, it has been shown the interfaces that break time-reversal symmetry have their gapless edge states replaced by (gapped) non-singular walls and solitons with spin textures protected by the chiral symmetry [34]. Finally, the appearance of spin textures in cubic structures based on the mirror symmetry is discussed in Refs. [12] and [13].

Applications:— Candidate compounds for topological Kondo insulators are formed from magnetic ions with ground states involving odd-parity orbitals. Concentrating onto the rare-earth $3^{+}$-ions with partially filled $4f$ shell, Ce-, Sm-, and Yb-based materials are of potential interest. The ground state Kramers’ doublet in case of the former two compounds arises from the $5/2$-sextet and in case of the latter from the $7/2$-octet. The necessary requirement for the appearance of a robust chiral symmetry as discussed here is then a crystal field which stabilizes the $\Gamma_{1/2}$-doublet in the ground state. Looking at representations of all possible point groups and their basis functions [37], we notice that from the $f$-electron multiplets a pure $\Gamma_{1/2}$-doublet only separates in tetragonal or hexagonal crystal symmetries. Specifically, the $\Gamma_{5/2}$-electrons. We have

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Crystal-Field & Point-Group & Multiplet \\
\hline
\text{tetragonal} & C_{4}, S_{4}, C_{4h}, D_{4}, C_{4v}, D_{2d}, D_{4h} & 5/2 \\
\hline
\text{hexagonal} & C_{6}, C_{3h}, C_{6h}, D_{3h} & 5/2, 7/2 \\
\hline
\end{tabular}
\caption{Point group symmetries which separate a pure $\Gamma_{1/2}$ Kramers’-doublet with lowest projection of angular momentum from the spin-orbit multiplets $J = 5/2$ and $7/2$. This Kramers’ doublet can split from the $5/2$-sextet in all of the seven point group symmetries of the tetragonal lattice, or four out of the seven point group symmetries of the hexagonal lattice. In case of the $7/2$-octet the Kramers’ doublet with lowest projection of angular momentum can only split in four out of point group symmetries of the hexagonal lattice.}
\end{table}

and that topological Kondo-insulators with chiral symmetry may only appear in crystals of odd-parity spin-orbit octets.

Experiments in combination with band structure calculations indicate that the $\Gamma_{5/2}$-doublet is the lowest energy state and inversion of bands occurs [39–41]. Moreover, the $4f$ occupancy near to integer value $n_{f} \sim 1$ and the low dispersive $f$-band, put this material into the topologically interesting region $|N| = 2$ of the phase diagram, Fig. 2. All known Sm-based Kondo insulators, on the other hand, have cubic symmetry and our analysis does not apply. Finally, Kondo insulators based on Yb can only exhibit chiral symmetry in the four hexagonal symmetries indicated in table I. Among the established Yb-based Kondo insulators there is none with hexagonal symmetry, i.e. these compounds can at most realize an approximate chiral symmetry. Recently, an interesting Yb compound with hexagonal symmetry, YbNi$_{4}$X$_{9}$ ($X = Al, Ga$), has been synthesized, but it appears to be metallic [42].

Discussion:— We have studied 3D Kondo insulators, where a wide conduction band hybridizes with a degenerate Kramers’ doublet of localized $f$-electrons. We have shown that in cases where the doublet is that of lowest angular momentum projection, $m_{J} = \pm 1/2$, the symmetry of orbitals involved allows for an improved characterization of the topological properties. The clean system is adiabatically connected with class DIII of Hamiltonians, which in turn are characterized by the Z-invariant. In this case, the winding number distinguishes the chirality of Dirac cones at the surfaces, providing further informations about the edge states. As an example, in cases where the band width of conduction electrons sets the largest energy scale, the tetragonal topological Kondo insulator is in a nontrivial phase with winding number $|N| = 2$, which means that we have two Dirac cones with the same chirality at each surface. Moreover, the phase diagram of this Kondo insulator shows a new weak topological phase when increasing the hopping anisotropy from the cubic to tetragonal structure. When other than the $m_{J} = \pm 1/2$-doublet is involved in the hybridization or when the crystalline field is other than one of those listed in table I, a chiral symmetry may only appear in a low order neighbor approximation. In supplementary material we exemplify with the 4-band model of a cubic structure as described in Ref. [12]. Relevant crystal structures for this work are thus those which allow for a pure $\Gamma_{1/2}$ doublet in the ground state. This implies that topological Kondo-insulators with chiral symmetry involving Kramers’ doublets from the $7/2$ spin-orbit octet can only exist in some of the crystalline hexagonal lattices (see table I). Kondo insulators forming from hybridization with a Kramers’ doublets from the $5/2$-sextet, on the other hand, can exist in all tetragonal and some of the hexagonal lattices. In practice, the crystal field splitting may not be strong enough to separate the ground state and (anisotropic) pressure may help to stabilize a topological chiral phase. We have discussed several implications for the rare-earth compounds, and indicated CeRu$_{4}$Sn$_{6}$ as a possible topological Kondo insulator of this kind.
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[1] M. Dzero, K. Sun, V. Galitski, and P. Coleman, Phys. Rev. Lett. 104, 106408 (2010).
[2] T. Takimoto, Journal of the Physical Society of Japan 80, 123710 (2011).
[3] M. Dzero, K. Sun, P. Coleman, and V. Galitski, Phys. Rev. B 85, 045130 (2012).
[4] M. Fruchart and D. Carpentier, Comptes Rendus Physique 14, 779 (2013).
[5] M. Dzero and V. Galitski, Journal of Experimental and Theoretical Physics 117, 499 (2013).
[6] D. J. Kim, J. Xia, and Z. Fisk, Nature Materials 13, 466 (2014).
[7] Y. Zhong, Y.-F. Wang, H.-T. Lu, and H.-G. Luo, Physical Review B 88, 045130 (2013).
[8] M. Dzero, J. Xia, V. Galitski, and P. Coleman, Annual Review of Condensed Matter Physics 7, 249 (2016).
[9] V. Alexandrov, M. Dzero, and P. Coleman, Phys. Rev. Lett. 111, 226403 (2013).
[10] M. Legner, A. Ruegg, and M. Sigrist, Phys. Rev. B 89, 085110 (2014).
[11] P. P. Baruselli and M. Vojta, Phys. Rev. B 90, 201106 (2014).
[12] P. P. Baruselli and M. Vojta, Phys. Rev. Lett. 115, 156404 (2015).
[13] M. Legner, A. Ruegg, and M. Sigrist, Phys. Rev. Lett. 115, 156405 (2015).
[14] N. Xu, P. K. Biswas, J. H. Dil, R. S. Dhaka, G. Landolt, S. Muff, C. E. Matt, X. Shi, N. C. Plumb, M. Rudovic, E. Pumplin, C. Conder, A. Amato, S. V. Borisenko, R. Yu, H. M. Weng, Z. Fang, X. Dai, J. Mesot, H. Ding, and M. Shi, Nature Communications 5, 4566 EP (2014).
[15] K. Shiozaki and S. Fujimoto, Phys. Rev. Lett. 110, 076804 (2013).
[16] Y. Zhong, Y.-F. Wang, H.-T. Lu, and H.-G. Luo, Phys. Rev. B 88, 235111 (2013).
[17] T. Yoshida, R. Peters, S. Fujimoto, and N. Kawakami, Phys. Rev. B 87, 165109 (2013).
[18] J. Werner and F. F. Assaad, Phys. Rev. B 88, 035113 (2013).
[19] G. Baskaran, ArXiv e-prints (2015), arXiv:1507.03477 [cond-mat.str-el].
[20] A. Thomson and S. Sachdev, Phys. Rev. B 93, 125103 (2016).
[21] A. M. Lobos, A. O. Dobry, and V. Galitski, Phys. Rev. X 5, 021015 (2015).
[22] Zhong, Yin, Liu, Yu, and Luo, Hong-Gang, Eur. Phys. J. B 90, 147 (2017).
[23] Inversion symmetry $T I h_k I^{-1} = h_{-k}$ restricts the diagonal blocks of $h_k$ in orbital-space to be even, and off-diagonal hybridization blocks to be odd functions in $k$. In presence of time reversal-symmetry, $T h_k T^{-1} = h_{-k}$, this excludes Pauli-spin matrices on the orbital diagonal blocks of $h$, while restrictions on hybridization blocks are different for symmetric and anti-symmetric hybridization combinations $c f \pm f c$. i.e. symmetric elements involve Pauli spin-matrices while anti-symmetric elements are independent of spin orientations. Notice that the choice of a relative phase-factor between $c$ and $f$-electrons, for which $T$ is of the indicated form, is reflected in coefficients $c_n, \bar{c}_n$ in Eq. (3), and one may alternatively work in a basis where $T = i \sigma_3 \otimes \gamma_2 K$.}

[24] T. Yamada and Y. Ono, Physical Review B Rev. B 85, 165114 (2012).
[25] I.e. without negative signs in the first line, and $c_n, \bar{c}_n$ now purely real/imaginary numbers for $n$ odd/even.
[26] For $J = 7/2$ it is the matrices $\gamma_i$ with $i = 1, 2, 5$.
[27] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008).
[28] M. Sato and Y. Ando, Reports on Progress in Physics 80, 076501 (2017).
[29] See appendix, where we review the Brouwer index, give details on hybridization-matrices, discuss the tetragonal Kondo insulator, and exemplify a non-zero winding number with spin textures in cubic structures.
[30] Such perturbations change class DIII to AIII without modifying its characterizing topological invariant.
[31] L. Fu and C. L. Kane, Physical Review B 76, 045302 (2007).
[32] The renormalization factor is e.g. found from expanding the self-energy due to interaction between localized $f$-electrons close to the Fermi surface, or alternatively using slave bosons or Gutzwiller’s approximation.
[33] G. Rosenberg and M. Franz, Phys. Rev. B 82, 035105 (2010).
[34] J. I. Väyrynen and G. E. Volovik, JETP Letters 93, 344 (2011).
[35] S. Shen, Topological Insulators: Dirac Equation in Condensed Matters, Springer Series in Solid-State Sciences, Vol. 174 (Springer, 2013).
[36] E. Fradkin, Field Theories of Condensed Matter Physics, 2nd ed. (Cambridge University Press, 2013).
[37] C. J. Bradley and A. P. Cracknell, The mathematical theory of symmetry in solids: representation theory for point groups and space groups (Oxford Clarendon Press, 1972).
[38] S. Paschen, H. Winkler, T. Nezu, M. Kriegisch, G. Hilser, J. Custers, A. Prokofiev, and A. Strydom, Journal of Physics: Conference Series 200, 012156 (2010).
[39] M. Sundermann, F. Strigari, T. Willers, H. Winkler, A. Prokofiev, J. M. Ablett, J-P. Rueff, D. Schmitz, E. Weschke, M. M. Sala, A. Al-Zein, A. Tanaka, M. W. Haverkort, D. Kasinathan, L. H. Tjeng, S. Paschen, and A. Severing, Scientific Reports 5, 17937 (2015).
[40] M. Sundermann, K. Chen, Y. Utsumi, Y.-H. Wu, K.-D. Tsuei, J. Haenel, A. Prokofiev, S. Paschen, A. Tanaka, L. H. Tjeng, and A. Severing, Journal of Physics: Conference Series 807, 022001 (2017).
Appendix A: Winding number and Brouwer index

For convenience of the reader we here review the calculation of the winding number, \( N = \int \frac{d^3k}{4\pi^2} \epsilon^{ijk} \text{tr} \left( \gamma_5 \mathcal{H}^{-1}(\partial_i \mathcal{H}) \mathcal{H}^{-1}(\partial_j \mathcal{H}) \mathcal{H}^{-1}(\partial_k \mathcal{H}) \right) \), via the Brouwer degree, Eq. (7) in the main text. Starting out from the Hamiltonian matrix \( \mathcal{H}(k) = \sum_{i=1}^{4} h_i(k) \gamma_i \) and the chiral symmetry operator \( \gamma_5 = \gamma_1 \gamma_2 \gamma_3 \gamma_4 \), we use anti-commutation relation, \( \{ \gamma_a, \gamma_b \} = 2 \delta_{ab} \), to simplify terms, e.g. \( h_a h_b \gamma_\alpha \gamma_\beta = \frac{1}{2} h_a h_b (\gamma_\alpha \gamma_\beta + \gamma_\beta \gamma_\alpha) = h_a h_b \delta_{\alpha\beta} = |h|^2 \), etc. One then arrives at \( N = \int \frac{d^3k}{4\pi^2} \epsilon^{ijk} h_{abc} \text{tr}(\partial_i h_b)(\partial_j h_c)(\partial_k h_d), \) with \( \epsilon^{ijk} = \epsilon^{ijk}_k \). This can be cast into the form

\[
N = \frac{1}{12\pi^2} \int \frac{1}{|h|^2} e^{abc} h_a dh_b \wedge dh_c \wedge dh_d. \tag{A1}
\]

Eq. (A1) is the pull-back of the (normalized) volume form on the three-sphere, i.e. \( N = \int h^* \omega_{S^3} \), where \( \omega_{S^3} = \frac{1}{\text{vol}(S^3)} \frac{1}{|k|^2} k^a e_a (dk_1 \wedge dk_2 \wedge dk_3 \wedge dk_4) \). The latter can be calculated from the Brouwer degree of the map \( h/|h| : T^3 \to S^3 \), \( k \mapsto (h/|h|)(k) \) with \( T^3 \) the 3D Brillouin zone torus and \( h^2 = (h_1, h_2, h_3, h_4) \). The Brouwer degree counts the number of intersections of a ray through the origin and the oriented surface spanned by the map, as discussed in the main text.

Appendix B: Hybridization matrix for the 5/2-doublets in tetragonal crystal field

Let us recall that matrices Eqs. (3) and (5) in the main text describe the hybridization

\[
\hat{H}_V(k) = \left( \begin{array}{cc}
\epsilon_k^1 & \epsilon_k^4 \\
\epsilon_k^4 & \epsilon_k^1
\end{array} \right) V_{mJ}(k) \left( \begin{array}{c}
\hat{f}_{k,+mJ} \\
\hat{f}_{k,-mJ}
\end{array} \right), \tag{B1}
\]

where \( mJ = n - \frac{1}{2} \) from Eq. (3) in the main text. Concentrating then on Kramers’ doublets separating from the \( J = 5/2\)-sexet and a tetragonal symmetry, we find in the nearest neighbor approximation the coefficient functions \( h^n_{1,2,3,5}(k) \) summarized in table II (see Eq. (4) in the main text). This situation was also considered in Ref. [47] up to first next neighbour approximation.

### Table II. Coefficient functions \( h^n_{1,2,3,5}(k) \) parametrizing the hybridization matrix \( V_{mJ}(k) \) for the \( mJ = 1/2, 3/2, 5/2 \) doublets of the \( J = 5/2\)-sexet in the nearest-neighbor approximation of a tetragonal lattice. Here \( v_\parallel \equiv v(r_\parallel^3) \) and \( v_\perp \equiv v(r_\perp^3) \) are the hybridization intensities within and perpendicular to the symmetry \((x,y)\)-plane, respectively.

| \( mJ \) | \( h^n_1 \) | \( h^n_2 \) | \( h^n_3 \) | \( h^n_5 \) |
|---|---|---|---|---|
| \( n = 1 \) | \( v_\parallel \sin(k_x) \) | \( v_\parallel \sin(k_y) \) | \(-2v_\parallel \sin(k_z) \) | 0 |
| \( n = 2 \) | 0 | 0 | \( v_\parallel \sin(k_x) \) | \( v_\parallel \sin(k_y) \) |
| \( n = 3 \) | \(-v_\parallel \sin(k_x) \) | \( v_\parallel \sin(k_y) \) | 0 | 0 |

We notice that in the nearest neighbor approximation hybridization with \( mJ = 3/2 \) and \( 5/2 \) doublets does not open a gap in the spectrum and the system remains metallic. As discussed in the main text, vanishing coefficient functions for \( mJ = 5/2 \) and \( 7/2 \) doublets are related to the specific values of spherical harmonics \( Y_3^0 \) at the angles of the nearest neighbor directions, here in the tetragonal lattice. In case of the \( mJ = 1/2 \) doublet, on the other hand, vanishing of \( h_3 \) is a consequence of the rotational symmetry of \( Y_3^0 \), and independent of the nearest neighbor approximation.

### Table III. Coefficient functions \( h^n_{1,2,3,5}(k) \) as in table II now including next-nearest neighbor contributions.

| \( mJ \) | \( h^n_1 \) | \( h^n_2 \) | \( h^n_3 \) | \( h^n_5 \) |
|---|---|---|---|---|
| \( n = 1 \) | \( F_a \sin(k_x) \) | \( F_a \sin(k_y) \) | \( -F_a \sin(k_z) \) | 0 |
| \( n = 2 \) | 0 | 0 | \( 5F_a \sin(k_x) \) | \( F_a \sin(k_y) \) | \( F_a \sin(k_z) \) | 0 |
| \( n = 3 \) | \(-F_a \sin(k_x) \) | \( F_a \sin(k_y) \) | \( -F_a \sin(k_z) \) | 0 | 0 |

Accounting for next-nearest neighbor contributions, a (small) gap also opens in case of hybridization with \( mJ = 3/2 \) and \( 5/2 \) doublets, as can be seen from table III where we summarize coefficient functions now including next-nearest neighbor contributions. Here we defined \( F_a = F_a(y-z) \), \( F_a' = F_a(-y+z) \), \( F_b = F_b(x-z) \), and \( F_b' = F_b(-x+z) \), with \( F_\pm(i \pm j) = v_\parallel + v_\perp(1 \mp 2C_{ij} - \sqrt{2} \cos(k_i)) \), \( C_{ij} = \sqrt{2}(\cos(k_i) \pm \cos(k_j)) \) \((i, j = x, y, z)\), and \( F_c = 2v_\perp + v_{2\perp}(2 - C_{xy}) \), \( F_c' = v_{2\perp} C_{xy} \). Here \( v_{2\parallel} \) and \( v_{2\perp} \) are the hybridization intensities within/perpendicular to the symmetry plane for first- and second-nearest neighbor sites, respectively (as also used in Eq. (4) of the main text). Notice that in this order of hopping approximation effective models for \( mJ = 3/2 \) and \( 5/2 \)-doublets also show a chiral symmetry, i.e. \( \gamma_1 \) and \( \gamma_5 \), respectively. Including, however, contributions from third-nearest neighbors all coefficient functions become non-vanishing in case of \( mJ = 3/2 \) and \( 5/2 \)-doublets. Only in case of the \( mJ = 1/2 \) doublet \( h_5 \) remains zero. Finally, a discussion similar to the above applies to coefficient functions parametrizing hybridization with doublets from the \( J = 7/2 \)-octet.
Appendix C: Tetragonal Kondo insulator

We here focus on a tetragonal Kondo insulator with the $t^{5/2}_{1/1}$-doublet in the ground state and calculate the winding number from the nearest neighbor model. Dispersion relations for conduction and (nearly) localized electrons then read $\varepsilon^{c,f}_k = \varepsilon_{c,f} + 2t^{c,f}_{\|}(\cos(k_x) + \cos(k_y)) + 2t^{c,f}_{\perp}(\cos(k_z))$, where $\varepsilon_{c,f}$ are the corresponding band-centers and $t^{c,f}_{\|}$ hopping parameters within/perpendicular to the symmetry plane of the tetragonal structure. Dispersion relations define coefficients $h_{0,4}(k)$ (see Eq. (2) in the main text) and coefficients $h_{1,2,3,5}^{c,f}(k)$ taken e.g. from table II or III of the previous section. With these functions Eq. (7) in the main text reads

$$N = \sum_{k \in \mathbf{h}^{-1}(n_0)} \text{sgn}(-F_a F_b F_c \cos k_x \cos k_y \cos k_z), \quad (C1)$$

where $F_a, F_b, F_c$ have been discussed in the previous section. To evaluate the sum (C1), it is then convenient to choose $n_0 = h_4(0)e_4$ whose pre-image, $\mathbf{h}^{-1}(n_0)$, are the eight time-reversal invariant points in the Brillouin zone. The result of this calculation is given in Eq. (8) of the main text.

Appendix D: Surface-states spin texture in the tetragonal Kondo insulator

The translational invariant tetragonal Kondo insulators allows for a characterization in terms of winding number, as described in Eq. (7) in the main text and appendix A. Here we apply the projection method to derive the surface Hamiltonian. Let us consider those time-reversal invariant momenta points $k_0$, as described in the previous section. In their vicinity the Hamiltonian reads $\mathcal{H}(k) = \sum_{i=1}^{3} v_i k_i \sigma_i \tau_z + m \tau_z$, with parameters $v_i$ and $m$ functions of $k_0$. As an illustration we consider the surface Hamiltonian at $z = \pm L/2$, where $L$ is the z-direction system size. Since translational invariance is broken in z-direction we substitute $k_z \rightarrow -i \partial_z$ and the zero energies eigenfunctions are obtaining by

$$\left(\tau_z [m - (P_+ - P_-)] v_z \partial_z \right) + \sum_{i=1}^{2} \psi_k (z) = 0,$$

where we have introduced the projection operators $P_{\pm} = \frac{1}{2} (\mathbb{1} \pm \sigma_z \tau_y)$. The spatially dependent part of the Schrödinger equation, with $\psi_k (z) = \psi (z) \psi (k)$, is solved by eigenfunctions of $P_{\pm}$, that is, introducing $P^{\pm} \psi^{\pm} = \pm \psi^{\pm}$ the z-coordinate dependent part reads

$$\psi (z) = e^{\frac{\varepsilon_{c,f}^{\pm}}{v_z} z} \psi^+ + e^{-\frac{\varepsilon_{c,f}^{\pm}}{v_z} z} \psi^-.$$

Depending on the sign of $\text{sgn}(m/v_z)$ is the first/second contribution accounts for the wave-functions exponentially localized at $z = \pm L/2$. Concentrating on either one of the surfaces we project the $k$-dependent part on the corresponding eigenspace $H^{\pm} = \mathbb{P}_s \mathcal{H}(k) \mathbb{P}_s$. In order to find an explicit expression it is convenient to introduce $U \equiv e^{i\pi v}$ such that the surface Hamiltonians are written in the rotated basis $H^\pm = U^\dagger H^\pm U$, explicitly

$$H^+ = \begin{pmatrix} 0 & 0 & v_x k_x - i v_y k_y \\ 0 & 0 & 0 \\ v_x k_x + i v_y k_y & 0 & 0 \end{pmatrix},$$

$$H^- = \begin{pmatrix} 0 & 0 & v_x k_x + i v_y k_y \\ 0 & 0 & 0 \\ v_x k_x - i v_y k_y & 0 & 0 \end{pmatrix}.$$

From this result we noticed that each of the two Hamiltonian describes a given surface depending on $\text{sgn}(v_z k_x)$ at $(k_0)$. The surface Hamiltonians on opposite surfaces have opposite chiralities, i.e. $\text{ch}_4 = \text{sgn}(v_x v_y)$ and $\text{ch}_2 = -\text{sgn}(v_x v_y)$. Thus, the chirality of the surface states at a given surface is fixed by the product $\text{ch} = \text{sgn}(mv_z v_y v_z)$. Coming back to our example in the previous section, the sum is over time-reversal invariant momenta where band inversion occurs, i.e. $m(k_0) < 0$. Having fixed the Brouwer’s formula $n_0 = h_4(0)e_4$ we noticed that each summand is related to the chirality of surface states such that

$$N = \sum_{k_0} \text{sgn}(-v_z (k_0) v_y (k_0) v_z (k_0)).$$

The absolute value of the winding accounts for the total chirality of surface states when present on a given surface. The latter is a well defined quantity, i.e. independent of the surface one looks at.

Appendix E: cubic Kondo insulator: low neighbor hopping approximation

As an example where the chirality appears in low neighbor hopping approximation, we apply our calculations to the 4-band model of a cubic structure as described in Ref. [12]. According to our notation, their Hamiltonian can be rewritten as $\varepsilon^{c,f}_k = \varepsilon^{c,f}_{0} - 2t^{c,f} \mu_1 (c_x + c_y + c_z) - 4t^{c,f} \mu_2 (c_y c_x + c_z c_y + c_z c_x)$, where $\varepsilon^{c,f}_k$ is dispersion relations for the conducting and localized bands, $\varepsilon^{c,f}_{0}$ are the corresponding band-centers, and $t^{c,f}_1 \mu_1^{c,f}$ and $t^{c,f}_2 \mu_2^{c,f}$ are the band-width for first and second nearest neighbors, respectively, finally $c_i = \cos (k_i)$ with $i = x, y, z$. Using notation of Table III with $n = 1$, the hybridization elements have their coefficient functions as $F_a = -2V (\eta^1 + \eta^2 (c_y + c_z))$, $F_b = -2V (\eta^1 + \eta^2 (c_x + c_z))$ and $F_c = 2V (\eta^1 + \eta^2 (c_y + c_x))$, where $V \eta^1$ and $V \eta^2$ are the hybridization amplitudes for nearest and next-nearest
neighbor hoppings, respectively. Finally, the parameters were set to $\epsilon_0^f - \epsilon_0^c = -2\text{eV}$, $t_c = 1\text{eV}$, $t_f = 0.003\text{eV}$, $\eta_1^c = \eta_1^f = 1$, $\eta_2^c = \eta_2^f = -0.5$, $V\eta^1 = 0.2\text{eV}$, and $V\eta^2 = 0$.

Now we intend to calculate the winding number according to Eq. [C1], where we evaluate the sum by choosing $n_0 = -h_4(0)e_4$, whose pre-image are the eight time-reversal invariant points in the Brillouin zone. The result of this calculation is $N = +3$, which characterizes the three Dirac cones with the same pseudo-spin chirality in Fig. 3(a) in Ref. [12].