A combined theoretical and experimental thermodynamic study of the Kondo insulator SmB$_6$ is pursued to elucidate the well-known anomalous low-temperature electronic-like specific heat contribution conjectured to arise from metallic surface states. A general thermodynamic description of topological Kondo insulators is developed using a mean-field slave-boson approximation and Hill thermodynamics to study the phase transitions with the critical exponents of the model, showing consistency with the Josephson hyper-scaling relation. Applying to SmB$_6$, the separation of bulk and boundary contributions to the heat capacity reveals that, while the surface states contribute to an increase in the heat capacity upon lowering temperature, the effect is unmeasurably small. A systematic experimental study of the dependence of SmB$_6$ heat capacity on surface to volume ratio confirms this to be true, and suggests an alternate explanation is required for the anomalous low-temperature contributions to specific heat in this material.

**Introduction** - Topological insulators are materials that are insulating in the bulk, but have conducting surface states at the boundaries. These surface states are protected by the symmetries of the bulk Hamiltonian against impurity scattering, and lead to fascinating phenomena, such as Majorana zero modes in 1D [1–2] or the quantum spin Hall effect in 2D [3–7]. In 3D, there are also several experimental realizations of topological insulators, such as Bi$_2$Se$_3$ and Bi$_2$Te$_3$ [8–9], but these materials have a residual bulk conductivity caused by impurities [10], and are therefore not truly gapped.

One of the most promising realizations of a 3D topological insulator with a fully gapped bulk is SmB$_6$ [11]. This material is a Kondo insulator, i.e. below the Kondo temperature, the otherwise metallic system becomes insulating. This transition is caused by a hybridization between conducting $d$-electrons and localized $f$-electrons that occurs at low temperatures, opening up a hybridization gap. In light of recent developments in the field of topological insulators, Dzero et al. [12] proposed that Kondo insulators could have a topological phase. This would naturally explain the puzzling behavior of the residual conductivity of SmB$_6$ in the low-temperature ($T$) regime. In addition, another obscure feature of SmB$_6$ that baffled scientists for many years, namely the resemblance of the low-$T$ heat capacity to that of a metal [13–14], motivated the search for an explanation in the topological nature of the system. In this view, the upturn in the heat capacity would be ascribed to the presence of metallic surface states, but this hypothesis still lacks confirmation.

Here, we address this issue by verifying both experimentally and theoretically whether the surface states are responsible for the upturn in the heat capacity. Experimentally, the dependence of the heat capacity of SmB$_6$ on the surface to volume ratio is studied by systematically breaking apart a single-crystal sample and remeasuring the total specific heat of the pieces. If the heat capacity increases as the surface increases, this would make it plausible that the presence of these surface states causes the upturn. Theoretically, one of the major difficulties is that topological systems have mostly been studied at zero $T$, whereas the heat capacity is a finite-$T$ property. Recently, a thermodynamic approach inspired by the pioneering work of Hill [15] has been proposed, which allows to separate the bulk and boundary contributions to the free energy [16], and describe the topological phase transition at zero and finite $T$. This approach will permit us to settle the discussion about the importance of surface states in determining the upturn in the heat capacity. Moreover, it was shown that the order of the topological phase transition in the bulk and at the boundary obeys a universal law for the five most common models for topological insulators, namely the Su-Schrieffer-Heeger and Kitaev models in 1D, the Kane-Mele and Bernevig-Hughes-Zhang (BHZ) in 2D and the BHZ in 3D [17]. Although the phase diagram of Kondo insulators has been determined previously [18–20], the order of the phase transition has not been considered. It is thus interesting to verify whether the universal rule also applies to topological Kondo insulators.

In the following, we first determine the phase diagram of a topological Kondo insulator and investigate the phase transition from a topological to a band-insulator phase using the thermodynamic approach. For this, we use a minimal Anderson-lattice model to study the topological Kondo insulator, accounting for only two $d$- and two $f$-bands. Using a mean-field slave-boson approach, we find that the order of the topological phase transition obeys the same universality as found in other topological-insulator models, and agrees with the Josephson-hyperscaling relations. Second, we examine SmB$_6$ in more detail both experimentally and theoretically.
sulators, such as SmB$_6$, are usually described using the Anderson lattice model (ALM) \cite{21}. In this tight-binding approach, an even number (spin up and spin down) of conducting $d$- and localized $f$-bands is considered. The different models available in the literature vary in the amount of bands that are included, the hybridization between the $f$- and $d$-bands, and in the range of hopping to which neighboring sites are incorporated \cite{12,22,23,24,25,27}. Here, we start with a minimal ALM \cite{24,25} and later describe how this should be altered to obtain a more appropriate model for SmB$_6$. The ALM Hamiltonian consists of three parts,

$$H_{ALM} = H_d + H_f + H_h.$$  

(1)

Here, $H_d$ describes the conducting $d$-electrons, $H_f$ the (almost) localized $f$-electrons, and $H_h$ the hybridization,

$$H_d = \sum_{i} \epsilon_i^d \sigma_{\alpha}^i \sigma_{\alpha}^i - \sum_{\langle ij \rangle \alpha \sigma \sigma'} \tilde{t}^d_{ij \sigma \alpha} (\sigma_{\alpha}^i \sigma_{\alpha}^j + \text{h.c}),$$

$$H_f = \sum_{i \sigma} \epsilon_i^f \sigma_{\alpha}^i \sigma_{\alpha}^i - \sum_{\langle ij \rangle \alpha \alpha'} \tilde{t}^f_{ij \alpha \alpha'} (\sigma_{\alpha}^i \sigma_{\alpha}^j + \text{h.c})$$

$$+ U \sum_{\langle i \alpha \rangle} \sigma_{\alpha}^i \sigma_{\alpha}^i,$$

$$H_h = \sum_{i} \sum_{\langle \alpha \rangle} (V_{i \sigma l, j \alpha} \sigma_{\alpha}^i \sigma_{\alpha}^j + \text{h.c}),$$  

(2)

where $\sigma_{\alpha}^i$ is the creation operator of a $d$-electron on site $i$, with spin $\sigma$, in orbital $l$, and $\sigma_{\alpha}^i$ creates an $f$-electron on site $j$ with pseudo-spin $\alpha$. Due to the presence of strong spin-orbit coupling, $\alpha$ is not a spin index, but defined by the total angular momentum $J$ and its $z$-component $M$ \cite{20}. Furthermore, $\epsilon$ and $t$ are the on-site energy and nearest-neighbor hopping amplitude respectively, $U > 0$ is the strength of the interaction between the $f$-electrons, and $V_{i \sigma l, j \alpha}$ is the hybridization-matrix element.

In order to obtain an effective model that is quadratic in the creation and annihilation operators, we use the slave-boson approximation \cite{24,25,27}, and take the limit $U \rightarrow \infty$. In the case of almost filled $f$-bands (the case we will consider later for SmB$_6$), this corresponds to projecting out the states with two or more $f$-holes per site. We apply this constraint using slave bosons, and then calculate the effective model by applying a mean-field approximation on the bosonic fields. This procedure results in the effective hole Hamiltonian,

$$H_{eff}(k) = \begin{pmatrix}
-\epsilon^f I + t^f_k - b V_k \\
-b V_k^\dagger \\
-(\epsilon^f - \lambda) I + b^2 t^f_k
\end{pmatrix} + \text{h.c.}$$

(3)

where $I$ is the unitary matrix, accounting for the (pseudo) spin species. Thus, the mean-field effect of the interaction is a rescaling of the $f$-electron hopping and the hybridization with $b$, and a shift $\lambda$ in the on-site energy of the $f$-electrons. Details of the derivation of the effective Hamiltonian and the corresponding mean-field equations for $b$ and $\lambda$ are described in the Sup. Mat.

**Phase diagram -** Now, we investigate the phase behavior of the minimal model that includes one $d$- and one $f$-orbital, and both spin up and down degrees of freedom \cite{12,28}. In this case,

$$\begin{align*}
-\epsilon^d I + t^d_k &= -1 \xi^d_k \\
-\epsilon^f I + b^2 t^f_k &= -1 \xi^f_k \\
V_k &= V(\sin k_x, \sin k_y, \sin k_z)^T \cdot \vec{\sigma},
\end{align*}$$

(4)

where

$$\begin{align*}
\xi^d_k &= -2t \sum_{k, \eta = x, y, z} \cos k_{\eta} - \mu, \text{ and} \\
\xi^f_k &= 2b^2 t_f \sum_{k, \eta = x, y, z} \cos k_{\eta} - \mu + \epsilon^f_0.
\end{align*}$$

(5)

Substituting Eq. (4) into Eq. (3), and using the numerical values $\epsilon^f_0 = -1.05t$ and $t_f = 0.1t$, we can calculate the topological invariant of the system, as described in the Sup. Mat.

![Figure 1. Temperature versus hybridization phase diagram of the four-band Kondo model. Four phases can be distinguished, a Kondo liquid (KL), a weak topological insulator (WTI), a topological Kondo insulator (TKI), and a band insulator (BI) phase.](image-url)

The resulting $T$ versus $V$ phase diagram for the four-band model is given in Fig. 1. As promptly observed in the phase diagram, the topological phase transitions in this model are driven by the hybridization $V$ or by the temperature $T$. For low $V$ and $T$, the system is a weak topological insulator (WTI). As $V$ increases, the mean-field solution for $\lambda$ increases, thus shifting the $f$-electron energy, which changes the topological index, giving rise to a (strong) topological Kondo insulator (TKI) for intermediate $V$. As $V$ increases even further, the $f$-bands move under the $d$-electron bands, resulting in a trivial topological index. The system then becomes a band insulator (BI). For sufficiently high $T$ and low $V$, the gap closes and the system becomes a Kondo liquid (KL). It
should be noted that the phase diagram is strongly dependent on the number of bands. As shown by Dzero et al. \[13\], inclusion of more bands leads to a disappearance of the WTI phase and an expansion of the stability region of the KL phase. The band structure for each phase is shown in the Sup. Mat.

Now, to gain more insight in these phases and their transitions, we analytically determine the order of the phase transitions for the bulk and boundary separately, and show the connection with the Josephson-hyperscaling relation explicitly. We focus on the phase transition from a TKI to a BI. The eigenvalues of the four-band Hamiltonian are relatively simple, and follow from diagonalizing Eq. (3),

\[ E_k = \frac{1}{2} (\xi_k^d + \xi_k^f - \lambda) \pm \sqrt{(\xi_k^d - \xi_k^f + \lambda)^2 + 4V^2} \sum_{\eta=x,y,z} \sin k_\eta. \] (6)

Using Eq. (3) we can calculate the free-energy contributions in the low-k limit. As the gap closes around the $\Gamma$ point at $\lambda = \lambda_c$, these are the relevant contributions for the thermodynamic behavior. The low-k free energy scales with $(\lambda - \lambda_c)^{1/4}$, and since $\lambda$ scales linearly with $V$, this indicates a fourth-order bulk phase transition (see Sup. Mat. for details). The fourth-order value for the transition indeed agrees with the universality unveiled previously for other topological models, where the bulk topological phase transition was of order $d + 1$, with $d$ the dimensionality of the model.\[17\].

We can understand this universality in a more general way. Near the critical point, the singular part of the free energy of the system $F(v) \propto |v|^{2-\alpha}$ scales with the dimensionless measure of the distance $v = (V - V_c)/V_c$ from the critical point.\[20\]. The quantum Josephson-hyperscaling relation connects the order of the phase transition at $T = 0$, which is equal to $2 - \alpha$ in the Ehrenfest classification, to the critical exponents $\nu$ and $z$\[30\,31\],

\[ 2 - \alpha = \nu(d + z). \] (7)

Here, $d$ is the dimensionality of the system, and $\nu$ and $z$ can be determined by investigating the behavior of the energy gap $\Delta G$ near the critical point.\[32\]. By considering $k_y = k_z = 0$ and redefining $k_x = k$, we find

\[ \Delta G(V = V_c) \propto k^z, \quad \Delta G(k = 0) \propto |v|^\nu. \] (8)

Next, we calculate how the gap closes as a function of $k$ and $v$, and find a linear behavior (see Sup. Mat.). Thus, we have $\nu = z = 1$, which leads to the order of the bulk phase transition $2 - \alpha = d + 1 = 4$ in our case. This result puts topological Kondo insulators in the same universality class as the topological models investigated by Kempkes et al.\[17\], which also had $\nu = z = 1$.

At the boundary, $F$ scales with the critical exponents $\nu$ and $z'$, where $z'$ characterizes the dispersion of the surface states, $E(k) \propto k^{z'}/z$ for $k \to 0$. Hence, the thermodynamic behavior of the boundary is dominated by the surface states that live in the gap, and we have

\[ F \propto \int_{E(k) | < \Delta} E(k) dk^{d-1} \propto \int_{|k^{z'}/z| < \Delta} k^{z'+d-2} dk \]

\[ \propto \Delta(z'+d-1)/z' \propto |v|^{\nu(z'+d-1)/z'}, \] (9)

where $\Delta = \Delta G(k = 0)$ is the gap size. For the four-band topological Kondo insulator, we find that $z' = 1$, as shown in the Sup. Mat. This indeed reproduces the universality for the boundary $2 - \alpha = d = \nu(z' + d - 1)$ found by Kempkes et al.\[17\] for systems with $\nu = z' = 1$. Hence, $F \propto |v|^{3\nu}$ and the phase transition at the boundary is of third order (a discontinuity occurs in the third derivative of the free energy).

Heat capacity - We now focus on a specific example of a Kondo insulator, namely SmB$_6$. The low-$T$ heat capacity of this material has long been known to present anomalous properties for a bulk insulator\[14\], including an apparent $T$-linear contribution that ranges from $\sim 10$ to 50 mJ/mol-K\[2\,33\]. In order to investigate the importance of the surface state contribution to the total measured heat capacity, we used an Al molten flux technique\[31\], studied by systematically cleaving into smaller pieces, thus increasing the surface area several times. The specific heat of each subsequent collection of pieces of the original crystal was measured down to 1.8 K using the relaxation technique in a Quantum Design Physical Properties Measurement System, measuring background addenda each time. As shown in Fig. 2 the collections of samples exhibit the telltale finite residual fermionic contribution of $\sim 10$ mJ/mol-K\[2\,33\]. In all cases, the variations between each sample count attributed to error in addenda determination. Normalizing all data to 15 K, where phonon conduction begins to dominate, reveals no discernible change in the specific heat as a function of estimated total surface area, indicating that the measured low-temperature specific heat is dominated by the bulk of the material.

We corroborate this experiment with a thermodynamic study with an approach that has recently been developed\[16\,17\]. Generally, thermodynamic quantities like the heat capacity are connected to the bulk of a system. However, in the case of topological insulators, the boundaries cannot be neglected. Hill thermodynamics solves this problem by allowing for contributions to the grand potential $\Phi$ that do not scale with the volume, but instead with the surface\[15\],

\[ \Phi = \mathcal{V} \Phi_V + \mathcal{A} \Phi_A, \] (10)

where $\mathcal{V}$ is the volume, $\mathcal{A}$ is the surface area, and $\Phi_V, \Phi_A$ is the bulk (surface) grand potential. It was recently
shown by Quelle et al. [16] that this formalism can be applied to describe the thermodynamic behavior of topological surface states once the Hamiltonian of the system is known.

Although the minimal model for a Kondo insulator used above involves only four bands [12], it was proposed that a realistic description of SmB$_6$ requires a ten-band model (2 $d$- and 3 $f$-electrons), with up to third nearest-neighbor hopping [35]. The parameters in this ten-band model are taken from ab-initio calculations [36], and the resulting in-gap surface states around both the $\Gamma$ and $X$ high-symmetry points in the Brillouin zone agree well with angle-resolved photoemission spectroscopy measurements [37-41]. The model is described in more detail in the Sup. Mat. and is used in the remainder of the discussion.

Next, we numerically solve the $T$-dependent mean-field equations for the ten-band model. Then, we apply these solutions to a model with periodic boundary conditions in all but one direction. In the non-periodic direction, the system consists of $n$ layers. If $n$ is large enough, such that there is no bulk-mediated interaction between the upper and lower layer, Eq. (10) is valid. In this case, the grand potential can be separated into a boundary and a bulk contribution

$$\Phi(T, n, l) = \Phi_V(T) nl^2 + \Phi_A(T) l^2,$$

(11)

where $l$ is the number of sites in the periodic directions. Using

$$\Phi(T, n, l) = \frac{1}{\beta} \log \left[ \text{Tr} \left( e^{-\beta H} \right) \right] = \frac{1}{\beta} \sum_{j,k} \log \left( 1 + e^{-\beta \epsilon_{jk}} \right),$$

(12)

where $\epsilon_{jk}$ is the $j$th eigenvalue of $H_{\text{eff}}(k)$, given in Eq. (3) we calculate the total grand potential, and then determine $\Phi_A(T)$ and $\Phi_V(T)$ by making a linear fit to Eq. (11) for several values of $n$. Once the grand potential is calculated, we can use the entire thermodynamic framework to calculate properties such as the density of states or the heat capacity.

Figure 2. Specific heat measurement of SmB$_6$ crystal as a function of surface area. In this experiment, a single-crystal sample is systematically broken into pieces and specific heat (top) is re-measured for collections up to 18 pieces. Analysis of the resultant increase in total sample surface area (bottom) is plotted as a function of the normalized specific heat normalized to 15 K data in order to remove errors in addenda subtraction and other systematic errors.

Figure 3. Bulk (pink) and surface (blue) contribution to the heat capacity of SmB$_6$ described by the minimal model from Baruselli et al. [35], where all first- and second-nearest neighbor hybridizations are included. Here, $v.(s.)f.$u. is an abbreviation for volume (surface) formula unit.

Calculating the grand potential with the method outlined above, we find the bulk (displayed pink) and surface (blue) contribution to the heat capacity $C_v = -T \frac{\partial^2 \Phi}{\partial T^2}$, with $i = V, A$ in Fig. 2. We observe two main features. First, the bulk contribution drops to zero for low $T$, which should indeed be the case for an insulator. Second, due to the metallic surface states, there is a peak in the heat capacity at low $T$. If we would stop the calculations at $T \approx 2$K, this would appear as an upturn, precisely as the one observed in the experiments, which go down to 2K. However, this quantity is calculated per surface area. Upon computing the total heat capacity for the experimentally used sample sizes, which are of
the order of nm, we see that the upturn caused by the surface states is seven orders of magnitude too small to explain the experimentally measured heat capacity.

**Conclusion and Outlook** - We investigated the thermodynamics of a Kondo system using (1) a simple four-band model to study the topological phase transitions, (2) a partitioned sample of SmB$_6$ to measure the heat capacity and (3) a more detailed ten-band model to compute the low-$T$ heat capacity of SmB$_6$. In both theoretical cases, we used a slave-boson mean-field approximation. We found that Kondo insulators obey the same universality rule as the five most common topological insulator models, namely, the phase transition from the topological to the trivial (BI) phase at the edge is one order lower than at the bulk [17]. Furthermore, we see that this universal behavior can be understood by considering the critical exponents of the system. Based on the experiment and the calculations for SmB$_6$, we conclude that topological surface states are not responsible for the puzzling upturn in the heat capacity. The idea that the anomalous heat capacity in SmB$_6$ is not a boundary effect is further supported by other recent papers by e.g. Knolle et al. [12], where it is shown that the heat capacity could be explained by considering bulk excitons, or the work by Tan et al. [13], where they look into bulk-like quantum oscillations. However, recent muon Knight shift experiments suggest the low-temperature excitonic mode would not contribute to thermodynamic quantities as previously thought [14]. According to our results, although the surface states provide a qualitative upturn in the heat capacity, it is nearly impossible to measure this effect, as it is extremely small, compared to the actual upturn of the surface states, even for a very thin sample of only a 100 atomic layers.

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Supplemental Material: Thermodynamic study of topological Kondo insulators

Appendix A: Slave-boson mean-field approximation

We approximate the interacting Hamiltonian given by Eq. 2 from the main text, by taking the limit of $U$ to infinity, which effectively imposes the constraint that there can be no more than one $f$-hole per site. In order to impose this constraint, we switch to the hole representation. We assume that the slave boson is filling up the place of the $f$-hole if it is not there. Thus, we get the transformation

\[ f_{i\alpha}^\dagger \rightarrow f_{i\alpha}^\dagger b_i, \]  

where $b_i$ is the slave-boson annihilation operator, and $f_{i\alpha}^\dagger$ creates an $f$-hole with pseudo spin $\alpha$ at site $i$. This procedure enables us to formulate the constraint that projects out the doubly occupied states,

\[ b_i^\dagger b_i + \sum_{\alpha} f_{i\alpha}^\dagger f_{i\alpha} = 1. \]  

As a consequence, $b_i^\dagger b_i$ and $f_{i\alpha}^\dagger f_{i\alpha}$ cannot be simultaneously nonzero, and the slave bosons drop out for the on site energy,

\[ f_{i\alpha}^\dagger b_i b_i f_{i\alpha} = (1 + b_i^\dagger b_i) f_{i\alpha}^\dagger f_{i\alpha} = f_{i\alpha}^\dagger f_{i\alpha}. \]  

We apply the transformation of the $f$-holes (Eq. S1) to the Hamiltonian and impose the constraint (Eq. S2) using the Lagrange multipliers $\lambda_i$. Then, we perform a mean-field approximation, in which we replace the $b_i$, $b_i^\dagger$ operators by their expectation values $\langle b_i \rangle = \langle b_i^\dagger \rangle = b_i$, and $i\lambda_i$ by $\lambda_i$. After implementing a Fourier transformation and dropping the constant terms, we obtain the effective Hamiltonian given by Eq. 3 from the main text.

Next, we show in detail how to derive and solve the mean-field equations that determine the value of $b$ and $\lambda$. Let us rewrite the effective hole Hamiltonian, but keep track of the constant term resulting from the mean-field approximation,

\[ H_{\text{eff}} = -\sum_{k\sigma l} \epsilon_l^d d_{k\sigma l}^\dagger d_{k\sigma l} + \sum_{k\alpha l'} t_{k\alpha l'}^f d_{k\sigma l}^\dagger d_{k\sigma l'}^f \]
\[ - \sum_{k\alpha} \left( \epsilon_k^f - \lambda \right) f_{k\alpha}^\dagger f_{k\alpha} + b^2 \sum_{k\alpha l'} t_{k\alpha l'}^f f_{k\alpha}^\dagger f_{k\alpha l'}^f \]
\[ - b \sum_{k\sigma l} \left( V_{k\sigma l} f_{k\sigma l}^\dagger + H.c. \right) + N_s (b^2 - 1) \lambda, \]  

where $N_s$ is the number of sites. We now minimize the free energy associated with this effective Hamiltonian. We start by calculating the partition function $Z$, since the free energy $F$ is given by $F = -k_B T \log Z$. The Euclidean action $S_{\text{eff}}$ corresponding to $H_{\text{eff}}$ is given by

\[ S_{\text{eff}} = \hbar \beta N_s (b^2 - 1) \lambda - \int_0^{\hbar \beta} d\tau \sum_k \int_0^{\hbar \beta} d\tau' \sum_{k'} \Psi^\dagger (\tau, k) G^{-1} (\tau, k, \tau', k') \Psi (\tau', k') , \]

where $\Psi (k, \tau)$ denotes the fermionic coherent state, and the inverse Green’s function $G^{-1}$ reads,

\[ G^{-1} (\tau, k, \tau', k') = \left( \begin{array}{cc} -\hbar \partial_\tau + \epsilon_k^d - t_k^d & \frac{bV_k^\dagger}{b} \\ \frac{bV_k}{b} & -\hbar \partial_\tau + \left( \epsilon_k - \lambda_1 \right) - b^2 t_k^f \end{array} \right) \delta (k - k') \delta (\tau - \tau'), \]  

with $1$ denoting the unitary matrix. This yields the partition function,

\[ Z = \text{Tr} \left( e^{-H_{\text{eff}}} \right) = \int D(\Psi, \Psi^\dagger) e^{-S_{\text{eff}}/\hbar} = \exp \left[ -\beta N_s (b^2 - 1) \lambda + \text{Tr} \log (-G^{-1}/\hbar) \right] , \]
which leads to the free energy,

\[ F = -k_b T \left[ -\beta N_s (b^2 - 1)\bar{\lambda} + \text{Tr} \log(-G^{-1})/\hbar \right]. \]  

(S8)

In order to minimize the free energy with respect to \( b \), we take the derivative,

\[
\frac{\partial}{\partial b} \left[ \text{Tr} \log(-G^{-1}) \right] = \text{Tr} \left[ -G \frac{\partial (-G^{-1})}{\partial b} \right] 
= \text{Tr} \left[ \int_0^\beta d\tau d\tau' \sum_{k,k'} G(\tau, k, \tau', k') \frac{\partial}{\partial b} G^{-1}(\tau', k', \tau, k) \right] 
= \text{Tr} \left[ \int_0^\beta d\tau d\tau' \sum_{k,k'} G(\tau, k, \tau', k') \left( 0 \begin{pmatrix} V_k^\dagger & -bt_k^f \end{pmatrix} \right) \delta(k - k') \delta(\tau - \tau') \right] 
= \text{Tr} \left[ h_\beta \sum_k G(k) \begin{pmatrix} 0 & V_k^\dagger \end{pmatrix} \right], \tag{S9}
\]

where in the last step we used that \( G(\tau, k, \tau', k) \) only depends on \( k \) and \( \tau - \tau' \). By setting \( dF/db = 0 \) and \( dF/d\bar{\lambda} = 0 \), we find the two mean-field equations

\[ 0 = bN_s \bar{\lambda} - \sum_k \text{Tr} \left[ \left\langle d_k^d \right\rangle V_k \right] + b \sum_k \text{Tr} \left[ \left\langle f_k^d \right\rangle t_k^f \right], \tag{S10} \]
\[ 1 = b^2 + \frac{1}{N_s} \sum_k \text{Tr} \left[ f_k^d f_k^\dagger \right], \tag{S11} \]

where the last is nothing but the averaged constraint condition, \( N_s \) is the number of sites, and we have used the notation for the propagator,

\[ G(\tau, \tau', k) = \begin{pmatrix} \left\langle d_k^d \right\rangle \left\langle d_k^d \right\rangle & \left\langle f_k^d \right\rangle \left\langle f_k^\dagger \right\rangle \\ \left\langle f_k^d \right\rangle \left\langle f_k^\dagger \right\rangle & \left\langle d_k^d \right\rangle \left\langle f_k^\dagger \right\rangle \end{pmatrix}. \tag{S12} \]

We consider specifically the regime where the number of holes per site is equal to the number of conduction bands \( N_d \). This gives the additional constraint

\[ N_d = \frac{1}{N_s} \sum_k \text{Tr} \left[ f_k^d f_k^\dagger \right] + \frac{1}{N_s} \sum_k \text{Tr} \left[ d_k^d d_k^\dagger \right], \tag{S13} \]

In practice, the use of this constraint may be avoided at low \( T \), by guaranteeing that the chemical potential \( \mu \) is inside the gap.

**Appendix B: Numerical results for the mean-field parameters**

Before we can use these equations to calculate the values of \( b \) and \( \bar{\lambda} \), we need to find an expression for the Green’s functions (the two-point expectation values). For this, we first investigate what happens when the Hamiltonian is diagonal in the \( \Psi_k \) basis \( H = \sum_k \Psi_k^\dagger D \Psi_k \), with \( D \) a diagonal matrix. In that case, we find the well known Dirac distribution,

\[ \left\langle \Psi_k^\dagger \Psi_k \right\rangle = \frac{\text{Tr}(\Psi_k^\dagger \Psi_k e^{-\beta H})}{\text{Tr}(e^{-\beta H})} = \sum_{n_{ik}=0,1} n_{ik} e^{-\beta n_{ik} \epsilon_{ik}} \sum_{n_{ik}=0,1} e^{-\beta n_{ik} \epsilon_{ik}} = \frac{1}{1 + e^{\beta \epsilon_{ik}}}. \]

However, the effective Hamiltonian is generally not diagonal in (pseudo)-spin space, and we need to apply a change of basis. If \( H_k \) is not diagonal in some basis \( C_k \), we can relate this basis to another basis, \( \Psi_k \), in which the Hamiltonian
values of $MG$ where the mean-field equations iteratively using a momentum space grid of evaluate all parts of the mean-field equations, reducing their solution to a numerical problem. We numerically solve the Green’s function from the eigenvalues and eigenvectors of $\sum$ is diagonal, by the unitary matrix of eigenvectors $U$. Furthermore, $k$-space grid used to calculate the solutions for $T/\epsilon_0$ equal to 0, 0.025, 0.049, and 0.074, respectively. Here, a $k$-space of $11^3$ points is used.

is diagonal, by the unitary matrix of eigenvectors $S_k$: $C_k = S_k \Psi_k$. For the elements of $C_k$, this means that $C_{ki} = \sum_{\alpha} S_{i\alpha k} \Psi_{\alpha k}$. Thus, we find that for a non diagonal basis $C_k$,

$$
\langle C_{jk}^\dagger C_{ik} \rangle = \sum_{\alpha \alpha'} \langle S_{j\alpha k}^\dagger \Psi_{\alpha k}^\dagger S_{i\alpha' k} \Psi_{\alpha' k} \rangle = \sum_{\alpha} S_{j\alpha k}^\dagger S_{i\alpha k} \langle \Psi_{\alpha k}^\dagger \Psi_{\alpha k} \rangle = \sum_{\alpha} S_{j\alpha k}^\dagger S_{i\alpha k} \frac{1}{1 + e^{\beta \epsilon_{\alpha k}}},
$$

where we used that $\langle \Psi_{\alpha k}^\dagger \Psi_{\alpha' k} \rangle = \langle \Psi_{\alpha k}^\dagger \Psi_{\alpha k} \rangle \delta_{\alpha, \alpha'}$. Thus, if we have a Bloch Hamiltonian $H_k$, we can now calculate the Green’s function from the eigenvalues and eigenvectors of $H_k$ \cite{S2}. These steps finally allow us to numerically evaluate all parts of the mean-field equations, reducing their solution to a numerical problem. We numerically solve the mean-field equations iteratively using a momentum space grid of $11^3$ points. In each step of the iteration, the values of $\lambda$, $\mu$ and $b$ were adapted accordingly, with respect to the iterative equations,

$$
\mu_{n+1} = MG(\lambda_n, \mu_n, b_n),
$$

$$
b_{n+1} = \sqrt{1 - \frac{1}{N_s} \sum_{k, \alpha} \langle f_{k\alpha} f_{k\alpha} \rangle (\lambda_n, \mu_{n+1}, b_n)},
$$

$$
\lambda_{n+1} = \frac{1}{b_{n+1} N_s} \left( \sum_{k} \text{Tr} \left[ \left( f_k^\dagger c_k \right) (\lambda_n, \mu_{n+1}, b_{n+1}) V_k \right] + b_{n+1} \sum_{k} \text{Tr} \left[ \left( f_k^\dagger f_k \right) (\lambda_n, \mu_{n+1}, b_{n+1}) t_k \right] \right),
$$

(S1)

where $MG$ calculates $\mu_{n+1}$, such that the center of the gap is at the Fermi energy for the system defined by $\bar{\lambda}$, $\mu$, and $b$, and the other equations are derived from the mean-field Eqs. (S10) and (S11).

The results are shown in Fig. S1. Here, we see that if the periodic $k$-space grid used to calculate the solutions is too small, the solution becomes unstable around $\frac{V}{\epsilon_0} = 4.1$. This is the point of the phase transition, where the correlation length diverges. Furthermore, kinks are visible in the $\mu$ solution. This is an artificial effect, caused by the approximation that $\mu$ is in the middle of the gap. Finally, we have that for $\frac{V}{\epsilon_0} > 0.04$, $b$ becomes zero for finite $\frac{V}{\epsilon_0}$ (see inset in fig. S1d). This signals a phase transition from a Kondo insulator to a Kondo liquid phase, in which the mean-field equations no longer hold.
Figure S2. Band structure of the four-band Kondo model for the three topological phases: (a) the weak topological insulator (WTI) phase at $V/\epsilon_0^f = 0.5$, (b) the strong topological Kondo insulator (TKI) at $V/\epsilon_0^f = 2.4$, and (c) the band insulator phase at $V/\epsilon_0^f = 4.3$. Here, green indicates the hybridized spectrum, blue the unhybridized $d$-electron spectrum and yellow the unhybridized $f$-electron spectrum. Figures (d)-(f) are zooming in on figures (a)-(c), respectively.

Appendix C: Topological invariant

The Anderson lattice model is inversion symmetric, and therefore the topological invariant $\tilde{\nu}$ can be calculated using \[ S1 \]

\[
(-1)^{\tilde{\nu}} = \prod_{i} \prod_{m=1}^{N} p_{2m}(\Gamma_i),
\]

where $p_{2m}(\Gamma_i) = \pm 1$ is the parity eigenvalue at the high-symmetry point $\Gamma_i$ of the $2m$’th energy band. Note that $p_{2m} = p_{2m-1}$, as this is a Kramers pair. The product involves all high-symmetry points in the Brillouin zone and the $2N$ occupied bands. If $\tilde{\nu}$ is one, the system is a strong topological Kondo insulator (TKI), and the topological surface states are protected. If $\tilde{\nu}$ is zero, but one of the products involving $\Gamma'_j$ at high symmetry points in the same plane is $-1$ i.e. $\prod_j \prod_{m=1}^{N} p_{2m}(\Gamma'_j) = -1$ the system is a weak topological insulator (WTI). In this case, the corresponding surface states are not protected from disorder. The band structure corresponding to each of the topological phases WTI, TKI and band insulator (BI) of the four band Kondo model is shown in Fig. S2. It is important to note here that the $d$- and $f$-electrons have opposite parity, thus the topological invariant changes when $d$- and $f$-bands are inverted at an odd number of high symmetry points.

Appendix D: Phase transitions and critical exponents

In the low-$k$ limit, near the topological Kondo insulator to band insulator phase transition, we can rewrite Eq. 6, \[ S1 \]

\[
E_{k\pm} = (t - b^2 t_f)k^2 + \delta_\mu \pm \sqrt{\delta_\lambda^2 + (2(b^2 t_f + t)\delta_\lambda + 4bV^2)k^2}. \]

Here, $\delta_\mu = \mu - \mu_c$ and $\delta_\lambda = \bar{\lambda} - \bar{\lambda}_c$, where the subindex $c$ stands for the value of the parameter at the critical point. This results in the zero-$T$ free energy

\[
\mathcal{F} = \int_{k<\Lambda} E_{k\pm} k^2 dk = G_1(V) + \frac{1}{8} \delta_\lambda^4(V) G_2(V)^{-3} \sinh^{-1} \left( \frac{G_2(V)}{|\delta_\lambda(V)|} \right),
\]
where $G_1$ and $G_2$ are smooth functions near the phase transition, assuming the mean field parameters vary smoothly with $V$, and $\Lambda$ is the cutoff enforcing the small-$k$ approximation. By solving the mean-field Eqs. (S10) and (S11) numerically, we find that $\bar{\lambda}$ scales linearly with $V$ near the phase transition (see Fig. S3a, where the red dots denote the numerical solution and the blue line is a linear fit to the numerical data). According to the Ehrenfest classification, the order of the phase transition is determined by the derivative of the free energy that exhibits a discontinuity or a divergence. Thus, since $\delta\bar{\lambda}$ is zero at the critical point, we expect a fourth-order bulk phase transition for this system. Furthermore, we can show that the dispersion of the surface states is linear, see Fig. S3c, leading to a third-order phase transition at the boundary, as derived in the main text.

To determine the critical exponents, we need to determine the dependence of the gap size. In Fig. S3c and Fig. S3d, the linear behavior of the gap size as a function of both $k_x$ and $v$ is shown, also leading to a fourth-order phase transition in the bulk of the system. It should be noted that when calculating the critical exponents, care should be taken to select the right parameter range: as $V_c$ is calculated with numerical precision, $\Delta G(V = V_c, k = 0)$ will only be zero up to the same precision, resulting in a seemingly quadratic band structure for extremely small $k$. In addition, to find a correct numerical solution to the mean-field equations, it is important that the chemical potential remains in the gap. Numerical errors that cause a slight overlap between the Fermi level and the energy bands result in an incorrect $T$ dependence. Moreover, the mean-field equations become unstable around the critical point, requiring larger system sizes as the distance to the critical point decreases.

**Figure S3.** Numerical values to determine the behavior of the mean-field solutions and critical exponents. (a) Numerical mean-field solution for $\bar{\lambda}$ at $T = 0$ in the four-band model. The dots indicate the numerical solutions, whereas the blue line represents a linear fit. (b) Surface state dispersion in the four-band model. The dots indicate the numerical calculations, the lines represent a linear fit to the data, and $a$ is the lattice constant. The dispersion was calculated for $V/\epsilon_f = 3.8$, using a 400-layer system. (c) and (d) Closing of the gap. The dots indicate the calculated gap size $\Delta G$ as a function of (c) the momentum $k_x$ for $k_y = k_z = 0$ and (d) the reduced hybridization $v$. The blue lines indicate a linear fit to the numerical data and $a$ is the lattice constant.

**Appendix E: Ten-band model for SmB$_6$**

The ten-band model for SmB$_6$ described in the main text is based on the minimal model in Ref. [S2]. This model is based on a full seventh nearest neighbor calculation where only the relevant hopping parameters were kept. As
the hybridization is highly relevant in the phase behavior. We have additionally included all first- and second-nearest neighbor hybridization terms. The resulting finite system band structure is shown in Fig. S4.

Figure S4. Finite-system band structure with 40 layers of the minimal model from Ref. [S2], where all first- and second-nearest neighbor hybridization terms are included.

[S1] L. Fu and C. L. Kane, Phys. Rev. B. 76, 045302 (2007)
[S2] P. P. Baruselli and M. Vojta, Phys. Rev. B. 90, 201106 (2014).