1. Introduction

Kondo insulators (KI) are a series of heavy-fermion compounds, in which the hybridization between conducting $d$ electrons and local $f$ moments generates a bulk energy gap at low temperatures [1]. In recent years, the proposal of topologically protected surface states in Kondo insulator SmB$_6$ has been gathering renewed interests [2–11], and the gapless surface states inside the bulk gap have been confirmed...
by spin- and angle-resolved photoemission spectroscopy (SARPES) [12, 13], which can explain the mystery plateau of resistivity at low temperatures.

Theoretically, topological Kondo insulators (TKI) can be described by the topological periodic Anderson model (T-PAM) with a spin–orbit coupled nonlocal hybridization between $d$ and $f$ orbitst [2, 3]. The spin–orbit-coupled nature and odd parity of such hybridization guarantee both time-reversal symmetry (TRS) and space-inversion symmetry of T-PAM, leading to a $Z_2$ topological classification of the insulating phases [2, 14]. According to the relative altitude between $d$ and renormalized $f$ levels at eight time-reversal invariant momenta (TRIM) in 3D Brillouin zone (BZ), insulating states can be classified into strong topological insulator (STI), weak topological insulator (WTI) and non-topological Kondo insulator (nKI) [2], in which STI and WTI exhibit gapless surface Dirac cones driven by band inversions between $d$ and $f$ bands at certain TRIM [3]. Since the effective $f$ level is strongly renormalized from the bare one $\epsilon_f$, the variations of hybridization strength $V$ and $\epsilon_f$ can cause successive topological transitions among STI, WTI and nKI [15], moreover, with different choices of electron-hopping amplitudes (EHA), the topological transition processes are quite distinct [16].

In a Kondo lattice at or near half-filling, antiferromagnetic (AF) order is quite favored in relative weak Kondo interaction region [17, 18], while in ordinary half-filled periodic Anderson model (PAM) with local $d$-$f$ hybridization, it is well-known that a ground-state magnetic transition occurs from AF to paramagnetic (PM) phase by enhanced hybridization, as revealed by numerical simulations and theoretical calculations [19–25]. For a TKI compound SmB$_6$, literature has witnessed an emergence of magnetic order under high pressure [26–33]. Similar to normal Kondo lattice systems, the pressure-induced magnetism in SmB$_6$ may be naturally considered to be AF ordered [34], although no clear experimental evidence is present to date. The topological essence of SmB$_6$ naturally reminds us of the possible non-trivial topology of the induced AF phase. Indeed, in some low-dimensional topological Kondo lattices, AF phases with non-trivial topologies have been verified theoretically [35]. These considerations motivate us to study the transition to AF phases in three-dimensional (3D) TKI, to classify these AF states and search topologically protected AF phase, then further reveal the transition processes among AF states and various PM topological insulating (TI) phases.

In a TI, once AF order sets in, TRS is broken, then the standard $Z_2$ classification is no longer applicable to AF phases. Nevertheless, Mong et al. have pointed out that if there is a translation $\mathbf{\theta}_D$ by lattice vector $\mathbf{D}$ which inverts the AF magnetization at all sites, then such AF state is invariant under a combined operation $S = \Theta \mathbf{\theta}_D$, since time-reversal operation $\Theta$ also inverts the magnetization [36–38], $S$ is antiunitary, and $S^2 = -1$ at four out of the eight high-symmetric points in 3D magnetic Brillouin zone (MBZ), ensuring Kramers degeneracy at these four momenta (KDM) [37]. These properties lead to a new type of $Z_2$ classification of these AF insulating states, in which an antiferromagnetic topological insulating phase (AFTI) arises by adding weak staggered magnetization into STI phase while maintaining an insulating bulk gap [36]. Since the proposal, a few AFTI phases have been suggested in some non-interacting models in which the AF orders are added artificially by Zeeman terms [39–42], or in low-dimensional models with electron correlation [43]. For a 3D AFTI candidate GdBInP [44], an AF phase has been suggested [45], but it is not a full-gapped insulating state. The explorations of AFTI in real systems, particularly in 3D strong-correlated systems in which AF orders can arise naturally, are still lacking.

The magnetism observed in pressured SmB$_6$ [26–33] sheds light on possible emergence of AFTI in 3D TKI. Recently, Peters et al. reported their study on bulk and surface magnetism in TKI by dynamic mean-field theory (DMFT), but the topologies of the magnetic states were not deduced explicitly [46]; Chang et al. proposed an interesting topological A-AF phase which is staggered along single axis in pressured SmB$_6$ by first-principle calculations [34], in which the strong correlation was not considered explicitly. Moreover, the AF phases suggested by Chang et al. are actually bulk-conducting states, essentially different from the topologically protected insulating AFTI state which requires a full bulk gap. Therefore, the possible AFTI in 3D TKI still lacks investigation.

As mentioned above, with different model parameters, distinct TI phases emerge in TKI in weak hybridization region [16], in which magnetic transitions may take place to induce AF states. Consequently, once TKI undergoes magnetic transitions, the induced AF orders grow from distinct TI phases, depending on the parameter regions, leading to topologically distinguishable AF phases, i.e. an AF order growing from STI leads to an AFTI state [36], if AF order grows from WTI or nKI, a non-topological AF insulator (nAFI) arises. Furthermore, if the magnetic transition occurs near the phase boundary between STI and WTI, varying the model parameters in a special way may induce a topological transition between AFTI and nAFI Therefore, in TKI, the existence of AFTI and nAFI, the topological-classification formula for them, and possible topological transition between AFTI and nAFI highly deserve investigations in a self-consistently manner from the original T-PAM model for TKI.

In this work, we verify the existence of AFTI in 3D TKI for the first time. We explore the transition to insulating AF states in 3D TKI, and present a $Z_2$ topological formula to classification these AF states. In some parameter region, we find a novel AFTI with topologically-protected gapless surface Dirac cones, exhibiting helical spin texture on the Fermi rings. We also obtain a topological transition from AFTI to nAFI. To our knowledge, the novel AFTI, and the topological transition between AFTI and nAFI in 3D TKI are reported for the first time by our work.

This paper is arranged as follows. In section 2, we adopt a mean-field Kotliar–Ruckenstein (K–R) slave-boson representation [23–25, 47] for T-PAM to describe the possible AF phases in 3D TKI in general parameter region. The AF configuration studied in this paper is staggered by adjacent sites, and meets the requirement of $S$-invariance. In section 3, we study the topological transitions among STI, WTI and nKI, and select two typical transition processes by choosing two sets of EHA, which are appropriate for studying AF transitions and will lead to topologically distinguishable AF phases. In section 4, by locating the four KDM, we derive the expression for $Z_2$ index in AF states, which is determined by the product
of parities at these KDM. In section 5, we perform a saddle-
point solution for AF phase to derive the evolution of stagger-
ged magnetization and determine the magnetic transition points on $\epsilon_f - V$ plane. By calculating the $Z_2$ index, we find that the two sets of EHA in section 3 lead to two topologically distinguishable AF phases, one is AFTI evolving from STI, and the other is nAFTI evolving from WTI. By diagonalizing parallel slabs with (001) surface, we observe the expected gapless surface Dirac cones with helical spin texture in AFTI, confirming its non-trivial topology. In section 6, we demonstrate a topological transition between AFTI and nAFTI driving by closing and reopening of bulk gap, and an insulator-metal transition inside the AF phases, then summarize the phase transitions in a global phase diagram.

Our work provides deeper understanding of AFTI in 3D TKI, and may account for the magnetism observed in pressurized SmB$_6$. Our algebra also helps to investigate richer AFTI phases in heavy-fermion systems, as well as in other strongly-correlated systems.

## 2. K–R representation for AF states

We consider a simplified model for 3D TKI: half-filled spin-
1/2 T-PAM with spin–orbit coupled hybridization between neighboring $d$ and $f$ electrons in cubic lattice, with lattice constant $a$ and $N$ sites [48]:

$$
\mathcal{H} = \sum_{i,j,\sigma} (t_{i,\sigma}' d_{i,j,\sigma}^\dagger d_{j,i,\sigma} + t_{j,\sigma}' f_{i,j,\sigma}^\dagger f_{j,i,\sigma}) + \epsilon_f \sum_{i,\sigma} f_{i,i,\sigma}^\dagger f_{i,i,\sigma}
+ U \sum_i n_{i,\uparrow} n_{i,\downarrow} - iV \sum_{i,\alpha,\beta} \bar{l} \cdot \sigma_{\alpha,\beta} d_{i,\alpha,\sigma}^\dagger d_{i+\bar{l},\beta,\sigma} + h.c.
- \mu \sum_{i,\sigma} (d_{i,i,\sigma}^\dagger d_{i,i,\sigma} + f_{i,i,\sigma}^\dagger f_{i,i,\sigma}),
$$

(1)

where $d_{i,\sigma}^\dagger$ and $f_{i,\sigma}^\dagger$ create a $d$ or $f$ electron at site $i$, with spin $\sigma = \pm 1$ representing spin up and down, respectively. The electron hopping amplitudes (EHA) include nearest-neighbor (NN) hopping, next-nearest-neighbor (NNNN) hopping, and next-next-nearest-neighbor (NNNNN) hopping for both $d$ and $f$ electrons, and we set $t_{i,j}' = -t_d$, $t_{j,i}' = -t_f$ for NN, $t_{i,j}'' = -t_d^\prime$, $t_{j,i}'' = -t_f^\prime$ for NNN, and $t_{i,j}''' = -t_d^\prime$, $t_{j,i}''' = -t_f^\prime$ for NNNN. In what follows, $t_d = 1$ is chosen as energy unit, and we consider $t_f/t_d < 0$ and keep $t_d''/t_d'\approx$ close to $t_d'/t_d$, and $t_f''/t_f'\approx$ close to $t_f'/t_f$ to get a full bulk gap [16, 48, 49], since we focus on the insulating phases at half-filling. $\mu$ denotes the chemical potential, which fits the total electron number per site to $n = 2$. $\epsilon_f$ is the energy level of $f$ orbit, $U$ is the on-site Coulomb repulsion between $f$ electrons. $\bar{L}$ are the six coordination vectors in cubic lattice, $\sigma$ stands for the Pauli matrix. In TKI, the opposite parities of $d$ and $f$ orbits cause the hybridization to acquire a non-local spin-dependent form, which is explicitly written as [48]

$$
\mathcal{H}_{\text{eff}} = -iV \sum_{i,j,\sigma,\tau} (\pm d_{i,\sigma}^\dagger Z_{i+\bar{j},\tau,\sigma} + \sigma d_{i,\sigma}^\dagger Z_{i+\bar{j},\tau,\sigma} + \pm \sigma d_{i,\sigma}^\dagger Z_{i+\bar{j},\tau,\sigma}) + h.c.,
$$

(2)

with $\sigma = -\sigma$ and $a_1, a_2, a_3$ are three lattice basic vectors along $x$, $y$, $z$ axis, respectively. $\mathcal{H}_{\text{eff}}$ can be written in momentum space by [48]

$$
\mathcal{H}_{\text{eff}} = V \sum_{k,\alpha,\beta} S_k \cdot \sigma_{\alpha,\beta} d_{k,\alpha}^\dagger f_{k,\beta} + h.c.,
$$

(3)

where the vector $S_k = (\sin k_x, \sin k_y, \sin k_z)$, with $k_x = k \cdot a_1$, $k_y = k \cdot a_2$, $k_z = k \cdot a_3$. Note that the particle-hole symmetry in T-PAM (equation (1)) has been broken even at half-filling, so the chemical potential term should be included in any case. In this paper, we focus on the large-$U$ limit and consider variable $\epsilon_f$, $V$ and EHA, which are appropriate to describe TKI compound SmB$_6$ with mixed valence.

It is well known that a half-filled PAM is usually AF-ordered in weak hybridization region [19–25], besides, in some topological Kondo lattices, AF orders are also favored [34, 35]. For pressurized SmB$_6$, an interesting topological A-AF state which is staggered along single axis has been suggested by first-principle calculations [34], unfortunately, such A-AF configuration is found to be unstable within our method, which may be ascribed to the large-$U$ limit we apply, while the Coulomb correlation was not considered explicitly in [34]. Under this context, we consider the more common AF state which is staggered between adjacent sites, and other AF configurations including A-AF state will not be considered explicitly, but we will still provide a brief topological description for these states.

The slave-boson technique has been widely used to study the TI phases and topological transitions in TKI [4, 9, 15, 16, 48], besides, Kotliar–Ruckenstein (K–R) slave-boson method has been applied successfully to include magnetic orders in studying the Hubbard model and PAM [23–25, 47]. In order to treat both PM and AF phases in TKI, we adopt the K–R slave-boson technique. Firstly the Hilbert space of $f$-electrons is decomposed into single occupancy, double occupancy and empty state, with two relations $\sum_\sigma P_{i,\sigma}^1 P_{i',\sigma}^1 + D_{i,i'}^1 + e_i^1 e_{i'}^1 = 1$ and $f_{i,\sigma}^1 f_{i',\sigma}^1 = P_{i,\sigma}^1 P_{i',\sigma}^1 + D_{i,i'}^1$, which are imposed by two Lagrange terms with Lagrange multipliers $\lambda_{1,\sigma}^1$ and $\lambda_{2,\sigma}^1$, respectively. In order to reproduce correct $f$-electron occupancy, each $f$-operator $f_{i,\sigma}^1$ ($f_{i,\sigma}^2$) in $d$-$f$ hybridization and $f$-$f$ hopping terms is multiplied by a renormalization factor $Z_{i,\sigma}$ ($Z_{i,\sigma}^\ast$).

By the definitions $P_{i,\sigma}^2 + P_{i',\sigma}^2 + 2D_{i,i'}^2 = n_{i,\sigma}^2$, $P_{i,\sigma}^2 - P_{i',\sigma}^2 = m_{i,\sigma}^2$, $(\lambda_{1,\sigma}^1 + \lambda_{2,\sigma}^1)/2 = \eta_{\sigma}$ and $(\lambda_{1,\sigma}^1 - \lambda_{2,\sigma}^1)/2 = -h_{\sigma}$, where $n_{i,\sigma}^2$ is $f$-electron number, $m_{i,\sigma}^2$ and $h_{\sigma}$ are staggered order parameters at site $i$, and $\eta_{\sigma}$ renormalizes the $f$ level, the Hamiltonian equation (1) is then rewritten as

$$
\mathcal{H} = \sum_i (h_{\sigma} m_{i,\sigma}^2 - \eta_{\sigma} n_{i,\sigma}^2) + \sum_{i,\sigma} (\epsilon_k + \mu) d_{i,\sigma}^\dagger d_{i,\sigma}
+ \sum_{i,\sigma} (\epsilon_f + \sigma h_{\sigma}) d_{i,\sigma}^\dagger f_{i,\sigma} + \sum_{i,\sigma} t_{i,j}^\prime Z_{\sigma}^\ast Z_{\sigma} d_{i,\sigma}^\dagger f_{j,\sigma}
- \frac{i}{2} V \sum_{i,\sigma,\tau,\alpha} (\pm d_{i,\sigma}^\dagger Z_{i+\bar{j},\tau,\alpha} + \sigma d_{i,\sigma}^\dagger Z_{i+\bar{j},\tau,\alpha} + \pm \sigma d_{i,\sigma}^\dagger Z_{i+\bar{j},\tau,\alpha}) + h.c.,
$$

(4)

in which we have set $U \rightarrow \infty$ then double occupancy is excluded, and $\lambda_{1,\sigma}^1$ term vanishes through mean-field
approximation. For our considered AF phases, we decompose the cubic lattice into two sublattices A and B (both are face-centered cubic lattices), and by using the mean-field approximation $n_i^f = n_i$, $m_i^f = (-1)^f m_i$, $h_i = (-1)^f h_i$, we have $Z_{A1} = Z_{B1} = Z_1$, and $Z_{A4} = Z_{B4} = Z_2$, with

$$Z_1 = \sqrt{\frac{2(1 - n_f)}{2 - n_f - m_f}}, \quad Z_2 = \sqrt{\frac{2(1 - n_f)}{2 - n_f + m_f}}.$$  

Through such mean-field treatment, we obtain the effective Hamiltonian in momentum space with a matrix form

$$\mathcal{H} = N(hm_f - \eta n_f) + \sum_{k \in \text{MBZ}} \Psi_k^\dagger H_k \Psi_k,$$  

where the summation of $k$ is restricted in the magnetic Brillouin zone (MBZ). A eight-component operator is defined as $\Psi_k = (d_{k\uparrow}, d_{k\downarrow}, d_{k\uparrow}, d_{k\downarrow})^T$, and the Hamiltonian matrix is given by

$$H_k = \begin{pmatrix} H_k^f & V_k^f \\ V_k^+ & H_k^\dagger \end{pmatrix},$$  

with

$$H_k^f = \begin{pmatrix} (t_f \gamma_k - \mu)I_2 & u_k^f I_2 \\ u_k^f I_2 & (t_f \gamma_k - \mu)I_2 \end{pmatrix},$$  

$$V_k = \begin{pmatrix} 0 & 0 & Z_2 \sin k_x & Z_2 \Gamma_k \\ 0 & Z_2 \Gamma_k & -Z_2 \sin k_x & 0 \\ Z_2 \Gamma_k & -Z_2 \sin k_x & 0 & 0 \\ Z_2 \sin k_x & Z_2 \Gamma_k & 0 & 0 \end{pmatrix},$$  

and

$$H_k^\dagger = \begin{pmatrix} e_{1k} & 0 & Z_1 Z_2 u_k^f & 0 \\ 0 & e_{2k} & 0 & Z_1 Z_2 u_k^f \\ Z_2 Z_2 u_k^f & 0 & e_{2k} & 0 \\ 0 & Z_1 Z_2 u_k^f & 0 & e_{1k} \end{pmatrix}.$$  

where $I_2$ is a two-order unit matrix, $\Gamma_k = \sin k_x - i \sin k_y$, $\gamma_k = -4(\cos k_x \cos k_y + \cos k_x \cos k_y + \cos k_x \cos k_y)$, $e_{1k} = \epsilon_f + \eta - h + \epsilon_f \Gamma_k$, $e_{2k} = \epsilon_f + \eta - h + \epsilon_f \Gamma_k$, $u_k^f = t_f^{(f)} \lambda_k + t_f^{(f)} g_k$ with $\lambda_k = -2(\cos k_x + \cos k_y + \cos k_x)$ and $g_k = -8 \cos k_x \cos k_y \cos k_y$. In general case, the Hamiltonian matrix (7) should be diagonalized numerically to obtain the four branches of dispersions $E_k^{(i)} (i = 1, 2, 3, 4)$ which are all two-fold degenerate. The mean-field parameters $n_f, m_f, h, \eta$ and the chemical potential $\mu$ in AF phase should be determined by saddle-point equations self-consistently, which are given in Appendix A, and the numerical solution of these equations will be performed later in section 5. With the calculated parameters, we can compute the ground-state energy of AF phase by

$$E_{gs}^{AF} = N(hm_f - \eta n_f + \mu n_f) + \sum_{k} \sum_{i=1,4} \theta(-E_k^{(i)})E_k^{(i)}.$$  

Table 1. Two sets of EHA used in this work

| $t_d$ | $t'_d$ | $t'_f$ | $t_f$ | $t'_f$ | $t''_f$ |
|------|-------|-------|------|-------|--------|
| EHA(I) | 1     | 0.15  | 0    | -0.2  | -0.02  |
| EHA(II)| -0.375 | -0.375 | -0.2 | 0.09  | 0.09   |

*In section 6, we also use other EHA.

3. Topological transitions between topological insulating phases

Before studying the magnetic transitions in TKI, we consider the topological transitions among various TI phases, then draw the topological phase diagrams, in order to select appropriate model parameters to further discuss magnetic transitions and AF phases. The K–R slave boson scheme for PM phases follows from equation (4), in which $m_f$ and $h$ should be eliminated, to arrive at the mean-field Hamiltonian in large-$U$ limit

$$\mathcal{H} = N(\eta n_f) + \sum_{k} \Psi_k^\dagger H_k \Psi_k,$$  

with $\Psi_k = (d_{k\uparrow}, d_{k\downarrow}, f_{k\uparrow}, f_{k\downarrow})^T$ and

$$H_k = \begin{pmatrix} (\epsilon_f - \mu)I_2 & V_k \\ V_k^+ & (\epsilon'_f - \mu)I_2 \end{pmatrix},$$  

in which the renormalized dispersion $\epsilon'_k = \epsilon_f + \eta + Z^2 \tilde{\epsilon}'_k$, the renormalization factor $Z = \sqrt{2(1 - n_f)/(2 - n_f)}$, the effective hybridization

$$V_k = VZ \begin{pmatrix} \sin k_x & \sin k_y - i \sin k_y \\ \sin k_x + i \sin k_y & -\sin k_y \end{pmatrix},$$  

and tight-binding dispersions $\epsilon_{i\pm} = t_{i\pm} \lambda_k + t_{i\pm} g_k$. The ground-state energy is then $E_{gs}^{PM} = N(\eta n_f + \mu n_f) + 2 \sum_{k, \pm} \theta(-E_k^\pm)E_k^\pm$, with quasi-particle dispersions

$$E_k^\pm = \frac{1}{2} \left[ (\epsilon'_k + \tilde{\epsilon}'_k)^2 + 4V^2Z^2 \sin'^2 k \right] - \mu.$$  

which are both two-fold degenerate. $n_f, \mu$ and $\gamma$ are computed through saddle-point solution of $E_{gs}^{PM}$, see appendix B.

The spin–orbit-coupled nature of effective hybridization $V_k$ guarantees TRS of Hamiltonian equation (12): $[\Theta, \mathcal{H}] = 0$ or equivalently $\Theta H_k \Theta^{-1} = H_k$. and the existence of inversion center ensures an additional space-inversion symmetry: $[\mathcal{P}, \mathcal{H}] = 0$ or $\mathcal{P} H_k \mathcal{P}^{-1} = H_k$. In which time-reversal operator $\Theta = i(I_2 \otimes \sigma_x)K (K$ is complex conjugation) and the parity matrix $\mathcal{P} = \sigma_z \otimes I_2$ in present basis. $\Theta$ is anti-unitary with $\Theta^2 = -1$, leading to Kramers degeneracy at eight TRIM in 3D BZ, resulting in $Z_2$ classification of the insulating states. The $Z_2$ invariants are calculated by parities of the occupied states at eight TRIM $k_m$ in the BZ [2, 14]. We use standard notation to denote $k_m$: $\Gamma$ for $(0, 0, 0)$, $X$ for $(\pi, 0, 0)$, $(0, 0, \pi)$, $M$ for $(\pi, \pi, 0)$, $(\pi, 0, \pi)$, $(0, \pi, \pi)$, and $R$ for $(\pi, \pi, \pi)$. For the 2D BZ of (001) surface, on which the surface states will be considered, there are four TRIM $k_p$, denoted by $\Gamma = (0, 0, 0)$, $X = (\pi, 0, 0)$, $(0, \pi, 0)$, and $M = (\pi, \pi, \pi)$. Due to its
odd-parity, the hybridization vanishes at TRIM, therefore at \( \mathbf{k}_m \), the occupied dispersion \( E\delta = \min\left(\epsilon_{\delta}^d, \epsilon_{\delta}^{\tilde{f}}\right) - \mu \) (see equation (15)). Since \( d \) (\( f \)) orbit has even (odd) parity, the parity at \( \mathbf{k}_m \) is expressed by (each pair of Kramers-degenerate states at \( \mathbf{k}_m \) is calculated once) \( \delta_m = -\text{sgn}(\epsilon_{\mathbf{k}_m}^d - \epsilon_{\mathbf{k}_m}^{\tilde{f}}) \) \cite{14, 15}, then the strong topological index \( \nu_0 \) is related to the product of all eight \( \delta_m \) by \((-1)^{\nu_0} = \prod \delta_m\), while the weak topological index \( \nu_f \) \((j = 1, 2, 3)\) is related to the product of four \( \delta_m \) on corresponding high-symmetry plane: \((-1)^{\nu_f} = \prod_{\mathbf{k}_m \in \mathcal{P}} \delta_m\), in which \( P_1, P_2, P_3 \) denote \( k_x = 0, k_y = 0, k_z = 0 \) planes, respectively. \( \nu_0 = 1 \) corresponds to a STI with odd number of surface Dirac cones, while \( \nu_0 = 0 \) and \( \nu_f = 1 \) indicate a WTI with even number of surface Dirac cones \cite{3}.

We choose two sets of EHA showing in table 1 to depict the topological transitions as functions of bare \( f \) level \( \epsilon_f \) and hybridization strength \( V \), and these two sets of EHA are denoted by EHA(I) and EHA(II) in the following, respectively. The reason to choose positive (negative) \( \epsilon_f \) in EHA(I) (EHA(II)) is that with physical \( \epsilon_f \) and \( V \) (e.g. \( \epsilon_f = -2 \) and \( V = 1 \)), a small positive \( \epsilon_f \) leads to a WTI phase, while \( \epsilon_f < -0.3 \) usually leads to a STI phase. Moreover, in EHA(I), for simplicity, we choose \( \epsilon_f' = \epsilon_f'' = 0 \), since small \( \epsilon_f' \) and \( \epsilon_f'' \) do not shift the topology. Actually, if \( \epsilon_f \) varies continuously (e.g. from \(-t_d\) to \( t_d\)), all possible TI phases in TKI can be induced on \( V - t_d \) or \( \epsilon_f - t_d \) planes \cite{16}. Since our work focuses on the AF phases in TKI, we select proper hopping amplitudes, and the PM phases will not be investigated deeply. We will show later that EHA(I) and EHA(II) will induce two topologically-distinct AF phases.

In figure 1(a), we display our numerical solutions of \( d \) dispersion \( \epsilon_{\delta}^d \) and renormalized \( f \) dispersion \( \epsilon_{\delta}^{\tilde{f}} \) at eight TRIM \( \mathbf{k}_m \) versus (a) bare \( f \)-level \( \epsilon_f \) or (c) hybridization strength \( V \). Model parameters are \( V = 3 \) with EHA(I) for (a), and \( \epsilon_f = -2 \) with EHA(II) for (c), respectively. In (a) and (c), the flat lines denote \( \epsilon_{\delta}^{\tilde{f}} \), while the curves show \( \epsilon_{\delta}^d \). The classification of TI phases is governed by \( Z_2 \) invariants, see the text. (b) and (d): corresponding bulk gap evolutions in (a) and (c), respectively. The reason to choose positive (negative) \( \epsilon_f \) and \( V \) is that with physical \( \epsilon_f \) and \( V \) (e.g. \( \epsilon_f = -2 \) and \( V = 1 \)), a small positive \( \epsilon_f \) leads to a WTI phase, while \( \epsilon_f < -0.3 \) usually leads to a STI phase.

Figure 1. \( d \) dispersion \( \epsilon_{\delta}^d \) and renormalized \( f \) dispersion \( \epsilon_{\delta}^{\tilde{f}} \) at TRIM \( \mathbf{k}_m \) versus (a) bare \( f \)-level \( \epsilon_f \) or (c) hybridization strength \( V \). Model parameters are \( V = 3 \) with EHA(I) for (a), and \( \epsilon_f = -2 \) with EHA(II) for (c), respectively. In (a) and (c), the flat lines denote \( \epsilon_{\delta}^{\tilde{f}} \), while the curves show \( \epsilon_{\delta}^d \). The classification of TI phases is governed by \( Z_2 \) invariants, see the text. (b) and (d): corresponding bulk gap evolutions in (a) and (c), respectively. The reason to choose positive (negative) \( \epsilon_f \) and \( V \) is that with physical \( \epsilon_f \) and \( V \) (e.g. \( \epsilon_f = -2 \) and \( V = 1 \)), a small positive \( \epsilon_f \) leads to a WTI phase, while \( \epsilon_f < -0.3 \) usually leads to a STI phase.
we consider (0 0 1) surface, the Dirac points locate at certain TRIM \( p_m \) in 2D BZ, with \((p_m, 0)\) and \((p_m, \pi)\) having opposite parities [14]. From figure 2(b) with EHA(I), on can see that the parity \( \delta_m \) changes sign between \((\pi, \pi, \pi)\) and \((\pi, \pi, 0)\), implying a band inversion at \( R \), inducing a single Dirac cone at \((\pi, \pi)\), and this phase is denoted by STI\( \bar{M} \) thereafter. For WTI with EHA(I) in figure 2(a), through similar analysis, we expect two Dirac cones at \((\pi, 0)\) and \((0, \pi)\), then this phase is denoted by WTI\( \bar{X} \). Besides STI\( \bar{M} \) with single Dirac cone, in the case of EHA(II), we find a STI\( \bar{\Gamma}\bar{X} \) phase with band inversions at three \( X \) points (figure 2(c)), leading to three Dirac cones, one at \( \bar{\Gamma} \), the other two at \( \bar{X} \), qualitatively coinciding with the surface states in SmB\(_6\) [12, 13, 50]. For nKI with no band-inversion (figure 2(d)), we expect no surface Dirac modes.

In order to verify the surface states in these TI phases, we compute the dispersions on (001) surface. We simulate the cubic lattice with (001) surface by 40 slabs perpendicular to \( z \) axis. With open boundary condition, we write the effective Hamiltonian in \( k_x - k_y \) space, then obtain the mean-field parameters and chemical potential self-consistently through saddle-point solution, and further diagonalize the Hamiltonian matrix to draw the bulk and surface spectrums. The surface dispersions are displayed in figure 3 by red solid lines inside the bulk gap, and the locations of Dirac cones confirm above analysis. At half-filling, the Dirac points in WTI\( \bar{X} \) and STI\( \bar{M} \) all cross the Fermi level (figures 3(a) and (b)), while in STI\( \bar{\Gamma}\bar{X} \) (figure 3(c)), the Dirac cones form small Fermi rings around \( \bar{\Gamma} \) and \( \bar{X} \), and the spin texture on these Fermi rings are obtained by calculating spin expectation values, shown in figure 9(b). The spin texture shows a helical structure and indicates strong spin-momentum locking in the surface states and reflects the topological nature of STI\( \bar{\Gamma}\bar{X} \). Furthermore, In STI\( \bar{\Gamma}\bar{X} \) phase, the size of Fermi rings can be enlarged by the difference between \( \eta_f/\tau_f \) and \( \eta_f/\tau_f \). The surface states of STI\( \bar{\Gamma}\bar{X} \) we demonstrated are in qualitatively agreement with the surface states of SmB\(_6\) derived by previous theoretical calculations [50–52].
Evolution of TI phases with $V$ and $\epsilon_f$ are summarized in figures S(a) and (b), with EHA(I) and EHA(II), respectively, in which the topological transitions are labeled by dashed lines. Here we should point out that the topological phase boundaries among STI, WTI and nKTI through our K-R solutions are very close to Coleman’s slase-boson solutions \[15, 16\], furthermore, the K–R method has the advantage to include magnetic order conveniently.

In T-PAM, AF order should emerge in the region $\epsilon_f < 0$ and weak $V$, thus, once AF order arises in the two phase diagrams in figure 5, it should evolve from WTI phase and STI$_{cK}$, respectively. Therefore, EHA(I) and EHA(II) may induce topologically distinct AF states, which will be verified in section 5.

4. $\mathcal{Z}_2$ invariant of AF states in 3D TKI

Before studying the magnetic transitions in TKI self-consistently, we should derive the expression of topological invariants for these expected AF insulating states by analysing the intrinsic symmetry of the AF Hamiltonian (equation (6)). Firstly, TRS is broken in AF states, because TRS operation $\Theta$ inverts the magnetization at all sites. Using $\Theta = i\Gamma_2 \otimes \sigma_y K$ in present basis (see equation (6)), where $I_k$ denotes $4 \times 4$ unit matrix and $K$ is complex conjugation, TRS-breaking in AF phase is manifested by $\Theta H_\kappa \Theta^{-1} \neq H_{-\kappa}$. Secondly, space inversion symmetry is preserved in our AF configuration due to existence of inversion center in the middle of a NNN bond: $\mathcal{P} H_\kappa \mathcal{P}^{-1} = H_{-\kappa}$, where the parity matrix is given by $\mathcal{P} = \sigma_z \otimes I_4$. Breaking of TRS prevents straightforward application of standard $\mathcal{Z}_2$ topological classification to AF states, so we should find alternative symmetric operation isomorphic to $\Theta$ in AF states.

Since a translation $T_0$ by a sublattice vector plus a basic vector of cubic lattice $D = R^* + \mathbf{a}_i$ ($i = 1, 2, 3$) inverts the magnetizations at all sites of our AF is staggered between all adjacent sites, the combined operation $S = \Theta T_0 \Theta^{-1}$ recovers the AF configuration, thus the AF states preserve the $S$-symmetry. The translation operation causes an interchange between two sublattices, so the corresponding operator is $T_D(k) = e^{ikD}I_2 \otimes (\sigma_z \otimes I_2)$. It is easy to check the $S$-symmetry of AF Hamiltonian by $S_k H_{\kappa} S^{-1}_k = H_{-\kappa}$, with $S_k = \Theta T_D(k) = e^{-ikD}I_2 \otimes (\sigma_z \otimes \sigma_y) K$. Secondly, $S_k$ is antiunitary because $T_D(k)$ is unitary, and $S^2 = S_k S_{-k} = e^{-2iD k}$. Therefore, if some of the eight high-symmetry points $k_{m0}$ in MBZ satisfy $e^{-2iD k} = 1$, Kramers degeneracy does exist at these points. Due to the antiunitary nature and squaring to minus of $S$ at these Kramers degenerate momenta (KDM) $k_{m0}$, the topology of AF states falls into $\mathcal{Z}_2$ topological class, following directly the $\mathcal{Z}_2$ algebra of TI with inverse symmetry \[14, 36, 37\]. In order to derive the explicit expression of $\mathcal{Z}_2$ invariant for AF states, we should first determine the KDM $k_{m0}$.

The AF sublattice is face-centered cubic lattice, and its basic vectors $\mathbf{a}_i$ and reciprocal basic vectors $\mathbf{b}_i'$ are expressed by unit vectors $\mathbf{x}, \mathbf{y}, \mathbf{z}$ through

\[
\mathbf{a}_1' = a(x + y) \quad \mathbf{b}_1' = \frac{\pi}{a} (x + y - z) \\
\mathbf{a}_2' = a(y + z) \quad \mathbf{b}_2' = \frac{\pi}{a} (-x + y + z) \\
\mathbf{a}_3' = a(x + z) \quad \mathbf{b}_3' = \frac{\pi}{a} (-x + y - z)
\]

satisfying $\mathbf{a}_i' \cdot \mathbf{b}_j' = 2\pi \eta_{ij}$. The eight high-symmetry points in MBZ are represented by

\[
k_{m0} = \frac{1}{2} (m_1 \mathbf{a}_1' + m_2 \mathbf{a}_2' + m_3 \mathbf{b}_3'),
\]

in which the subscript $m$ represents a combination of $m_i$ ($i = 1, 2, 3$), with $m_i$ either 1 or 0. Using the translation vector $D = n_1 \mathbf{a}_1' + n_2 \mathbf{a}_2' + n_3 \mathbf{a}_3' + n_4 (n_1, n_2, n_3)$ are integer numbers, we have

\[
2k_{m0} \cdot D = 2\pi \sum_{i=1,2,3} m_i n_i + \pi (m_1 - m_2 + m_3). 
\]

To satisfy $e^{-2iD k} = 1$, requires $(m_1 - m_2 + m_3)$ is even, corresponding to four sets of $(m_1, m_2, m_3) = (0, 0, 0), (1, 1, 1), (0, 1, 0)$ and $(1, 1, 0)$, leading to four KDM: $\Gamma = (0, 0, 0)$ and three X points $(\pi, 0, 0), (0, \pi, 0)$, $(0, 0, \pi)$, which are just four out of eight TRIM in PM phases. The other four high-symmetry points in MBZ are not KDM thus are irrelevant to determine the topological invariant.

At four KDM $k_{m0}$, $H_{-k_{m0}} = H_{k_{m0}}$, the inverse symmetry ensures the commutation relation $[H_{k_{m0}}, \mathcal{P}] = 0$, hence the eigenstates at KDM are also parity eigenstates with parities $\pm 1$. The $S$ and $\mathcal{P}$ symmetries lead to a new topological classification of AF states by the $\mathcal{Z}_2$ invariant \[36, 37\], determined by the quantities $\delta_{m0}$ at four KDM $k_{m0}$, which are calculated by the parities at $k_{m0}$ through

\[
\delta_{m0} = \prod_{i} \xi_i (k_{m0}').
\]

where $\xi_i (k_{m0}')$ is the parity of the occupied state $i$ at $k_{m0}'$, and each Kramers pair is multiplied only once in $\delta_{m0}$. Similar to the PM phases in TKI, effective hybridization in AF states also vanishes at KDM, then the AF dispersions $E^{(i)}_{k_{m0}'}$ equal either $\epsilon_{k_{m0}'}^e$ or $\epsilon_{k_{m0}'}^\xi$, so the parity is determined by

\[
\xi_i (k_{m0}') = \begin{cases} 
1, & \text{if } E^{(i)}_{k_{m0}'} = \epsilon_{k_{m0}'}^e \\
-1, & \text{if } E^{(i)}_{k_{m0}'} = \epsilon_{k_{m0}'}^\xi.
\end{cases}
\]

The $\mathcal{Z}_2$ invariant $\nu'$ in AF state is then defined by

\[
(\neg)^{\nu'} = \prod_{k_{m0} \in \text{KDM}} \delta_{m0}'.
\]

$\nu'$ is the only topological index in AF states, and it is strongly related to the strong topological index $\nu_0$ in PM TI phases. Near the AF transition point, an infinitesimal AF order arises, then the 3D BZ is folded into MBZ, and the eight TRIM in PM phases are also folded into four KDM in AF phases, explicitly, $R$ and three $M$ are folded into $\Gamma$ and three $X$ points,
respectively. In addition, the spectrums are also folded, leading to two occupied dispersions under Fermi level, then the quantity $\delta_m$ at a KDM $k_{m}$ is essential the product of two $\delta_m$ of two corresponding TRIM which are folded into $k_{m}$, therefore the product of parities at four KDM in AF state equals the product of parities at all eight TRIM in PM phase, in this sense, near the magnetic boundaries, $\nu'$ of AF phase is equivalent to strong topological index $\nu_0$ of PM phase from which AF order grows. Then we can draw to a conclusion that an AF order growing from STI (by reducing $V$, etc) leads to an AFTI with $\nu' = 1$; if AF order is induced from WTI or nKI, a nAFI arises with $\nu' = 0$, which helps us to search AF states with different topologies. When leaving the magnetic boundaries, AF magnetization increases, then $\nu'$ should be calculated by equation (21), and it may be shifted by varying model parameters to arouse a topological transition between AF states, which is to be discussed in the following sections.

The topologies of AF states will be reflected by the surface states. On AF-ordered (001) surface, the $\mathcal{S}$ symmetry is conserved, with vector $\mathbf{D}$ parallel to the surface, then the surface MBZ has two KDM: $\Gamma = (0,0)$ and $X = (0,\pi)$. As AF vector $\mathbf{Q} = (\pi,\pi)$ on this surface, $M = (\pi,\pi)$ is equivalent to $\Gamma$ due to folding of 2D BZ, and another $X$ point $(\pi,0)$ is equivalent to $(0,\pi)$, therefore the four TRIM $(\Gamma, M$ and two $X$) in surface BZ of PM phases now become $\mathcal{S}$-invariant momenta, and they are KDM which may support gapless Dirac cones [37]. Analogous to STI, on the AF-ordered surfaces in AFTI, on which $\mathcal{S}$-symmetry is preserved, there are odd number of gapless Dirac cones at certain KDM which are robust against $\mathcal{S}$-preserving perturbations. We remind that the topological classification requires insulating AF states with full bulk gap [36, 37], otherwise the topological argument will be meaningless.

5. Magnetic transitions, $\mathbb{Z}_2$ classification of AF phases, and the surface states

Based on the topological phase diagrams of TI phases in figure 5, we now turn to the magnetic transitions in TKI. We perform a saddle point solution for the ground-state energy of AF state (equation (11)) to determine the mean-field parameters $n_f, m_f, h, \eta$ and the chemical potential $\mu$, and obtain the bulk dispersions by diagonalizing the Hamiltonian matrix (equation (7)), then further calculate $\nu'$ by equation (21) to classify the solved AF phases.

In figures 4(a) and (b), we display the calculated order parameters $m_f$ and $h$ as functions of $V$, for EHA(I) at fixed $\epsilon_f = -3$, and for EHA(II) at $\epsilon_f = -1$, respectively. The critical behavior of $m_f$ with respect to $V$ clearly indicates a second-order magnetic transition. In figures 5(a) and (b), the critical hybridization $V_c$ of magnetic transition is plotted as $\epsilon_f$ varies. The suppression of $V_c$ as $\epsilon_f$ approaches the Fermi level is attributed to the enhancement of valence fluctuation of $f$ electrons which suppresses the AF order.

The phase diagrams are then summarized on $\epsilon_f - V$ plane in figures 5(a) and (b), for EHA(I) and EHA(II), respectively, including both AF phases and TI phases. For EHA(I), we find that the AF phase is in proximity to WTI, indicating a nAFI with $\nu' = 0$; while for EHA(II), the AF phase is in proximity to STI, indicating an AFTI with $\nu' = 1$. The bulk dispersions of three typical AF states (two for nAF and one for AFTI) are demonstrated in figures 7(b), (d) and (f), through which we can calculate $\delta_m$ at four KDM using equation (19), then obtain $\nu'$ by equation (21). The results are shown in table 2, confirming our analysis.

In figure 6, we display the phase evolution with $V$ and temperature $T$ at fixed $\epsilon_f = -3$ with EHA(I). It shows that
while \( V \) is enhanced, the Néel temperature of nAFI phase is suppressed continuously, then vanishes at \( V_c \), which is the critical value of magnetic transition at zero temperature. Therefore, besides by the enhancement of \( V \) or ascent of \( \epsilon_f \) at zero temperature, the nAFI-WTI transition (and AFTI-STI transition) can also be driven by increasing temperature. In addition, the phase boundaries among WTI, STI and nKI are slightly shifted by finite temperatures.

Now we calculate the surface states of AF phases. With three sets of model parameters listed in table 2 (two for nAFI with bulk spectrums displayed in figures 7(b) and (f), and one for AFTI shown in figure 7(d)), we have performed saddle-point solutions of 40 slabs to derive the mean-field parameters and chemical potential, then diagonalize the Hamiltonian matrix to obtain the surface dispersions on (0 0 1) surface. The bulk and surface dispersions are given in figures 7(a) and (e) for nAFI, and (c) for AFTI, in which the bulk spectrums are all full-gapped. For nAFI, the surface states remain gapless within present solution. The original Dirac cone at \( \bar{X} \) in WTI \( _X \) (see figure 3(a)) is decomposed upwards and downwards into two Dirac cones by AF magnetization, leading to two Dirac points at \( \bar{X} \), one above and another below the Fermi level, similar to that reported in [34]. Since \( \bar{X} \) is now KDM, therefore, in nAFI, Kramers degeneracy takes place at these two Dirac points on both sides of the Fermi level. However, such surface states cross the Fermi level even times from \( \bar{X} \) to any other KDM, revealing the non-topologically-protected

### Table 2. \( Z_2 \) classification and surface Dirac points of the AF states demonstrated in figure 7. The last two columns show critical hybridization of the magnetic transitions under EHA and \( \epsilon_f \) in the second column, and topologies of the PM phases near the magnetic transitions.

| Classification | Model parameters | Dispersions | \( \delta'_m \) at \( \bar{\Gamma} \) | \( \delta''_m \) at three \( \bar{X} \) | \( \nu' \) | Dirac points | Critical \( V \) | PM phase |
|---------------|-----------------|-------------|-----------------|-----------------|-------|-------------|--------------|----------|
| nAFI          | EHA(I), \( \epsilon_f = -3 \), \( V = 2 \) | figures 7(a) and (b) | -1 | -1 | 0 | — | 2.27 | WTI \( _X \) |
| AFTI          | EHA(II), \( \epsilon_f = -2 \), \( V = 1.6 \) | figures 7(c) and (d) | 1 | -1 | 1 | \( \bar{\Gamma} \) and \( \bar{M} \) | 1.71 | STI \( _{\bar{X}} \) |
| nAFI          | \( \epsilon_f = -2 \), \( V = 2.05 \) | figures 7(e) and (f) | -1 | -1 | 0 | — | 2.22 | WTI \( _{\bar{X}} \) |

a The surface dispersions are showing on (001) surface.

b The \( Z_2 \) index \( \nu' \) is calculated by equation (21).

c Showing topologically protected Dirac points in the AF phases.

d With EHA: \( t'_d = t''_d = -0.375 \), \( t_f = -0.1 \), \( t'_f = t''_f = 0.0375 \).

Figure 5. Phase diagrams on \( \epsilon_f - V \) plane, showing magnetic transitions (solid blue lines) and topological transitions among TI phases (dashed lines). EHA(I) for (a) and EHA(II) for (b). Depending on whether the AF order arises from WTI or STI, AF phases are classified into nAFI or AFTI, respectively.

Figure 6. Phase evolution with hybridization strength \( V \) and temperature \( T \). Parameters: \( \epsilon_f = -3 \) and EHA(I).
the nature of nAFI, in the manner that these surface states can be deformed adiabatically by perturbations which conserve $S$ symmetry (e.g. adding contact potential on surface) [37], to gap the surface dispersions [14], see figure 8. Hence, although the surface states in nAFI remain gapless by present solution, nAFI is topologically undistinguishable from other AF states with gapped surface states (such as adding an AF order to nKI). AFTI shown in figure 7(c) is in the vicinity of STI $\bar{\Gamma}\bar{\Pi}$ phase, and the Dirac point at $\bar{\Gamma}$ persists, because $\bar{\Gamma}$ point shares opposite $\delta^\prime_m$ with other three KDM (see table 2). Another Dirac point at $\bar{M}$ is formed by folding of surface BZ, and these two Dirac cones in AFTI are topologically protected against $S$-conserving perturbations. In addition, the original Dirac cones at $\bar{X}$ are decomposed in AFTI, and the surface states around $\bar{X}$ in AFTI are also topologically trivial, similar to nAFI.

Although bulk gap persists, the gapless surface states in AFTI induce metallic Fermi rings, as shown in figure 9(a), comparing with the Fermi rings in STI $\bar{\Gamma}\bar{X}$ shown in figure 9(b). For AFTI, the Fermi ring around $\bar{\Gamma}$ evolves continuously to that in STI $\bar{\Gamma}\bar{X}$, when approaching the magnetic boundary. It should be noted that since the surface states around $\bar{X}$ in AFTI are topologically trivial, corresponding Fermi surfaces around $\bar{X}$ can be destructed by $S$-conserving perturbations such as contact potential on the surfaces; on the contrary, the Fermi rings around $\bar{\Gamma}$ and $\bar{M}$ in AFTI are topologically protected and are robust under $S$-conserving perturbations. The spin texture on the Fermi ring around $\bar{\Gamma}$ in AFTI is illustrated by the inset of figure 9(a), showing a helical spin structure and indicating spin-momentum locking in the surface Dirac states, however, on (0 0 1) surface, large Néel energy suppresses the projection of spins on this surface, therefore, the spin-momentum locking in AFTI is much weaker than in STI $\bar{\Gamma}\bar{X}$ (figure 9(b)). On the Fermi rings around $\bar{X}$ points in AFTI, we found that the spins are greatly suppressed, and no clear signal of spin-momentum locking is observed.

As revealed by previous theoretical calculations [50–52] and SARPES observations [13, 53], the TKI compound SmB$_6$ is in a STI $\bar{\Gamma}\bar{X}$ phase, hence the pressure-induced magnetic phase in SmB$_6$ is most probably an AFTI, but under two conditions: firstly, no former topological transition takes place before the magnetic transition, secondly, there is a lattice translation which flips the magnetization at all sites, allowing the application of $Z_2$ classification to the AF phase. However, during the high-pressure-induced magnetic transition, tracking the evolution of model parameters is a complicated task, so the existence of AFTI in SmB$_6$ requires further first-principle investigations and experimental confirmation.

**Figure 7.** Left column: surface dispersions (red lines) on (001) surface through slab-calculations. Right column: corresponding 3D bulk spectrums comparing with $d$- (red lines) and renormalized $f$- dispersions (green lines). The upper and down rows are for nAFI states, while the middle row is for AFTI. Parameters: (a) and (b) with $\epsilon_f = -3, V = 2$ and EHA(I); (c) and (d) with $\epsilon_f = -2, V = 1.6$ and EHA(II); (e) and (f) with $\epsilon_f = -2, V = 2.05, t'_d = t''_d = -0.375, t_f = -0.1, t'_f = t''_f = 0.0375$. 

---

**Figure 9.** (a) and (b) Fermi rings around $\bar{\Gamma}$ and $\bar{M}$ in AFTI. Parameters: $\epsilon_f = -2, V = 2.05, t'_d = t''_d = -0.375, t_f = -0.1, t'_f = t''_f = 0.0375$. (c) and (d) Fermi rings around $\bar{X}$ in AFTI. Parameters: $\epsilon_f = -2, V = 1.6, t'_d = t''_d = -0.375, t_f = -0.1, t'_f = t''_f = 0.0375$. (e) and (f) Fermi rings around $\bar{X}$ in STI. Parameters: $\epsilon_f = -3, V = 2$.
In an AFTI, the surface states are strongly anisotropic to surface orientation [37]. AF-ordered (0 0 1) surface we studied above conserves the $S$ symmetry, leading to topologically protected gapless Dirac cones on it, namely these surface states are stable under additional interactions which do not violate $S$ symmetry. On ferromagnetically (FM) ordered surfaces which violate $S$ symmetry (e.g. (1 1 1) surface), no KDM exists, so the surface states are generally gapped [36, 37], similar to the surface states in magnetic topological insulators [54].

The topologies of the AF phases depend on the topologies of the PM phases from which the AF orders grow, therefore, the AFTI phase only emerges below the critical $V_{c}$ of a parameter region in which STI phase is favored. Consequently, AFTI only emerges in a narrow parameter region. The nAFI and AFTI states we derived are close to WTI $\bar{X}$ and STI $\bar{\Gamma}\bar{X}$, respectively. From figure 5, one can see that for physical $\epsilon_f < 0$, STI phase emerges at relative strong $V$ at which magnetic order has already been suppressed. By adding further EHA properly, we expect to realize an AF transition inside STI $\bar{X}$ phase, then the arising AF state is an AFTI, with protected Dirac points at $\bar{\Gamma}$ and $\bar{M}$ in AFTI are topologically protected.

In an AFTI, the surface states are strongly anisotropic to surface orientation [37]. AF-ordered (0 0 1) surface we studied above conserves the $S$ symmetry, leading to topologically protected gapless Dirac cones on it, namely these surface states are stable under additional interactions which do not violate $S$ symmetry. On ferromagnetically (FM) ordered surfaces which violate $S$ symmetry (e.g. (1 1 1) surface), no KDM exists, so the surface states are generally gapped [36, 37], similar to the surface states in magnetic topological insulators [54].

6. Topological transition between AF states

In the above, we have shown that with EHA(I) or EHA(II), a magnetic transition takes place to induce nAFI or AFTI, respectively. Particularly, in figure 5(b), one can see that with EHA(II), although the magnetic transition occurs between STI $\bar{X}$ and AFTI, the magnetic boundary is quite close to STI $\bar{X}$ − WTI $\bar{X}$ boundary. On the other hand, we find that the critical $V_{c}$ of magnetic transition increases rapidly with
and can shift the magnetic boundary from nearby STI
nAFI-AFTI transition at $\bar{\Gamma}$ to $-0.1$ and keep the relation $t'_f = t'_f = -0.525t_f - 0.015$ which EHA(II) obeys, then find a magnetic transition at $V_c = 2.22$, now from WTI to nAFI state (see top right corner on the red line in figure 11). Therefore, a continuous change of $t_f$ (and associated change of $t'_f$ and $t''_f$) can shift the magnetic boundary from nearby STI$_F$ to nearby WTI$_F$, shown by the two segments of red line in figure 11. From knowledge of the $Z_2$ classification of AF states discussed in section 4, upon reduction of $V$ from these two segments of magnetic boundaries, we obtain an AFTI and nAFI states, respectively. Therefore, by varying $t_f$ in such way, we can realize a topological transition between AFTI and nAFI.

To verify this topological transition, we set $t_f = -0.144$ and $\epsilon_f = -2$ to calculate the phase evolution with $V$, the result is illustrated in figure 10. Magnetic transition occurs between AFTI and STI$_F$ at $V = 1.989$. With decreasing $V$, we find two successive topological transitions between AF phases: an AFTI-nAFI transition at $V = 1.941$ and a following nAFI-AFTI transition at $V = 1.826$. At these two topological transitions, the bulk gap is closed, while at the magnetic transition, bulk gap persists. When further reducing $V$ after nAFI-AFTI transition, bulk gap increases then decreases rapidly to generate an insulator-metal transition at $V = 1.707$, and the metallic AF state is similar to the AF states proposed in [34, 45]. Phase diagram summarizing the magnetic transition, topological transitions, and insulator-metal transitions are shown in figure 11.

To see explicitly what happens during the topological transition between AFTI and nAFI, we depict the bulk and surface dispersions of the two phases on both sides of this transition in figures 7(c)–(f). We find that AFTI-nAFI transition is accompanied by closing of bulk gap at $\Gamma$ and equivalent $R$ points. On AFTI side of this transition (figures 7(c) and (d)), $\delta'_m = 1$ at $\Gamma$, while at three X points, $\delta'_m = -1$, inducing a topological index $\nu' = 1$. By closing and reopening of the bulk gap at $\Gamma$ (and $R$) during AFTI-nAFI transition, in nAFI phase, $\delta'_m$ is shifted to $-1$ at $\Gamma$ and remains $-1$ at $X$, leading to $\nu' = 0$. So gap-closing during AFTI-nAFI transition causes a parity inversion at $\Gamma$, shifts the topological index, consequently leading to the vanishing of Dirac cones at $\Gamma$ and $M$ in nAFI.

In this work, the nAFI-AFTI topological transition is achieved by special setting and variation of some model parameters. When applying pressure to real TKI materials, the variation of model parameters can be quite complicated to track, so whether such nAFI-AFTI topological transition is realizable deserves further first-principle calculations and experimental verification. Besides, quantum phase transitions between topological trivial and nontrivial AF phases and the metal-insulator transition in other system have been reported in literature [40, 55].

### 7. Conclusion and discussion

In conclusion, we have verified a novel topologically protected AFTI phase in 3D TKI, and realized a topological transition between AFTI and nAFI, for the first time. We have performed an extended slave-boson mean-field solution of 3D TKI modeling by the half-filled periodic Anderson model with spin–orbit coupled $d$-$f$ hybridization in large $U$ limit. In a wide parameter region, we have found second-order transitions from TI phases to AF phases. Although time-reversal symmetry $\Theta$ is broken, the AF phases preserve the symmetry under combined operation $\hat{S} = \Theta \hat{T}_D$, in which a translation by vector $D$ flips the magnetization at all sites. $\hat{S}$ operator is antiunitary and squares to minus at four out of eight high-symmetry points in MBZ, leading to Kramers degeneracy at these momenta. The Kramers degeneracy at four KDM and the inverse symmetry of AF result in a new type of $Z_2$ classification for AF states by invariant $\nu'$ calculated by product of parities at four KDM, and $\nu'$ is in analogy to the STI index $\nu_0$. By applying $Z_2$ classification to the slave-boson solutions...
of AF phases. The magnetic transitions, the topological transitions between nAFI and AFTI, and the topological transitions between TI phases have been summarized in a global phase diagram. We should emphasize that our derived AFTI in 3D TKI is an insulator with full bulk gap, distinct from the AF phases with metallic bulk previously reported in SmB$_6$ and GdBiPtn by other authors [34, 45].

In this paper, we have so far discussed an AF structure which is staggered between adjacent sites. Actually, other AF configurations have also been discussed in literature, e.g. the so-called A-AF state which is staggered along one axis [34]. We have pointed out that as long as an insulating AF phase possesses a translation by a certain lattice vector which flips the magnetization at all sites, plus it has an inversion center, then this AF state can be classified by the $Z_2$ invariant calculated by the parities at four KDM in its MBZ. Under these conditions, we can always reach the conclusion that if an insulating AF phase evolves from STI, it is an AFTI; while it arises from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations. Therefore, once an insulating A-AF state emerges from WTI, it is nAFI, regardless of the detailed AF configurations.

In terms of topology and topological transitions. The limitation of this mean-field approach lies in low efficiency to describe the dynamic behaviors such as Kondo resonance, Kondo screening and spin or charge correlations, which may require more rigorous methods such as Monte Carlo simulation [19].

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Appendix A. The saddle-point equations for AF phases

Here we discuss the equations for saddle point solution of AF phase based on the mean-field Hamiltonian equation (6). Since the Hamiltonian matrix $H_k$ (equation (7)) has no analytical expression for its eigenvalues, we have to solve it numerically to get the unitary transformation matrix $U_k$ which diagonalize $H_k$: $U_k^H H_k U_k = \Lambda_k$, or $\Psi_k^\dagger H_k \Psi_k = \Phi_k^\dagger \Lambda_k \Phi_k$, where $\Lambda_k$ is a diagonal matrix with the eigenvalues $E_k^{(i)} (i = 1, ..., 8)$ as its diagonal elements. $\Phi_k^\dagger$ is the eight-component creation operator for elementary excitations. Now we can calculate the ground-state expectation values for quadratic combinations of $d$ and $f$ operators $(n, m = 1, ..., 8)$:

$$\langle nm \rangle_k \equiv \langle \langle \Psi_k^\dagger \rangle_j \langle \Psi_k \rangle_m \rangle = \langle \langle \sum_j (\Phi_k^\dagger)_i (U_k)^m (\Phi_k)_j \rangle \rangle = \langle \langle \sum_{i=1}^8 (U_k^m)^* (U_k)_m (\Theta(-E_k^{(i)})) \rangle \rangle. \quad \text{(A.1)}$$

Using these expectation values $\langle nm \rangle_k$ which can be extracted from numerical diagonalization, we can write the free energy $F$ as the expectation value of the Hamiltonian equation (6):

$$F = N(\eta n_f - m_f) + \sum_{k \in \text{MBZ}} (H_k)_{nm} \langle nm \rangle_k. \quad \text{(A.2)}$$

then derive the saddle-point equations of the mean-field parameters $n_f, m_f, h, \eta$ and chemical potential $\mu$ from knowledge of the elements of $H_k$. For example, the equation from $\partial F/\partial h = 0$ is derived as

$$m_f = \frac{1}{N} \sum_{k \in \text{MBZ}} \langle \langle 55 \rangle_k + \langle 88 \rangle_k - \langle 66 \rangle_k - \langle 77 \rangle_k \rangle = 0. \quad \text{(A.3)}$$

the equation from $\partial F/\partial \eta = 0$ is

$$n_f = \frac{1}{N} \sum_{k \in \text{MBZ}} \langle \langle 55 \rangle_k + \langle 66 \rangle_k + \langle 77 \rangle_k + \langle 88 \rangle_k \rangle = 0. \quad \text{(A.4)}$$

and equation from $\partial F/\partial \mu = -n_f$ is
\[ n_t - \frac{1}{N} \sum_{\mathbf{k} \in \text{MBZ}} \sum_{i=1}^{8} \langle \hat{n}_i \rangle_{\mathbf{k}} = 0. \tag{A.5} \]

The other two equations corresponding to \( \partial F / \partial n_f = 0 \) and \( \partial F / \partial m_f = 0 \) have much complex expressions. In this paper, we restrict the discussion to \( n_t = 2 \).

\section*{Appendix B. The saddle-point equations for PM phases}

For PM phase, the Hamiltonian matrix equation (13) can be easily diagonalized analytically, leading to the expression for dispersions \( E_k^\pm \) and ground-state energy \( E_{gPM} \) in and above equation (15). Then the saddle-point equations can be derived by minimizing of \( E_{gPM} \) with respect to \( n_f, \mu \) and \( \eta \), to obtain

\[ n_f = \frac{1}{N} \sum_{\mathbf{k} \pm} \Theta(-E_k^\pm) \]

\[ n_f = \frac{1}{N} \sum_{\mathbf{k} \pm} \Theta(-E_k^\pm)[1 + \frac{\epsilon_k^d - \epsilon_k^f}{\sqrt{(\epsilon_k^d - \epsilon_k^f)^2 + 4 V^2 Z_s^2 S_k^z}}] \]

\[ \eta = \frac{2Z}{N} \frac{\partial Z}{\partial n_f} \sum_{\mathbf{k} \pm} \Theta(-E_k^\pm) \frac{\epsilon_k^d - \epsilon_k^f}{\sqrt{(\epsilon_k^d - \epsilon_k^f)^2 + 4 V^2 Z_s^2 S_k^z}} \]

in which

\[ \frac{\partial Z}{\partial n_f} = \left( \frac{1 - n_f}{2(1 - n_f)^3} \right) - \frac{1}{2(2 - n_f)(1 - n_f)}. \tag{B.2} \]

The self-consistent equations of AF and PM phases should be solved by numerical iteration.

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