Magnetic and topological transitions in three-dimensional topological Kondo insulator*

Huan Li1,1, Zhi-Yong Wang,1 Xiao-Jun Zheng†1, Yu Liu2,3, and Yin Zhong4

1College of Science, Guilin University of Technology, Guilin 541004, China
2Institute of Applied Physics and Computational Mathematics, Beijing 100088, China
3Software Center for High Performance Numerical Simulation, China Academy of Engineering Physics, Beijing 100088, China
4Center for Interdisciplinary Studies & Key Laboratory for Magnetism and Magnetic Materials of the MoE, Lanzhou University, Lanzhou 730000, China

By using an extended slave-boson method, we draw a global phase diagram summarizing both magnetic phases and paramagnetic (PM) topological insulating phases (TI) in three-dimensional topological Kondo insulator (TKI). By including electron hopping (EH) up to third neighbor, we identify four strong topological insulating (STI) phases and two weak topological insulating (WTI) phases, then the PM phase diagrams characterizing topological transitions between these TI are depicted as functions of EH, f-electron energy level and hybridization constant. We also find an insulator-metal transition from a STI phase which has surface Fermi rings and spin textures in qualitative agreement to TKI candidate SmB6. In weak hybridization regime, antiferromagnetic (AF) order naturally arises in the phase diagrams, and depending on how the magnetic boundary crosses the PM topological transition lines, AF phases are classified into AF topological insulator (AFTI) and non-topological AF insulator (nAFI), according to their Z2 indices. In two small regions of parameter space, two distinct topological transition processes between AF phases occur, leading to two types of AFTI, showing distinguishable surface dispersions around their Dirac points.

PACS numbers: 75.30.Mb, 75.30.Kz, 75.70.Tj, 73.20.-r

Over the recent years, searching topological phases of matter has becoming one of the central topics in condensed matter physics. Among the enlarging family of topological matters, the strongly correlated electron systems offer as important basis, because they naturally involve rich kinds of mechanism, hence can generate a variety of interacting topological phases, such as interacting topological insulator, topological Mott insulator, interacting topological superconductor, Weyl semimetal, topological Kondo insulator, antiferromagnetic topological insulator (AFTI), etc.

Topological Kondo insulator (TKI), a heavy-fermion system with strong Coulomb interaction and d-f hybridization governing by spin-orbit coupling, preserves time-reversal symmetry (TRS), therefore can generate topological insulating phases (TI) with Kondo screening effect. As revealed by previous works, variation of electron hopping (EH) strength, f-electron energy level εf and hybridization constant V can drive topological transitions among phases of strong topological insulator (STI), weak topological insulator (WTI) and normal Kondo insulator (nKI). However, existing works in literature are restricted to their interested parameter regime, hence the studied TI are still confined to a limited number of STI and WTI, and the full STI and WTI phases in TKI have not been explored adequately, particularly at the presence of strong electron-electron correlation. In this work, by considering adequate parameter space of periodic Anderson model (PAM), we uncover all possible TI in three-dimensional (3D) TKI: four STI and two WTI, each possessing distinct surface states and Dirac cones. We also present the paramagnetic (PM) phase diagrams characterizing topological transitions between these TI, as functions of EH, εf and V. By proper fitting of EH, we verify a STI phase with Fermi surfaces and spin textures which can qualitatively simulate the TKI material SmB6, confirming the applicability of PAM to TKI, and it is find that this STI phase is in vicinity to an insulator-metal transition driving by enhancement of V.

In heavy-fermion systems, the interplay and competition between Kondo screening and magnetic correlation can motivate magnetic transitions when the Kondo interaction is reduced. Similarly, in half-filled TKI, theoretical calculations have verified a transition to AF phase when the hybridization interaction V is weakened, reminiscent of the induced magnetism in pressurized SmB6. Besides, our earlier work has proved that due to the combined S symmetry of time reversal and translation operations, the AF states in TKI remain topological distinguishable, regardless of the breaking of TRS by magnetic order. We has developed a Z2 topological classification to the AF states in TKI and proposed a novel AFTI phase under unique setting of model parameters, together with an AFTI-nontopological AF insulator (nAFI) topological transition while EH was shifted in some way. Unfortunately, why AFTI should appear in such parameter region is still not clear, and it remains confused whether new AF phases exist in other parameter regions. We have shown that at least near the magnetic boundary (MB), the Z2 index for AF directly relies on that of TI phase from which the AF order develops, therefore, in order to investigate all possible AF phases with distinct topologies, the magnetic transition and classification of AF phases should be discussed on the basis of the PM phase diagrams summarizing all TI, i.e., the four

*Supported by the National Natural Science Foundation of China under Grant Nos 11764010, 11504061, 11564008, 11704084, 11704166, Guangxi NSF under Grant Nos 2017GXNSFAA198169, 2017GXNSFBA198115, and SPC-Lab Research Fund (No. XKFZ201605).
†Corresponding author, Email: lihuan@glut.edu.cn
‡Corresponding author, Email: zhengxiaojun323@foxmail.com

PACS numbers: 75.30.Mb, 75.30.Kz, 75.70.Tj, 73.20.-r
STI and two WTI should be included properly to study the AF transition as well as the topological transitions between AF phases.

We use the spin-1/2 PAM to characterize the 3D TKI in cubic lattice:  

$$H = H_d + H_f + H_{df} + H_U,$$  (1)

where $H_d = \sum_{k,\alpha} (\epsilon_k - \mu) d_{k\alpha}^\dagger d_{k\alpha}$, $H_f = \sum_{k,\alpha} (\epsilon_f + \epsilon_k - \mu) f_{k\alpha}^\dagger f_{k\alpha}$. $H_{df} = V \sum_{k,\alpha\beta} S_k \cdot \sigma_{\alpha\beta} d_{k\alpha}^\dagger f_{k\beta} + h.c.$ is the Kondo hybridization with spin-orbit coupling, in which $S_k = (\sin k \cdot a_1, \sin k \cdot a_2, \sin k \cdot a_3)$, with the element vectors $a_1, a_2, a_3$ for cubic lattice. $H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}$ is the on-site coulomb repulsion between $f$ electrons, and we consider infinite $U$ in this work. We includes EH up to third neighbor, with $t_{d(\bar{f})}, t_{d(\bar{f})}''$ denote nearest-neighbor (NN), next-nearest-neighbor (NNN), and next-next-nearestneighbor (NNNN) hopping amplitudes, respectively, which determine the tight-binding dispersions $\epsilon_k^{d(\bar{f})}$. The chemical potential $\mu$ is used to fix the total electron number to half filling $n_f = 2$, and variable EH, hybridization interaction $V$ and $f$ energy level $\epsilon_f$ are considered. In what follows, $t_d = 1$ is set as energy unit, and we choose $t_f = -0.2$ and keep $t_{d(\bar{f})}'/t_d = t_{d(\bar{f})}'/t_d$ to get a medium gapped insulating phase (unless when the insulator-metal transition is discussed).

We employ the Kotliar-Ruckenstein (K-R) slave-boson method to solve PAM. Similar to Coleman’s slave boson theory, the mean-field approximation of PAM Eq. 1 in large-U limit reads

$$H_{MF} = N(-\eta n_f) + \sum_{k,\alpha,\beta} (d_{k\alpha}^\dagger f_{k\beta}^\dagger) \left( \begin{array}{cc} (\epsilon_k - \mu) \delta_{\alpha\beta} & \tilde{V} S_k \cdot \sigma_{\alpha\beta} \epsilon_k^{\dagger} \delta_{\alpha\beta} \\ \tilde{V} S_k \cdot \sigma_{\alpha\beta} \epsilon_k^{\dagger} \delta_{\alpha\beta} & (\epsilon_k^d - \mu) \delta_{\alpha\beta} \end{array} \right),$$  (2)

where the effective hybridization $\tilde{V} = V Z$ is renormalized by factor $Z = \sqrt{2(1 - n_f)}/(2 - n_f)$, and the effective $f$ dispersion $\epsilon_k^f = \epsilon_f + \eta Z^2 \epsilon_k^d$, in which $\eta$ shifts the $f$ level. $n_f$ is the density of $f$ electron per site, $N$ is the number of lattice sites. The PM mean field parameters $n_f, \eta, \mu$ are solvable through saddle-point solution for $H_{MF}$, where the quasi-particle dispersions are the eigenvalues of the Hamiltonian matrix in Eq. 2 (in a modified form) are used to identify the $Z_2$ index.

In last two rows of Fig. 1, we show six types of distinct quasi-particle spectra of PM TI, each with different model parameters listed in Tab. 1, comparing with $d$ and $f$ dispersions. The eight high symmetric points (HSP) $k_{\text{HSP}}$ in 3D Brillouin zone (BZ) (i.e., $\Gamma = (0,0,0)$; $\bar{X} = (\pi,0,0)$, $(0,\pi,0)$, $(0,0,\pi)$; $M = (\pi,\pi,0)$, $(\pi,0,\pi)$, $(0,\pi,\pi)$; and $R = (\pi,\pi,\pi)$), the hybridization vanishes (due to its odd parity), consequently the quasi-particle energy equals either $\epsilon_k^d$ or $\epsilon_k^f$, leading to the parity of occupied states $\delta = 1$ or $-1$ at $k_{\text{HSP}}$, respectively. Therefore, the strong topological index $\nu_0$ can be easily obtained by observing the bulk dispersions in Fig. 1 via $(-1)^{\nu_0} = \prod_{m \in \text{HSP}} sign_m$, and the weak topological indices $\nu_j$ ($j = x, y, z$) are calculated from the HSP on $k_j$ plane $P_j$ through $(-1)^{\nu_j} = \prod_{m \in \text{HSP}} \delta_m$. The quantities $\delta_m$ and $Z_2$ indices for six TI are listed in Tab. 1.

By diagonalizing 40 slabs to simulate the 3D lattice with opened (001) surface, the surface states of the six TI are solvable through $\bar{X}$-dispersion, respectively. Parameters and $Z_2$ invariants for each TI are listed in Tab. 1.

In the first row of Fig. 1, with varying $t_{d(\bar{f})}'/t_f$ and $V$, we have located the topological boundaries among all possible TI, determined by the change of $Z_2$ index. The topological transitions between TI are generated by closing and reopening of the insulating gap at certain HSP, leading to an inversion of parity and consequently the shifting of $Z_2$ index.

In above, we have set $t_{d(\bar{f})}'/t_f = t_{d(\bar{f})}'/t_d$, under which the Dirac points in TI, all cross the Fermi energy, leading to the vanishment of Fermi surface. For TKI candidate SnB$_6$, medium-
The surface dispersions are calculated on (001) surface.

Based on the PM phase diagrams of TI\(_s\), we now study the AF transitions in TKI. In our previous work, the original K-R method of symmetric PAM\(^{19,20}\) has been generalized to treat AF phases in non-symmetric case,\(^{16}\) which can be applied to TKI. The resulting mean-field Hamiltonian is rather complicated in that in addition to \(n_f, \eta\) and \(\mu\), two AF order parameters \(n_\|=\h\) should be determined, besides, two renormalization factors \(Z_1\) and \(Z_2\) arise. Due to the \(S\) symmetry combined by TRS and lattice translation, the AF phases in TKI fall into \(Z_2\) topological class, and the \(Z_2\) index \(\nu\) is calculated from the parities of the occupied spectrums at four Kramers degenerate momenta (KDM) \(p_m\) (\(\Gamma\) and three \(X\) points) via 
\[
(-1)^\nu = \prod_{p_m \in \text{KDM}} \delta_m, \text{ in which } \delta_m = \prod_{i} \xi_i(p_m), \text{ with}
\]
the parity \(\xi_i(p_m)\) of \(i\)-th occupied state at \(p_m\) equals either 1 or -1, when quasi-particle energy equals that of \(d\) or \(f\) at \(p_m\), respectively.\(^{10}\) Particularly, the strong topological index \(\nu_0\) on the PM side of the MB directly determines \(\nu\) of the AF phase near MB, namely, \(\nu_0 = 1\) (STI) leads to \(\nu = 1\) (AFTI), while \(\nu_0 = 0\) (WTI or nKl) leads to \(\nu = 0\) (nAFI),\(^{10}\) giving a straightforward verification of the AF phases near MB.

### TABLE I: Parameters and \(Z_2\) invariants of the TI phases shown in Fig. 1. In all phases, \(t_f = -0.2\).

| phase     | \(t'_d\) | \(t'_d\) | \(t'_f\) | \(t'_f\) | \(\epsilon_f\) | \(V\) | \(\delta_f\) | \(\delta_\eta\) | \(\delta_M\) | \(\delta_\eta\) | \(\nu_0\) | \(\nu_f\) | Dirac points\(^a\) |
|-----------|----------|----------|----------|----------|---------------|------|-------------|-------------|-------------|-------------|----------|-------------|----------------|
| STI\(_\Gamma\) | 0.26     | 0.26     | -0.052   | -0.052   | -2            | 0.7  | 1           | -1          | -1          | -1          | 1        | 1           | \(\Gamma\)     |
| STI\(_\bar{\Gamma}\) | -0.35   | -0.35   | 0.07     | 0.07     | -2            | 1    | -1          | 1           | -1          | -1          | 1        | 1           | \(\bar{\Gamma}, \bar{\chi}\) |
| STI\(_X\) | 0.252    | 0.252    | -0.0504  | -0.0504  | -2            | 1.5  | 1           | 1           | 1           | 1           | 1        | 1           | \(X\)        |
| WTI\(_X\) | -0.6     | 0        | 0.12     | 0         | -1            | 1    | 1           | -1          | 1           | -1          | 1        | 0           | \(M, \bar{X}\) |
| WTI\(_\bar{X}\) | -0.2     | 0        | 0.04     | 0         | -2            | 1    | 1           | -1          | 1           | 1           | 0        | 1           | \(\Gamma, \bar{M}\) |

\(^{a}\)The surface dispersions are calculated on (001) surface.

**FIG. 2:** (a) Insulator-metal transition from STI\(_\bar{\Gamma}\) to conducting phase. (b) Closing of bulk gap during this transition. (c) Slab dispersions of STI\(_\bar{\Gamma}\). (d) Surface Fermi rings and spin textures of STI\(_\bar{\Gamma}\). \(t'_d = t'_d = -0.375, t'_f = -0.23, t'_f = t'_f = 0.2, \epsilon_f = -4\) for (b) to (d), and \(V = 1\) for (c) and (d).

**FIG. 3:** (a) Magnetic boundary in 3D TKI (blue lines). Near \(t'_d = 0.25\) and \(-0.35\), topological transitions between AF phases take place (green solid lines). Parameters: \(\epsilon_f = -1.5, t'_d = t'_d, t'_f = t'_f = -0.2\) and \(t'_f/t'_f = t'_d/t'_d\).

**FIG. 4:** Surface dispersions (left column) and quasi-particle dispersions (right column) of AFTI and nAFI near the AF topological boundary in lower inset of Fig. 3. \(V = 1.4, t'_d = -0.37\) for AFTI, and \(t'_d = -0.35\) for nAFI.
The magnetic critical hybridization $V_c$ is calculated as a function of $t'_d$, then the MB plotted by $V_c$ is added to the phase diagram, see Fig. 3. The MB crosses the topological boundaries of TI$_s$ in two parts, one near $t'_d = 0.25$, the other around $t'_d = -0.35$, see insets of Fig. 3 for details.

Around $t'_d = -0.35$, the MB is divided by the STI$_{FX}$-WTI$_X$ transition line into two parts, leading to AFTI and nAFI just below the two parts of MB, respectively. While $V$ is lowered further from MB, $\nu$ of AF phases should be computed from the 3D spectrums (e.g., Fig. 4(b) and (d)) to determine the AFTI-nAFI topological boundary, which is demonstrated by the green line near $t'_d = -0.35$ in Fig. 3. The AFTI-nAFI transition is realized via parity inversion during gap closing and reopening at $\Gamma$, and it converges with STI$_{FX}$-WTI$_X$ boundary at the MB, see the lower inset in Fig. 3.

Near $t'_d = 0.25$, the MB is separated by WTI$_X$-STI$_M$, and STI$_M$-nKI lines into three parts. Below the middle part of MB (which touches STI$_M$), an AFTI arises, while below the other two parts of MB, nAFI emerges. The AFTI-nAFI transition forms a narrow water-drop-shaped area in which AFTI survives (green solid line in the upper inset in Fig. 3). Besides, though nAFI$_s$ above and below $t'_d = 0.25$ have quite different dispersions (compare Fig. 5(b) with (f)), they still have equal $\nu = 0$, since their magnetic orders grow from nKI and WTI, respectively. Though band gap is closed at the boundary between two nAFI$_s$, no parity inversion occurs, consequently no topological transition takes place (see the green dashed line in upper inset of Fig. 3).

The surface states of AF phases are shown in Fig. 4(a), (c) near $t'_d = -0.35$, and in Fig. 5(a), (c), (e) around $t'_d = 0.25$, respectively. In AFTIs, the Dirac points at $\Gamma$ and $M$ are protected by topology hence are robust, see Fig. 4(a) and Fig. 5(c). Furthermore, the Dirac surface states of two AFTI$_s$ (one near STI$_M$ and the other near STI$_{FX}$) disperse quite differently, in which the former constructs a valley shape (Fig. 5(c)). In contrast, the gapless surface states at X in both AFTI and nAFI (Fig. 4(a), (c) and Fig. 5(a)) are not robust, since they can be gapped by additional factor such as gate voltage.\(^\text{10}\)

In summary, we have performed a slave-boson mean-field analysis of the 3D TKI using spin-orbit coupled PAM, and presented the phase diagrams including all possible PM TI$_s$ in TKI: four STI and two WTI, each with distinguishable locations of Dirac points. We also obtained a STI$_{FX}$ phase with similar surface states to SmB$_6$, and found it can be driven to conducting state through an insulator-metal transition by enhanced hybridization. We also investigated the magnetic boundary of AF phases in TKI, and found the topological transitions between AFTI and nAFI in two narrow regions in parameter space. Besides, we found two types of AFTI with distinct dispersions at the Dirac points. Though our work is based on an uniform mean-field approximation, any site-dependent treatment will not break the application of $Z_2$ classification of both PM and AF states.\(^\text{14,17}\) We hope our work can help to reach a comprehensive understanding of novel AFTI phases in strongly correlated electrons systems.

---

1. Qi X L and Zhang S C 2013 Rev. Mod. Phys. 83, 1057
2. Go A et al 2012 Phys. Rev. Lett. 109, 066401
3. Yu S L, Xie X C and Li J X 2011 Phys. Rev. Lett. 107, 010401
4. Wang Z and Zhang S C 2012 Phys. Rev. B 86, 165116
5. Wan X G et al 2011 Phys. Rev. B 83, 205101
6. Dzero M et al 2012 Phys. Rev. B 85, 045130
7. Mong R S K, Essin A M and Moore J E 2010 Phys. Rev. B 81, 245209
8. Fang C, Gilbert M J and Bernevig B A 2013 Phys. Rev. B 88, 085406
9. Li Z et al 2015 Phys. Rev. B 91, 235128
10. Li H et al 2018 J. Phys.: Condens. Matter https://doi.org/10.1088/1361-648X/aae17b
11. Legner M, Rüegg A and Sigrist M 2014 Phys. Rev. B 89, 085110
12. Xu N, Ding H and Shi M 2016 J. Phys.: Condens. Matter 28, 363001
13. Vekic M et al 1995 Phys. Rev. Lett. 74, 2367
14. Peters R, Yoshida T and Kawakami N 2018 Phys. Rev. B 98, 075104
15. Zhou Y Z et al 2017 Science Bulletin 62, 1439
16. Butch N P et al 2016 Phys. Rev. Lett. 116, 156401
17. Chang K W and Chen P J 2018 Phys. Rev. B 97, 195145
18. Alexandrov V, Coleman P, and Erten O 2015 Phys. Rev. Lett. 114, 177202
19. Kotliar G and Rudenberg A E 1986 Phys. Rev. Lett. 57, 1362
20. Sun S J, Yang M F and Hong T M 1993 Phys. Rev. B 48, 16127
21. Paraskevas P, Martin B and Mohamed M 2015 Europhys. Letts. 110, 66002