Article

On Strong f -Electron Localization Effect in a Topological Kondo Insulator

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Abstract: We study a strong f -electron localization effect on the surface state of a generic topological Kondo insulator (TKI) system by performing a mean-field theoretic (MFT) calculation within the framework of the periodic Anderson model (PAM) using the slave boson technique. The surface metallicity, together with bulk insulation, requires this type of localization. A key distinction between surface states in a conventional insulator and a topological insulator is that, along a course joining two time-reversal invariant momenta (TRIM) in the same BZ, there will be an intersection of these surface states, an even/odd number of times, with the Fermi energy inside the spectral gap. For an even (odd) number of surface state crossings, the surface states are topologically trivial (non-trivial). The symmetry consideration and the pictorial representation of the surface band structure obtained here show an odd number of crossings, leading to the conclusion that, at least within the PAM framework, the generic system is a strong topological insulator.

Keywords: topological Kondo insulator; surface state; periodic Anderson model; slave boson technique; time-reversal invariant momenta

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1. Introduction

We investigate the effects of a strong f -electron localization on the surface state of a generic topological Kondo insulator (GTKI). The boride SmB_6 is a typical example of this class of compound. Its d band metallic counterpart is LaB_6 . In fact, it was proposed in 2008—after the discovery of topological insulators (TIs)—that SmB_6 is a topological band insulator [1] supporting metallic surface states with an insulating bulk. The angle-resolved photoemission spectroscopy (ARPES) [2,3] and the transport measurement [4] on SmB_6 seem to authenticate the topological interpretation of SmB_6 , providing persuasive affirmation of metallic surface states with an insulating bulk. In this paper, our focal point is a generic topological Kondo insulator (GTKI) and its band structure. We study the strong f -electron localization effect on the surface state of this system. At times, in the course of the discussion, we will refer to SmB_6 to clarify issues that come into view. For example, the issue of categorization (in regard to weak and strong TI). A TKI, such as SmB_6 , needs to display an odd number of band-crossings between the Sm 4 f - and 5 d -bands (or, is it overwhelmingly 2 p B? [5]) to be categorized as a strong TI; an even number of crossings corresponds to a weak TI. Our analysis is based on the Periodic Anderson Model (PAM) [6,7], which is well-suited to discuss a Kondo insulator (KI) [7]. In Section 3, we show how the strong f -electron localization makes GTKI fall into the former category.

A KI basically corresponds to periodic array (Kondo lattice) of localized spin states, which hybridize with itinerant electron sea leading to an energy gap in the electronic density of states (DOS) whose magnitude is strongly temperature-dependent and only fully developed at low temperatures. Interestingly, KIs display metallic behavior at a high temperature regime. Upon reducing temperature, the resistivity decreases to a minimum value, followed by a divergence of the form $-\ln(T)$. As concluded by Kondo [8], such

a strange variation can be ascribed to strong dependence on the conduction electron scattering by the localized magnetic moments. The *s*-*d* hybridization model put forward by Kondo displays a similar trend in resistivity up to a certain temperature, generally referred to as the Kondo temperature (T_K). At temperatures less than T_K , the resistivity is found to diverge. The proximity of periodic ions brings into play an additional strong correlation effect (SCE), which leads to the renormalization of band structure and reconstruction of the hybridization gap in the density of states (DOS). While for heavy fermion metals, the Fermi level coincides with a finite DOS (the chemical potential is located in the conduction band), for KI, the Fermi level falls in the hybridization gap, which could be direct or indirect [9]. Most studied Kondo insulators [9] are FeSi, Ce₃Bi₄Pt₃, SmB₆, YbB₁₂, and CeNiSn. Upon decreasing the temperature further, there would be coupling of the spins of the itinerant electrons, and those of the impurities, leading to the spin-flip scattering (SFS) and the disappearance of the $-\ln(T)$ behavior. The near disappearance of local magnetic moments will also occur, due to the screening by the sea of conduction electrons. In fact, the spin-spin coupling, and SFS, also cause formation of spin singlets. This eventually leads to a typical Doniach-like phase diagram [10] (see Section 2). The topological Kondo insulator [11,12] (TKI), on the other hand, is a class of narrow gap insulators, in which the gap is created by strong *f*-electron correlations, which are, at the same time, topologically ordered due to large spin orbit coupling (and the odd/even-parity of the localized *f*-states/conduction band). The strongly localized *f* electrons and the spin-momentum locked helical liquid-like band structure in the surface of these systems give rise to exquisite electronic properties. In Figure 1, we present a qualitative sketch of DOS (eV⁻¹) as a function of energy (eV) for a GTKI. It should be mentioned that the hybridization gap on Sm-terminated and B-terminated surfaces exhibit very similar behavior, including the display of a finite DOS at $E = 0$, compatible with an additional (surface) conductance channel. Supposing Figure 1 corresponds to an Sm-terminated surface, all other features are shifted toward smaller absolute values of energy on a B-terminated surface.

The periodic Anderson model [6,7], used in this communication for a GTKI [1–5], ignores the complicated multiplet structure of the *d* and *f* orbitals, usually encountered in real TKIs, such as SmB₆. As a quick side note, we present the structure of SmB₆ to apprise the readers with the complications involved: electrons in a rare earth occupy shells of either [Xe]4f^{*n*}5d¹6s² or [Xe]4f^(*n*+1)5d⁰6s². The states have multiplet energy levels: Sm4f levels split into 4f_{5/2} and 4f_{7/2} bands with large energy separation. There is strong onsite repulsion of *f* electrons. We assume in PAM that the *f* electrons locally interact via a Hubbard-*U* repulsion, while the *d* electrons are practically non-interacting. The crystal field splits Sm 4f_{5/2} bands into a Γ_7 doublet and a Γ_8 quartet. Away from the Γ point, the Γ_8 quartet further splits into Γ_8^1 and Γ_8^2 doublets. Furthermore, Sm 5d states exhibit with t_{2g} and e_g symmetry. These splittings are depicted in a cartoon caricature in Figure 2. In a realistic description, the starting Hamiltonian *H* must involve terms representing this complex multiplet structure of the *d* and *f* orbitals, including the strong correlation effect. In that case, however, the analysis will be an unenviable task. Besides, such an analysis is beyond the scope of this communication. We note that the 4f electrons are closer to the nucleus in comparison with the 5d or 6s electrons. Thus, the electrons in the 4f shell are more localized (than the 5d or 6s electrons) and, consequently, their orbital angular momentum behaves like that of a free atom. On the other hand, the outer ones, such as the ones in 5d orbital, are in the midst of the crystalline environment. For this reason, the angular momentum average is almost zero due to its precession in the crystal field. As regards the boride SmB₆, it possesses inversion symmetry (see Section 3). The Z_2 topological invariants were computed via parity analysis by previous researchers [2–4], who found that $Z_2 = 1$. Based on this, it was predicted by Dzero et al. [13–16] that SmB₆ is a topologically non-trivial system. Furthermore, within the bulk hybridization gap, the signatures of two-dimensional Fermi surfaces on (100) and (101) surface planes, supporting the presence of topological surface states, were obtained in the quantum oscillation experiments of Li et al. [17]. Regarding quantum oscillations, it should be noted that Tan et al. [18] and, subsequently, Sebastian et al. [19], uncovered

a deep mystery associated with the insulating bulk of SmB_6 , which is the formation of a large three-dimensional (solely) conduction electron Fermi surface (FS), given that, thus far, such FSs have been considered the preserve of metals, in the absence of the long-range charge transport. This is possibly due to the residual density of states at the Fermi energy (shown in Figure 1) in SmB_6 . The existence of the residual DOS was indicated through measurements of heat capacity [20] long ago. Now, coming back to our original focus—a recent study [5] by Maiti et al. argued that the observed metallic surface states have trivial origins, rendering SmB_6 a trivial surface conductor. The symmetry consideration and the pictorial representation of the surface band structure obtained show an odd number of crossing (presented in Section 3 of this paper), which leads to the conclusion that this is not true for a GTKI.

Figure 1. A qualitative sketch of DOS (eV^{-1}) as a function of energy (eV) for a GTKI. While for TI and TKI, the Fermi level falls in the hybridization gap of total density of states (DOS), heavy fermion metals, the Fermi level coincides with a finite DOS. The position of the Fermi energy E_F is set at zero energy. There is a finite DOS-value at energy $E = E_F$. This might indicate an incomplete (or pseudo) gap, but it is also compatible with an additional conductance channel at the surface.

Figure 2. A cartoon caricature representation of the bulk band structure without self-energy broadening in SmB₆. An alternative, conventional representation of the evolution of energy levels of the f -states in SmB₆, due to intervention of the spin–orbit coupling and the crystal field, is shown in the lower panel for greater clarity. The f -states are split into $J = 7/2$ and $J = 5/2$ states by spin–orbit coupling (SOC). The $J = 5/2$ state, slightly below the Fermi energy E_F , is split into a Γ_7 doublet and a Γ_8 quartet by the crystal field (CF). Away from the Γ point, the Γ_8 quartet is further split into $\Gamma_8^{(1)}$ and $\Gamma_8^{(2)}$ doublets. The hybridization between the Γ_7 , $\Gamma_8^{(1)}$ bands and the conduction band opens two gaps, which are denoted as Δ (typically around 15 meV) and $\Delta' \sim 3$ meV.

We now present the organization of the paper: in Section 2, we begin with dispersive f and d bands involving hopping (t_f, t_d) for f , and d electrons with $t_d \gg t_f$. The d bands correspond to bath, which can be described by Bloch states. The assumption that the correlation between electrons on the impurity ion (f band), much greater than all hopping terms, has the effect of favoring the single occupation of the impurity level. The correlation, being important for the formation of a magnetic moment on the localized f -orbital, arises from the Coulomb repulsion $U \gg t_d$ between the electrons. The next term involves the f band, and d/p bands, which hybridize at cryogenic temperatures (a strong spin-orbit overlap) forming an insulating gap, with the Fermi level residing in the hybridization gap. The hybridization V , between an odd-parity nearly localized band and an even-parity delocalized conduction band, plays the role of band-inversion, yielding a 3D TI. These terms together constitute PAM Hamiltonian, where there are two different species of electrons, namely conduction electrons and localized electrons. When U is very large ($U \gg t_d$) and $V \ll t_d$, the weight of configurations with the number of f electrons, significantly different from the average number, is few and far between in the ground-state wave function, and charge fluctuations become effectively non-existent. This results in transformation of the PAM Hamiltonian H^{PAM} to Kondo lattice Hamiltonian H_K [21,22] that describes the interaction between spins of localized and conduction electrons. The Hamiltonian H_K is obtained by using a second-order perturbation, with respect to hybridization V of PAM, where the localized f electrons can exchange with the conduction electrons bath, allowing both charge and spin fluctuations to occur. Whereas the Hamiltonian H_K leads to Kondo singlet formation, H^{PAM} constitutes our minimalistic Hamiltonian H^{bulk} which captures essential physics of GTKI in the presence of strong f -electron localization, such as the bulk and surface band-structure topology. In Section 3, we investigate the surface state Hamiltonian H_s in slab geometry, starting from H^{bulk} . We use the Dirac-matrix Hamiltonian (DMH) method [23] to ascertain whether SmB_6 is a weak or strong TKI. We should note that when a slab of finite thickness is considered, two surface states overlap, such that off-diagonal mass-like term M_0 must be included in the surface Hamiltonian H_s above. For this, the matrix $\gamma_5 M_0$ is suitable, where $\gamma_5 \equiv i\gamma_0\gamma_1\gamma_2\gamma_3$ and γ_j are Dirac matrices in the Dirac basis. As an important step of the DMH method, one needs to check anti-commutativity of the matrix $\gamma_5 M_0$ with H_s . We obtain here $\{H_s, \gamma_5 M_0\} \neq 0$ and, therefore, the topological stability of the band crossing is possible [23]. The combined surface state Hamiltonian that we proceed with is $H^{\text{slab}}(k_x, k_y) = H_s(k_x, k_y) + \gamma_5 M_0$. We find that $H^{\text{slab}}(k_x, k_y)$ preserves time reversal symmetry (TRS) and the inversion symmetry (IS). The pictorial representation of the surface band structure obtained by us leads to the conclusion that, at least within the single impurity PAM framework, the GTKI system under consideration is a strong topological insulator. The paper ends with a discussion and concluding remarks in Section 4.

2. Kondo Screening

A Kondo system exhibits the Kondo screening. Thus, while investigating a Kondo system, the possibility of the Kondo screening needs to be explored. In effort to do this, we calculate the Kondo singlet density below within the PAM-Kondo framework. The PAM model [6,7,24] on a simple cubic lattice for d and f electrons in momentum-space is as follows:

$$\begin{aligned} \mathcal{N} = & \sum_{k,\zeta=\uparrow,\downarrow} (-\mu - \epsilon_k^f) f_{k,\zeta}^\dagger f_{k,\zeta} + \sum_{k,\zeta=\uparrow,\downarrow} (-\mu - \epsilon_k^d) d_{k,\zeta}^\dagger d_{k,\zeta} \\ & + \sum_{k,\zeta=\uparrow,\downarrow} \left\{ \Gamma_{\zeta=\uparrow,\downarrow}(\mathbf{k}) d_{k,\zeta}^\dagger f_{k,\zeta} + \text{H.C.} \right\} + \mathcal{N}_{\text{int}} \end{aligned} \quad (1)$$

$$\begin{aligned}
\epsilon_k^d &= [2t_{d1} c_1(k) + 4t_{d2} c_2(k) + 8t_{d3} c_3(k)], \\
\epsilon_k^f &= [-\epsilon_f + 2t_{f1} c_1(k) + 4t_{f2} c_2(k) + 8t_{f3} c_3(k)], \\
c_1(k) &= (\cos k_x a + \cos k_y a + \cos k_z a), \\
c_2(k) &= (\cos k_x a \cos k_y a + \cos k_y a \cos k_z a + \cos k_z a \cos k_x a), \\
c_3(k) &= (\cos k_x a \cos k_y a \cos k_z a), \\
\aleph_{int} &= U_f \sum_{i(\text{site index})} f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow}
\end{aligned} \tag{2}$$

We have assumed that, whereas the coulomb repulsion between f electrons on the same site could be approximated by a term involving the Hubbard- U , the d electrons are practically non-interacting. In rest of the terms, in momentum-space, d and f electrons are represented by creation (annihilation) operators $d_{k\zeta}^\dagger$ ($d_{k\zeta}$) and $f_{k\zeta}^\dagger$ ($f_{k\zeta}$), respectively. Here, the index ζ ($=\uparrow, \downarrow$) represents the spin or pseudo-spin of the electrons with a as the lattice constant. The first and the second term, respectively, describe the dispersion of the f and d electrons. The parameters (t_{f1} , t_{f2} , t_{f3}), and (t_{d1} , t_{d2} , t_{d3}) correspond to the (NN, NNN, NNNN) hopping for the f and d electrons, respectively. The hybridization between the f -electrons ($l = 3$ and, hence, odd parity) and the conduction d -electrons ($l = 2$ and, hence, even parity) [6,7,24] are given by the third term. The parity is a good quantum number. It follows that, at high symmetry points (HSP) in the Brillouin zone (BZ), where odd and even parity states cannot mix, the third term is zero. The presence of the hybridization node at HSP is an important feature of TKI. Furthermore, since the f - and d -states have different parities, the momentum-dependent form-factor matrix $\Gamma_{\zeta=\uparrow, \downarrow}(k)$ involved in the third term in (1) must be odd: $\Gamma_{\zeta=\uparrow, \downarrow}(-k) = -\Gamma_{\zeta=\uparrow, \downarrow}(k)$. This is required in order to preserve time reversal symmetry (TRS), as the matrix involves coupling with the physical spin of the electron. Therefore, we write $\Gamma_{\zeta=\uparrow, \downarrow}(k) = -2V(s(k) \cdot \zeta)$, where V is a constant parameter characterizing the hybridization, $s(k) = (\sin k_x a, \sin k_y a, \sin k_z a)$ and $\zeta = (\zeta_x, \zeta_y, \zeta_z)$ are the Pauli matrices in physical spin space. In Section 4, we outline what to use as more complicated odd-parity expressions for Γ , to reinvestigate the present problem, expecting newer information.

The system shows the bulk metallic as well as the bulk insulating phases determined by the sign of t_{f1} . It is positive for the former and negative for the latter phase [24]. The negative sign of t_{f1} is also necessary for the band inversion, which induces the topological state [25]. Since the bandwidth of the f electrons needs to be smaller than the bandwidth of the conduction electrons, we assume that $|t_{f1}| \ll |t_{d1}|$. Similar relations hold for second- and third-neighbor hopping amplitudes. For the hybridization parameter V , we assume $|V| < |t_{d1}|$. **Throughout the paper, we choose t_{d1} to be the unit of energy, except in the investigation of Kondo screening.** We further assume that, while the d electrons are non-interacting, the on-site coulomb repulsion of f -electrons is given by Hubbard U [24]. Under the assumption that U is considerably greater than $|t_{d1}|$, one may write the thermal average of the TKI slave boson mean-field Hamiltonian [24] in the following form (see also Section 4):

$$\begin{aligned}
\aleph_{sb}(b, \lambda, \zeta) &= \sum_{k\zeta=\uparrow, \downarrow} (-\mu - \zeta - \epsilon_k^d) \langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle \\
&\quad + \sum_{k,\zeta=\uparrow, \downarrow} (-\mu + \zeta - b^2 \epsilon_k^f + \lambda) \langle s_{k,\zeta}^\dagger s_{k,\zeta} \rangle \\
&\quad + b \sum_{k,\zeta,\sigma=\uparrow, \downarrow} \{ \Gamma_{\zeta=\uparrow, \downarrow}(k) \langle d_{k,\zeta}^\dagger s_{k,\zeta} \rangle + \text{H.C.} \} + \lambda N_s (b^2 - 1)
\end{aligned} \tag{3}$$

where the additional terms, in comparison with (1), are $\lambda \left[\sum_{k,\sigma=\uparrow, \downarrow} s_{k,\zeta}^\dagger s_{k,\zeta} + N_s (b^2 - 1) \right] - \zeta [N_d - N_s] - \mu [(N_d + N_s) - N]$ where λ is a Lagrange multiplier, μ is the chemical potential, N_d is the number of lattice sites for d electrons, and N_s corresponds to that for f -electrons. The first term describes the constraint on the pseudo-particles due to the infinite Coulomb repulsion. This ensures strong localization of f electrons. The second term compels observance of the fact that the d and f fermions are equal in number ($N_d = N_s$). The reason simply is the key requirement for a Kondo insulator, viz. the formation of singlet pairing states between d and f fermions at each lattice site for which the number of d and f fermions must be equal on average. The third term is the constraint that

fixes the total number of particles N ($N = N_d + N_s$). An explanation to highlight the physical mechanism underlying the second constraint, and the physical interaction that enforces it, perhaps will not be irrelevant: we investigate the Kondo screening under the assumption “large on-site repulsion ($U_f \gg t_{d1}$) between the f -electrons” (and no interaction U_d between conduction electrons). In this situation, each impurity simply becomes an isolated magnetic moment correlated with an itinerant electron spin. The necessity of “chemical potential” ξ is rooted in the correlation between impurity and conduction electron spins. The interaction involved is the spin–spin exchange interaction. It is clear from Equation (3) that the hybridization parameter is renormalized by the c -number b . It is also clear that the dispersion of the f -electron is renormalized by λ and its hopping amplitude by b^2 . The total parameters are, thus, the Lagrange multiplier λ , auxiliary chemical potentials ξ and μ (μ is a free parameter), and slave boson field b . In order to make this paper self-contained, we found it necessary to include these facts, though these are explained clearly in reference [24]. The minimization of the thermodynamic potential per unit volume, relative to the parameters (b, λ, ξ) yields equations to determine them: $\partial \Omega_{sb} / \partial b = 0, \partial \Omega_{sb} / \partial \lambda = 0$, and $\partial \Omega_{sb} / \partial \xi = 0$, where $\beta = (k_B T)^{-1}$, k_B is the Boltzmann constant and T is temperature. The method outlined in references [26,27] was used to calculate the thermodynamic potential.

The equations $\partial \Omega_{sb} / \partial b = 0, \partial \Omega_{sb} / \partial \lambda = 0$, and $\partial \Omega_{sb} / \partial \xi = 0$, respectively, can be written as $2\lambda b = N_s^{-1}(\alpha_1 + \alpha_2 + \alpha_3)$, $(1-b^2) = N_s^{-1}(\beta_1 + \beta_2 + \beta_3)$, and $0 = N_s^{-1}(\gamma_1 + \gamma_2 + \gamma_3)$ where

$$\begin{aligned}\alpha_1 &= \sum_k \frac{\partial}{\partial b} [2V(s_x - i s_y) \langle d_{k\uparrow}^\dagger b s_{k,\downarrow} \rangle + 2V(s_x - i s_y) \langle b s_{k,\uparrow}^\dagger d_{k\downarrow} \rangle + \text{H.C.}] \\ \alpha_2 &= \sum_{k,\zeta} \frac{\partial}{\partial b} [\epsilon_k^f \langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \epsilon_k^d \langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle] \\ \alpha_3 &= \sum_{k,\zeta} \frac{\partial}{\partial b} [2V s_z \zeta \langle d_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \text{H.C.}],\end{aligned}\quad (4)$$

$$\begin{aligned}\beta_1 &= \sum_k \frac{\partial}{\partial \lambda} [2V(s_x - i s_y) \langle d_{k\uparrow}^\dagger b s_{k,\downarrow} \rangle + 2V(s_x - i s_y) \langle b s_{k,\uparrow}^\dagger d_{k\downarrow} \rangle + \text{H.C.}] \\ \beta_2 &= \sum_{k,\zeta} \frac{\partial}{\partial \lambda} [\epsilon_k^f \langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \epsilon_k^d \langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle] \\ \beta_3 &= \sum_{k,\zeta} \frac{\partial}{\partial \lambda} [2V s_z \zeta \langle d_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \text{H.C.}],\end{aligned}\quad (5)$$

$$\begin{aligned}\gamma_1 &= \sum_k \frac{\partial}{\partial \xi} [2V(s_x - i s_y) \langle d_{k\uparrow}^\dagger b s_{k,\downarrow} \rangle + 2V(s_x - i s_y) \langle b s_{k,\uparrow}^\dagger d_{k\downarrow} \rangle + \text{H.C.}] \\ \gamma_2 &= \sum_{k,\zeta} \frac{\partial}{\partial \xi} [\epsilon_k^f \langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \epsilon_k^d \langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle] \\ \gamma_3 &= \sum_{k,\zeta} \frac{\partial}{\partial \xi} [2V s_z \zeta \langle d_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \text{H.C.}]\end{aligned}\quad (6)$$

$$\epsilon_k^d = [2t_{d1} c_1(k) + 4t_{d2} c_2(k) + 8t_{d3} c_3(k)] \quad (7)$$

$$\epsilon_k^f = [-\epsilon_f + 2t_{f1} c_1(k) + 4t_{f2} c_2(k) + 8t_{f3} c_3(k)]. \quad (8)$$

The averages $\langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle$, $\langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle$, etc., were calculated below in the finite temperature formalism. Here the time evolution an operator O is given by $O(\tau) = \exp(\mathfrak{N}\tau) O \exp(-\mathfrak{N}\tau)$, where τ is imaginary time. The equations for the operators $\{d_{k,\zeta}(\tau), s_{k,\zeta}(\tau)\}$ can be written down easily, for the Hamiltonian is completely diagonal. Starting with this Hamilton, the thermal averages in the equations above are determined in a self-consistent manner. The Green's functions $G_{sb}(k\zeta, k\zeta, \tau) = -\langle T_\tau \{d_{k,\zeta}(\tau) d_{k,\zeta}^\dagger(0)\} \rangle$, $F_{sb}(k\zeta, k\zeta, \tau) = -b^2 \langle T_\tau \{s_{k,\zeta}(\tau) d_{k,\zeta}^\dagger(0)\} \rangle$, etc., are of primary interest. Here T_τ is the time-ordering operator acting on

imaginary times τ . It arranges other operators, such as $d_{k,\zeta}(\tau)$, etc., from left to right with descending imaginary time arguments. We obtain

$$\begin{aligned}
 G_{sb}(k \uparrow, k \uparrow, \tau \rightarrow 0^+) &= u_{k,+}^{(-)^2} f_-^{(-)}(k, \mu) + u_{k,-}^{(-)^2} f_+^{(-)}(k, \mu), \\
 G_{sb}(k \downarrow, k \downarrow, \tau \rightarrow 0^+) &= u_{k,+}^{(+)^2} f_-^{(+)}(k, \mu) + u_{k,-}^{(+)^2} f_+^{(+)}(k, \mu), \\
 F_{sb}(k \uparrow, k \uparrow, \tau \rightarrow 0^+) &= (u_{k,+}^{(+)^2} - v_{k,+}^{(+)^2}) f_-^{(+)}(k, \mu) + (u_{k,-}^{(+)^2} + v_{k,-}^{(+)^2}) f_+^{(+)}(k, \mu) \\
 &\quad + v_{k,+}^{(+)^2} f_+^{(-)}(k, \mu) - v_{k,-}^{(-)^2} f_-^{(-)}(k, \mu), \\
 F_{sb}(k \downarrow, k \downarrow, \tau \rightarrow 0^+) &= (u_{k,-}^{(+)^2} + v_{k,-}^{(+)^2}) f_+^{(-)}(k, \mu) + (u_{k,+}^{(+)^2} - v_{k,+}^{(+)^2}) f_-^{(-)}(k, \mu) \\
 &\quad + v_{k,-}^{(-)^2} f_+^{(+)}(k, \mu) - v_{k,+}^{(+)^2} f_-^{(+)}(k, \mu), \\
 f_-^{(-)}(k, \mu) &= (e^{\beta(\in_-^{(-)}(k) - \mu)} + 1)^{-1}, \quad f_+^{(-)}(k, \mu) = (e^{\beta(\in_+^{(-)}(k) - \mu)} + 1)^{-1} \\
 f_-^{(+)}(k, \mu) &= (e^{\beta(\in_-^{(+)}(k) - \mu)} + 1)^{-1}, \quad f_+^{(+)}(k, \mu) = (e^{\beta(\in_+^{(+)}(k) - \mu)} + 1)^{-1}.
 \end{aligned} \tag{9}$$

Here

$$\begin{aligned}
 u_{k,\pm}^{(\zeta)^2} &= \frac{1}{2} [1 \pm \frac{(2\zeta + \epsilon_k^d - b^2 \epsilon_k^f + \lambda)}{2\{\epsilon(k, b, \lambda, \zeta)\}}], \quad v_k^{(\zeta)^2} = \frac{-2V^2 b^2 s_z^2}{\epsilon(k, b, \lambda, \zeta) [\frac{(2\zeta + \epsilon_k^d - b^2 \epsilon_k^f + \lambda)}{2} + \zeta \epsilon(k, b, \lambda, \zeta)]}, \\
 \epsilon(k, b, \lambda, \zeta) &= \sqrt{\frac{(2\zeta + \epsilon_k^d - b^2 \epsilon_k^f + \lambda)^2}{4} + 4V^2 b^2 (s_x^2 + s_y^2 + s_z^2)}, \\
 \in_a^{(\zeta)}(k) &= -\frac{(\epsilon_k^d + b^2 \epsilon_k^f - \lambda)}{2} + \alpha \sqrt{\frac{(2\zeta + \epsilon_k^d - b^2 \epsilon_k^f + \lambda)^2}{4} + 4V^2 b^2 (s_x^2 + s_y^2 + s_z^2)}, \\
 \langle d_{k\uparrow}^\dagger b s_{k\downarrow} \rangle &= \frac{V(s_x + i s_y)}{\epsilon(k, b, \lambda, \zeta)} [f_-^{(-)}(k, \mu) - f_+^{(-)}(k, \mu)], \\
 \langle b s_{k\uparrow}^\dagger d_{k\downarrow} \rangle &= \frac{V(s_x + i s_y)}{\epsilon(k, b, \lambda, \zeta)} [f_-^{(+)}(k, \mu) - f_+^{(+)}(k, \mu)],
 \end{aligned} \tag{10}$$

and $\alpha = 1$ (-1) for upper band (lower band), $\zeta = \pm 1$ labels the eigenstates ($\uparrow, \downarrow$) of ζ_z .

The expressions for the averages $\langle d_{k\uparrow}^\dagger b s_{k\downarrow} \rangle$ and $\langle b s_{k\uparrow}^\dagger d_{k\downarrow} \rangle$, etc., show that, in the zero-temperature and the long-wavelength limits, their contributions to the derivatives in (4)–(6) are insignificant in comparison with those of $\sum_{k,\zeta} [\epsilon_k^f \langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \epsilon_k^d \langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle]$. The observation allows us to approximate the equations $\partial' \Omega_{sb} / \partial b = 0$, $\partial' \Omega_{sb} / \partial \lambda = 0$, and $\partial' \Omega_{sb} / \partial \zeta = 0$ as

$$2 \lambda b \approx N_s^{-1} \sum_{k,\zeta} \frac{\partial}{\partial b} [\epsilon_k^f \langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \epsilon_k^d \langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle] \tag{11}$$

$$(1 - b^2) \approx N_s^{-1} \sum_{k,\zeta} \frac{\partial}{\partial \lambda} [\epsilon_k^f \langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \epsilon_k^d \langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle] \tag{12}$$

$$0 \approx N_s^{-1} \sum_{k,\zeta} \frac{\partial}{\partial \zeta} [\epsilon_k^f \langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle + \epsilon_k^d \langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle] \tag{13}$$

in these limits. The restriction $\int dr \sum_\zeta s_\zeta^\dagger(r) s_\zeta(r) \cong N_s (1 - b^2)$ needs to be imposed for the conservation of auxiliary particle number. This has been noted above. Here $s_\zeta(r) = N_s^{-\frac{1}{2}} \sum_k e^{ik \cdot r} s_{k,\zeta}$. This is the fourth equation with (11)–(13) as the first three, and we have four unknowns, viz. $(b, \lambda, \zeta, ak_F)$, where $a \approx 4.13 \text{ \AA}$ is the lattice constant and ak_F is the Fermi wave number. We will briefly explain why a single value to the Fermi wave vector (ak_F) is assigned. In view of the fact that the chemical potential is a free parameter and could be somewhere between the valence and the conduction bands ($\mu > \in_-^{(+)}(k)$, $\in_-^{(-)}(k)$), once again, it is easy to see that in the long wavelength (i.e., low-lying states) and the zero-temperature limit, one may write the imposed restriction as $2 N_s^{-1} \sum_{k,\zeta} 1 = b^2 - b^4$. The integration on the left-hand-side is non-trivial, for assigning a single value to the Fermi wave vector (ak_F), of an anisotropic (lattice) band structure whose Fermi surface (FS) may not be a sphere, is inappropriate. However, as mentioned in Section 1, the formation of a

large three-dimensional (solely) conduction electron FS takes place in the insulating bulk of SmB₆. Deriving support of this mysterious finding, we assume FS to be a sphere in the first approximation. This leads to the equation

$$b^2 = \frac{1}{2} \left[1 \pm \sqrt{1 - \left(\frac{8}{3}\right) (a^3 k_F^3)} \right]. \quad (14)$$

With a little algebra, we find that, whereas (11) and (12) together yield $\lambda = -6t_{f1} + 6b^2 t_{f1}$, Equation (13) yields $\xi = -3t_{d1} + 3t_{f1}$. This equation for ξ will be extremely useful in Section 3. We now estimate (ak_F) in the following manner: since the effective mass m^* (Fermi velocity v_F^*) of the particles in low-lying states is known to be about $100 m_e$ (<0.3 eV-Å) [24], the relation $m^* = \frac{\hbar k_F}{v_F^*}$ yields $(ak_F) \sim 0.2$, which is consistent with the long wavelength limit we have taken. The two values of b^2 obtained from (14) are 0.9430 and 0.0565. As we see below in Equation (15), when b is non-zero, the system corresponds to a Kondo state, and, when b is zero, the system is a non-interacting, dispersive lattice gas mixture of itinerant electrons and charge carrying heavy bosons (see Section 4). Thus, the admissible value of b^2 will be 0.9430. As all of the unknown parameters have been determined, the stage is set to consider the Kondo screening.

We calculate the Kondo singlet density, which is defined as $K_{\text{singlet}}(k, b, \lambda, \mu, \xi) = [\langle d_{k\uparrow}^\dagger b s_{k,\downarrow} \rangle + \langle b s_{k,\uparrow}^\dagger d_{k\downarrow} \rangle]$. This average is the ultimate signature of the Kondo insulating state, where there is precisely one conduction electron paired with an impurity spin. The important point now is that a large U puts down charge fluctuations on the local moment site. The corresponding “charge degree of freedom” is “quenched”. The degree of freedom that remains at the impurity is its spin. Naturally, the Hamiltonian should contain a term H_k comprising of the spin operator of the impurity and the conduction electron spin. Suppose, S_m denotes the m th-site impurity spin operator, and $s_m = (\frac{1}{2}) d_{m\zeta}^\dagger \zeta_z d_{m\zeta}$ is that for the conduction electron spin, where $d_{m\zeta}$ is the fermion annihilation operator at site- m and spin-state ζ ($=\uparrow, \downarrow$) and ζ_z is the z -component of the Pauli matrices. The required term H_k can now be written [28] as $[-|J|/t_{d1}] \sum_m S_m \cdot s_m$. This is an anti-ferromagnetic exchange-coupling term representing the exchange interaction between the itinerant (conduction) electrons and impurity magnetic moment in the system. For $|S| > 1$, we may approximate the impurity spins as classical vectors. This allows us to replace the exchange coupling constant J by $M = -(|J|/t_{d1})$. It follows that the exchange field term gives the dimensionless contribution $[M \sum_{k,\zeta} \text{sgn}(\zeta) d_{k,\zeta}^\dagger d_{k,\zeta}]$ to the Hamiltonian in (3), in the basis $(d_{k\uparrow}^\dagger f_{k\uparrow} d_{k\downarrow}^\dagger f_{k\downarrow})^T$ in the momentum space. We notice that since a band electron hops on to the impurity site to gain kinetic energy or the impurity electron hops on to the band to lose kinetic energy, the spin flip during such hopping gives rise to an anti-ferromagnetic (AFM) exchange interaction term. Another important point is that in the local moment limit, the Anderson and Kondo couplings describe the same physics. A fundamental difference between them, however, is that the Anderson model includes charge fluctuations that determine the coupling, while there is absence of the spin-orbit coupling ($V \ll t_{d1}$) in the Kondo model, which includes only spin-spin interactions [28]. The interaction is non-zero only in the local moment regime. The complete derivation of the AFM interaction can be found in terms of the Schrieffer–Wolff transformations [28]. The averages $\langle d_{k,\zeta}^\dagger d_{k,\zeta} \rangle$, $\langle b s_{k,\zeta}^\dagger b s_{k,\zeta} \rangle$, etc. have been calculated below in the finite-temperature formalism, as outlined above in page 8. We find

$$K_{\text{singlet}}(k, u) = A_- [f_-^{(-)}(k, \mu) - f_+^{(-)}(k, \mu)] + A_+ [f_-^{(+)}(k, \mu) - f_+^{(+)}(k, \mu)], \quad (15)$$

$$A_- = \frac{2V^2(s_x^2 + s_y^2)}{\varepsilon_-(k, b, \lambda, \mu, \xi)}, \quad A_+ = \frac{2V^2(s_x^2 + s_y^2)}{\varepsilon_+(k, b, \lambda, \mu, \xi)}, \quad (16)$$

$$\varepsilon_{\pm}(k, b, \lambda, \xi) = \sqrt{\frac{(2\xi + \epsilon_k^d - b^2 \epsilon_k^f + \lambda \mp M)^2}{4} + 4V^2 b^2 (s_x^2 + s_y^2 + s_z^2)} \quad (17)$$

$$\epsilon_{\alpha}^{(\zeta)}(k) = \frac{-\frac{(\epsilon_k^d + b^2 \epsilon_k^f - \lambda + \zeta M)}{2} + \alpha \sqrt{\frac{(2\zeta + \epsilon_k^d - b^2 \epsilon_k^f + \lambda + \zeta M)^2}{4} + 4V^2 b^2 (s_x^2 + s_y^2 + s_z^2)}}{2} \quad (18)$$

With help from Equations (16)–(18), we obtain non-zero values of K_{singlet} defined in Equation (15). As a function of anti-ferromagnetic exchange field energy (M) and (Boltzmann constant Temperature) (kT) in eV, we have contour/3D plotted K_{singlet} in Figure 3 for (a) $\mu = 0.00$ eV, $t_{d1} = 0.38$ eV, and $t_{f1} = -0.02$ eV, and (b) $\mu = 0.00$ eV, $t_{d1} = 0.60$ eV and $t_{f1} = -0.03$ eV, at $ak_x = ak_y = ak_z = 1$. The anti-ferromagnetic quantum critical point (AFM QCP) is, respectively, at $M = M_C = 0.035$ eV and 0.060 eV in (a), and (b), respectively. The two diagrams below show that the location of QCP is strongly dependent on t_{d1} and t_{f1} . The anti-ferromagnetic quantum critical point (AFM QCP) at $T = 0$ K, in the former case, is at $M_{c1} = 0.03$ eV, and in the latter case is at $M_{c2} = 0.060$ eV. The contour plot appears as the Doniach-like phase diagram [10]: close to 0 K, approximately, the region $M > M_c$ corresponds to the heavy-fermion liquid, while the region $M < M_c$ corresponds to anti-ferromagnetic liquid with the quantum critical region in between. We also notice that the location of QCP depends on μ and t_{f1} . For example, the QCP value increases with a decrease in $|t_{f1}|$ when t_{d1} and μ are held fixed.

Figure 3. Cont.

(b)

Figure 3. The contour/3D plots of Kondo singlet term given by Equation (15) as a function of anti-ferromagnetic exchange field energy (M) and (Boltzmann constant temperature) (kT) in eV for (a) $\mu = 0.00$ eV, $t_{d1} = 0.38$ eV, and $t_{f1} = -0.02$ eV, and (b) $\mu = 0.00$ eV, $t_{d1} = 0.60$ eV and $t_{f1} = 0.03$ eV, at $ak_x = ak_y = ak_z = 1$. The anti-ferromagnetic quantum critical point (AFM QCP) is, respectively, at $M = M_C = 0.035$ and 0.060 eV in (a,b). Other parameters in terms of electron volts, in the graphical representations, are $b = 0.95$, $t_{d2} = 0.001$, $t_{f2} = 0.001$, $t_{d3} = 0.0001$, $t_{f3} = 0.0001$, $\varepsilon_f = -0.002$, and the hybridization parameter $V = 0.0001$ (negligible compared to t_{d1}).

3. Surface State Hamiltonian

The next important issue is how to get the surface state Hamiltonian $\hat{H} = \aleph^{slab}(k_x, k_y)$ for slab geometry from that of bulk $\aleph^{bulk}(k_x, k_y, k_z)$ in the non-local moment limit. To explain, we first consider a slab with a length, breadth, and thickness in the x , y , and z directions, respectively. The thickness is limited in $z \in [-d/2, d/2]$. We further assume the non-open boundary conditions. We can thus replace k_z by $-i\partial_z$, as in this case, k_z is not a good quantum number. The Hamiltonian $\aleph^{slab}(k_x, k_y)$ can be obtained from the Hamiltonian $\aleph^{bulk}(k_x, k_y, k_z = -i\partial_z)$ considering a set of ortho-normal basis states $\{|\varphi_n\rangle, n = 1, 2, 3, 4\}$ satisfying the completeness condition $I = \sum_n |\varphi_n\rangle\langle\varphi_n|$. The issue of obtaining the surface state Hamiltonian is thus settled. In terms of the basis states, an arbitrary state vector $|\Phi\rangle$ can be written as $|\Phi\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\Phi\rangle$. We now turn to the operator equation $\hat{H}|\psi\rangle = |\Phi\rangle$, where $|\psi\rangle$ is an arbitrary state vector. Again, in view of the completeness condition, one can write

$$|\Phi\rangle = \hat{H}|\psi\rangle = \hat{H} \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle = \sum_n \hat{H} |\varphi_n\rangle\langle\varphi_n|\psi\rangle. \quad (19)$$

Now, form the inner product $\langle\psi|\Phi\rangle$, where $\langle\psi|\Phi\rangle = (\langle\Phi|\psi\rangle)^*$. We have

$$\langle\psi|\Phi\rangle = \sum_{m,n} \langle\psi|\varphi_m\rangle \langle\varphi_m|\hat{H}|\varphi_n\rangle\langle\varphi_n|\psi\rangle. \quad (20)$$

We can write the last equation as $\langle \psi | \Phi \rangle = \sum_n \psi_n^* H_{mn} \psi_n$, where $H_{mn} = \langle \varphi_m | \hat{H} | \varphi_n \rangle$ and $\psi_n = \langle \varphi_n | \psi \rangle$. Here, ψ_n is an inner product and H_{mn} is the Hamiltonian matrix sought for. We choose the product as

$$\left(\frac{2}{d}\right)^{\frac{1}{2}} \left[\sin \left\{ \frac{n\pi \left(z + \frac{d}{2} \right)}{d} \right\} \right] \quad (n = 1, 2, 3, 4) \quad (21)$$

With this ansatz, the matrix elements may be written as

$$\aleph_{mn}^{slab}(k_x, k_y) = \left(\frac{2}{d}\right) \int_{-d/2}^{d/2} \left[\sin \left\{ \frac{m\pi \left(z + \frac{d}{2} \right)}{d} \right\} \right] \aleph_{mn}^{bulk}(k_x, k_y, -i\partial_z) \left[\sin \left\{ \frac{n\pi \left(z + \frac{d}{2} \right)}{d} \right\} \right] dz. \quad (22)$$

Since there are several examples of complete orthogonal systems, viz., the Legendre polynomials over $[-1, 1]$, and Bessel function over $[0, 1]$, and so on, one may ask why show preference for $\{\sin(nx), \cos(nx)\}$ over $[-\pi, \pi]$. The reason is—this is simpler to handle and it replicates the model of a periodic crystal potential, terminating at the surface, where it undergoes a jump abruptly to the vacuum level. Now, from the expectation value of the bulk Hamiltonian in (3), in the basis $(d_{k,\uparrow}^\dagger, d_{k,\downarrow}^\dagger, s_{k,\uparrow}^\dagger, s_{k,\downarrow}^\dagger)^T$, the Hamiltonian could be written in the matrix form as

$$\begin{pmatrix} \Gamma_{10} & 0 & -2Vbs_z & -2Vb(s_x - is_y) \\ 0 & \Gamma_{10} & -2Vb(s_x + is_y) & 2Vbs_z \\ -2Vbs_z & -2Vb(s_x - is_y) & \Gamma_{20} & 2Vbs_z \\ -2Vb(s_x + is_y) & 2Vbs_z & 0 & \Gamma_{20} \end{pmatrix}, \quad (23)$$

$$\Gamma_{10} = -\mu - \xi - \varepsilon_k^d,$$

$$\Gamma_{20} = -\mu + \xi - b^2 \varepsilon_k^f + \lambda.$$

In the basis $(d_{k,\uparrow}^\dagger, s_{k,\uparrow}^\dagger, d_{k,\downarrow}^\dagger, s_{k,\downarrow}^\dagger)^T$, the same bulk Hamiltonian will be given as

$$\begin{pmatrix} \Gamma_{10} & -2Vbs_z & 0 & -2Vb(s_x - is_y) \\ -2Vbs_z & \Gamma_{20} & -2Vb(s_x - is_y) & 0 \\ 0 & -2Vb(s_x + is_y) & \Gamma_{10} & 2Vbs_z \\ -2Vb(s_x + is_y) & 0 & 2Vbs_z & \Gamma_{20} \end{pmatrix} \quad (24)$$

Therefore, upon using (24), $\aleph_{mn}^{slab}(k_x, k_y)$ consistent with Equation (22) is given by H_s , which is equal to

$$\begin{pmatrix} \Gamma_1 & -i c_{\zeta=+1} & 0 & 0 \\ i c_{\zeta=+1} & \Gamma_2 & 0 & 0 \\ 0 & 0 & \Gamma_1 & i c_{\zeta=-1} \\ 0 & 0 & -i c_{\zeta=-1} & \Gamma_2 \end{pmatrix} \quad (25)$$

where $c_{\zeta=+1} = \frac{16Vba}{3d}$, $c_{\zeta=-1} = \frac{96Vba}{7d}$, $K = (k_x, k_y)$, and in the long wavelength limit $\Gamma_1(K) = -\mu - \xi - 6t_{d1} + t_{d1}K^2$, and $\Gamma_2(K) = -\mu + \xi + b^2\varepsilon_f - 6b^2t_{f1} + b^2t_{f1}K^2 + \lambda$. It may be noted that, in view of (14), $\Gamma_1(K) \approx \Gamma_2(K)$.

The Dirac matrices in Dirac basis is given by γ_j , where $j = (0, 1, 2, 3)$, and

$$\gamma_0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \gamma_j = \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix} \quad (26)$$

where σ_j are Pauli matrices. A fifth related matrix is usually defined as $\gamma_5 \equiv i\gamma_0\gamma_1\gamma_2\gamma_3 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$. We use below the Dirac-matrix Hamiltonian (DMH) method [23] to ascertain whether SmB_6 is a weak or strong TKI. It must be emphasized here that when a slab is

considered, the top and bottom of the slab interface with vacuum, and hopping events between the surface states on the top and bottom opens a finite gap at the Γ point ($k = 0$). If there is breaking of inversion symmetry (IS), then lifting the degeneracy of the surface state sub-bands with opposite spin angular momenta occurs. In this case, as we shall show, there is no IS breaking and, therefore, the two surface states overlap without spin flip. Off-diagonal mass-like terms must be included in the surface Hamiltonian H_s in a suitable basis, say, $(d^\dagger_{k,\zeta} s^\dagger_{k,\zeta} d^\dagger_{k,\zeta} s^\dagger_{k,\zeta})^T$ to characterize the opening of the finite gap at the Γ point. A matrix of the form

$$\begin{pmatrix} 0 & 0 & M_0 & 0 \\ 0 & 0 & 0 & M_1 \\ M_0 & 0 & 0 & 0 \\ 0 & M_1 & 0 & 0 \end{pmatrix}$$

where M_1 (hopping parameter for f -electrons) $\ll M_0$ (hopping parameter for d electrons) perhaps will be suitable to take care of the overlap scenario. In what follows we, however, choose the simpler matrix, namely $\gamma_5 M_0$, hoping that the choice is not going to affect the aim stated above. The outcome of the inclusion of the mass-like term is that there would not be chiral liquid on the surface. There is, however, possibility of helical liquid provided we are able to see that the system is a strong TI. We will show below the suitability of the matrix $\gamma_5 M_0$. As a first step of the DMH method, one needs to check the following: we consider non-spatial symmetries. These are symmetries that do not transform different lattice sites into each other. There are three different non-spatial symmetries that need to be considered: particle-hole symmetry (PHS) P , chiral symmetry (CS), and anti-unitary time-reversal symmetry Θ (TRS) [23]. If a complex conjugation operator K is multiplied on the left side by a unitary matrix U , the resultant matrix UK is referred to as anti-unitary. It can be easily seen that for 4×4 matrices $\Theta = \sum_j K$ (this definition ensures Θ anti-unitary), $P = \sum_x K$, and

$C = \text{diag}(1, 1, -1, -1)$ where $\sum_j = \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix}$ and σ_j are Pauli matrices. The properties

of Pauli and four-by-four $\sum$ matrices are similar. The mass term $\gamma_5 M_0$ that leads to the opening of a gap at the band crossing must satisfy $[\Theta, \gamma_5 M_0] = 0$, $[P, \gamma_5 M_0] = 0$, and $\{C, \gamma_5 M_0\} = 0$, which we find they do. The second step is to check the anti-commutativity of the matrix $\gamma_5 M_0$ with the surface Hamiltonian H_s given by (25). If they do not anti-commute (do anti-commute), i.e., any sort of correlation does not exist (exists) between $\gamma_5 M_0$ and H_s , then the band crossing cannot be gapped out (can be gapped out) which means the band crossing is topologically stable (unstable). We obtain here $\{H_s, \gamma_5 M_0\} \neq 0$ and, therefore, the topological stability of the band crossing is seemingly possible. The surface state Hamiltonian that we proceed with now is $H^{slab}(k_x, k_y) = H_s(k_x, k_y) + \gamma_5 M_0$. It is easy to see that the Hamiltonian $H^{slab}(k_x, k_y)$ commutes with the operator Θ . Consequently, $H^{slab}(k_x, k_y)$ needs to satisfy the identity $H(-k) = \Theta H(k) \Theta^{-1}$. In view of $\Gamma_1(K) = \Gamma_2(K)$, it can be easily checked that $H^{slab}(-k_x, -k_y) = \Theta H^{slab}(k_x, k_y) \Theta^{-1}$. The identity implies that if energy band $E(k)$, of a time-reversal (TR) symmetric system, satisfies $E(k) = E(-k)$ for a TR-invariant momentum (TRIM) pair $(k, -k)$, called Kramers pair, the relation $-k + G = k$ (where G is a reciprocal lattice vector) is satisfied by such a pair due to the periodicity of the BZ. Moreover, one can gap out the helical edge states by introducing a Zeeman term that explicitly breaks the protecting time-reversal symmetry. As we show below, we obtain a term referred to as the pseudo-Zeeman term (PZT) in the single-particle spectrum, which has different sign for opposite spins and no connection with momentum. Now, usually, the effects of an external magnetic field, B , perpendicular to the TI film are captured by two additional terms in the film Hamiltonian. The first term describes the orbital coupling to magnetic field through the minimal coupling $k_x \rightarrow k_x + (e/c)A_x$, where $A = [-By, 0]$ is the vector potential in the Landau gauge. The second term describes the coupling of the spins to the magnetic field and is given by the Zeeman contribution. Thus, the PZT term in question does not act like a magnetic field here in a real sense. The Hamiltonian $H^{slab}(k_x, k_y) = H_s(k_x, k_y) + \gamma_5 M_0$ is spin non-conserving, as $[H^{slab}(k_x, k_y), \sum_z] \neq 0$. The reason is the presence of the spin-orbit coupling. In fact, due to the spin-orbit coupling,

the f-states are eigenstates of the total angular momentum J and, hence, hybridize with conduction band states with the same symmetry. Furthermore, we find that

$$C^{-1}H^{slab}(k_x, k_y)C \neq H^{slab}(k_x, k_y). \quad (27)$$

The absence of chiral symmetry ensures that the Hamiltonian $H^{slab}(k_x, k_y)$ could not be brought to an off-diagonal form by a unitary transformation. For example, in a Su-Schrieffer-Heeger [29] chain, one can move the end states away from zero energy by breaking the chiral symmetry at the surface and/or in the bulk. We also obtain

$$P^{-1}H^{slab}(-k_x, -k_y)P \neq -H^{slab}(k_x, k_y), \quad (28)$$

i.e., P-H symmetry breaking. We wish to identify the effects of P-H symmetry breaking on the magneto-optical conductivity of the system in a sequel to this paper. Finally, the space inversion operator Π (the eigenvalue of the Π operator is ± 1 as $\Pi^2 = 1$), acting on a state vector in position/momentum representation, brings about the transformations $x \rightarrow -x$, $\sigma \rightarrow \sigma$, and $k \rightarrow -k$, where x stands for the spatial coordinate, σ signifies the spin, and k stands for momentum. For $H^{slab}(k_x, k_y)$, it follows that $\Pi H^{slab}(k_x, k_y) \Pi^{-1} = H^{slab}(k_x, k_y)$, where $H^{slab}(-k_x, -k_y) = H^{slab}(k_x, k_y)$. Hence, the system preserves inversion symmetry (IS).

The surface state Hamiltonian that we proceed with now is $H^{slab}(k_x, k_y) = H_s(k_x, k_y) + \gamma_5 M_0$. This is TRS and IS invariant. However, it breaks PHS and CS. We definitely require a version of surface state Hamiltonian better than $H^{slab}(k_x, k_y)$, say, under open boundary condition, by guessing an improved ansatz. The work is under way in this direction. The equation to find the eigenvalues of the Hamiltonian is a quartic. After conducting lengthy algebra, this yields the following roots $E_{\alpha, surface}^{(\zeta)}(K) = \{E_1, E_2, E_3, E_4\}$ in view of Ferrari's solution of a quartic equation

$$E_{\alpha, surface}^{(\zeta)}(K) = \zeta \sqrt{\frac{z_0(K)}{2}} + \frac{(\Gamma_1(K) + \Gamma_2(K))}{2} + \alpha \left(b_0(K) - \left(\frac{z_0(K)}{2} \right) + \zeta c_0(K) \sqrt{\frac{2}{z_0(K)}} \right)^{\frac{1}{2}}, \quad (29)$$

where $\zeta = \pm 1$ is the spin-index and $\alpha = \pm 1$ is the band-index. The first term $\sqrt{z_0/2}$ acts as an in-plane Zeeman term. The pseudo-Zeeman term of the spectrum (29) comes into being due the presence of the mass-like term M_0 . Without this term, the spectrum reduces to a bi-quadratic rather than a quartic. The possible role of this term is that of the polarization-usurer. The other functions appearing in (29) are defined as follows:

$$\begin{aligned}
E_{\alpha, \text{ surface}}^{(\zeta=+1)}(K) &= \{E_1(K), E_2(K)\} = \sqrt{\frac{z_0(K)}{2}} + \frac{(\Gamma_1(K) + \Gamma_2(K))}{2} \\
&\quad + \alpha \sqrt{b_0(K) - \left(\frac{z_0(K)}{2}\right) + c_1^2}, \\
E_{s, \text{ surface}}^{(\zeta=-1)}(K) &= \{E_3(K), E_4(K)\} = -\sqrt{\frac{z_0(K)}{2}} + \frac{(\Gamma_1(K) + \Gamma_2(K))}{2} + \\
&\quad + \alpha \sqrt{b_0(K) - \left(\frac{z_0(K)}{2}\right) - c_1^2}, \\
c_1^2 &= c_0(K) \sqrt{\frac{2}{z_0(K)}}. \\
z_0(K) &= \frac{2b_0(K)}{3} + \left(\frac{1}{2}\Delta^{\frac{1}{2}}(K) - A_0(K)\right)^{\frac{1}{3}} - \left(\frac{1}{2}\Delta^{\frac{1}{2}}(K) + A_0(K)\right)^{\frac{1}{3}}, \\
A_0(K) &= \left(\frac{b_0^3(K)}{27} - \frac{b_0(K)d_0(K)}{3} - c_0^2(K)\right), \quad b_0(K) = \frac{3B^2(K) - 8C(K)}{16}, \\
c_0(K) &= \frac{-B^3(K) + 4B(K)C(K) - 8D}{32}, \\
d_0(K) &= \frac{-3B^4(K) + 256E(K) - 64B(K)D(K) + 16B^2(K)C(K)}{256}, \\
\Delta(K) &= \left(\frac{8}{729}b_0^6 + \frac{16d_0^2b_0^2}{27} + 4c_0^4 - \frac{4d_0b_0^4}{81} - \frac{8c_0^2b_0^3}{27} + \frac{8c_0^2b_0d_0}{3} + \frac{4}{27}d_0^3\right), \\
B(K) &= -2(\Gamma_1(K) + \Gamma_2(K)), \\
C(K) &= [(\Gamma_1(K) + \Gamma_2(K))^2 + 2\Gamma_1(K)\Gamma_2(K) - \left(\frac{96Vba}{7d}\right)^2 - \left(\frac{16Vba}{3d}\right)^2 - 2M_0^2], \\
D(K) &= (\Gamma_1(K) + \Gamma_2(K)) \left[-2\Gamma_1(K)\Gamma_2(K) + 2M_0^2 + \left(\frac{96Vba}{7d}\right)^2 + \left(\frac{16Vba}{3d}\right)^2\right], \\
E(K) &= M_0^4 + 2M_0^2\Gamma_1(K)\Gamma_2(K) + (\Gamma_1(K)\Gamma_2(K))^2 - \left(\left(\frac{96Vba}{7d}\right)^2 + \left(\frac{16Vba}{3d}\right)^2\right)(\Gamma_1(K)\Gamma_2(K)) - \\
&\quad M_0^2(\Gamma_1(K) + \Gamma_2(K))^2 + \left(\left(\frac{96Vba}{7d}\right)^2 \times \left(\frac{16Vba}{3d}\right)^2\right) - 2M_0^2 \times \left(\left(\frac{96Vba}{7d}\right) \times \left(\frac{16Vba}{3d}\right)\right).
\end{aligned} \tag{30}$$

The surface states correspond to the eigenstates corresponding to the eigenvalues in (29). In an effort to examine the possibility of helical spin liquids, we plotted the surface state energy spectrum given by Equation (29) for the dimensionless wave vector as a function of the dimensionless wave vector (aK) in Figure 4, for finite mass-like coupling and the various values of the chemical potential μ . Since the conduction bands are partially empty, the surface state will be metallic. In all figures, t_{f1} is negative and, therefore, the figures correspond to insulating bulk. The important question is, have we been able to show SmB_6 as a strong/weak TI? The answer is not yet. For this purpose, we recall that there is a key distinction between surface states in a conventional insulator and a topological insulator. The explanation is given below: we first recall what has been stated above. The TRS identity $H^{\text{slab}}(-k_x, -k_y) = \Theta H^{\text{slab}}(k_x, k_y) \Theta^{-1}$ satisfied here means that the energy bands come in (Kramers) pairs. The pairs are degenerate at the TR-invariant momentum (TRIM) where $+\mathbf{K}$ becomes equivalent to $-\mathbf{K}$ due to the periodicity of the BZ, i.e., $\mathbf{K} + \mathbf{G} = -\mathbf{K}$ where $\mathbf{G}$ is a reciprocal lattice vector. Now, consider Figure 4a–d. An inspection yields that, in the band structure displayed in Figure 4a, TRIM is $\mathbf{K} = (\pm 1, 0) / (0, \pm 1)$, in Figure 4b also $\mathbf{K} = (\pm 1, 0) / (0, \pm 1)$, in Figure 4c $\mathbf{K} = (\pm 2, 0) / (0, \pm 2)$, and in 4(d) $\mathbf{K} = (\pm 3, 0) / (0, \pm 3)$. The reason is that $\mathbf{K}'$ s satisfy the condition $\mathbf{K} + \mathbf{G} = -\mathbf{K}$. For example, $\mathbf{K} = (\pm 1, 0)$ and $\mathbf{G} = (\pm 2, 0)$ added together will give $-\mathbf{K} = (\pm 1, 0)$. In Figure 4c, the momentum $\mathbf{K} = (\pm 2, 0)$ or $(0, \pm 2)$ obey $\mathbf{K} + \mathbf{G} = -\mathbf{K}$ where $\mathbf{G}$ is the reciprocal lattice vector $(\pm 4, 0)$ or $(0, \pm 4)$. Similarly, in Figure 4d, the momentum $\mathbf{K} = (\pm 3, 0)$ or $(0, \pm 3)$ obey $\mathbf{K} + \mathbf{G} = -\mathbf{K}$ where $\mathbf{G}$ is $(\pm 6, 0)$ or $(0, \pm 6)$. Let us now note that the Fermi energy E_F inside the gap intersects these surface states (in the surface multi-band structures) in the same BZ, either an even or an odd number of times. If there are odd numbers of intersections at TRIMs, which guarantees the time reversal invariance, the surface state is topologically non-trivial (strong topological insulator), for disorder or correlations cannot remove pairs of such surface state crossings (SSC) by pushing the surface bands entirely above or below the Fermi energy E_F . This has been checked in Figure 4 by assigning different values to the chemical potential. We notice that the number of paired SSCs in each of the figures in Figure 4 is three (odd). However, amongst the three pairs of momenta $(\mathbf{K}, -\mathbf{K})$, only one in each

of the figures satisfies the relation $-\mathbf{K} = \mathbf{K} + \mathbf{G}$. Thus, the number of TRIM involved in SSC is one (odd). When there are an even number of pairs of surface-state crossings, the surface states are topologically trivial (weak TI or conventional insulator), for disorder or correlations can remove pairs of such crossings. The inescapable conclusion is that the system under consideration is a strong topological insulator. The material band structures are also characterized by Kane–Mele index $Z_2 = +1$ ($\nu_0 = 0$) and $Z_2 = -1$ ($\nu_0 = 1$). The former corresponds to weak TI, while the latter to strong TI. The symmetry analysis and graphical representations lead to the conclusion that the system considered here is a strong TI. The TKI surface, therefore, comprises of ‘helical liquids’ [30] in the slab geometry, which (helicity) is one of the most unique properties of a topologically protected surface. A recent report of a spin-signal on the surface by the inverse Edelstein effect [31] has confirmed the helical spin-structure.

Figure 4. *Cont.*

(b)

(c)

Figure 4. Cont.

Figure 4. The plots of the surface state single-particle excitation spectrum given by Equation (29) versus the dimensionless wave vector for the various values of chemical potential μ and the mass-like term M_0 : (a) $\mu = 0.00$, $t_{f1} = -0.5$, and $M_0 = 0.02$; (b) $\mu = 0.00$, $t_{f1} = -0.50$ and $M_0 = 0.50$; (c) $\mu = -0.32$, $t_{f1} = -0.1$, and $M_0 = 0.50$; and (d) $\mu = 0.50$, $t_{f1} = -0.10$, and $M_0 = 0.50$. The other parameters are $b = 0.95$, $t_{d1} = 1$, $\varepsilon_f = -0.05$, $V = 0.10$, $V_p = \left(\frac{Vab}{d}\right) = 0.05$. Since the conduction bands are partially empty, the surface state will be metallic in all cases. The hopping integral t_{f1} is negative and, therefore, the system corresponds to insulating bulk. The TRIM involving pair crossings in each figure is one (odd).

4. Discussion and Conclusions

We started with the periodic Anderson model (PAM)—a model for a generic TKI in Section 2. The model is quadratic in creation, showing annihilation operators without the on-site repulsion (U_f) between the f -electrons. The quadratic Hamiltonian makes calculating the relevant Matsubara propagators extremely simple. To investigate the model with U_f , the slave boson technique (SBT) [24] was employed in the mean-field theoretic (MFT) framework. The technique falls on the conjecture that electrons can transmute into spinons and chargons (s – c). The s – c bound state needs to be fermionic to preserve the Fermi–Dirac statistics of the electrons. The two ways to have it on board are: (i) if the spinon is fermionic, the chargin should be bosonic (slave boson). On the other hand, (ii) if the spinon is bosonic, the chargin should be fermionic (slave fermion). Suppose that the operators $b^\dagger$ (light slave boson creation operator) and $c^\dagger$ (heavy slave boson creation operator), respectively, create empty bosonic impurity states and doubly occupied states. Since the latter is prohibited for large on-site repulsion ($U_f \gg t_{d1}$) between the f -electrons, the operators $c^\dagger$ and c need not be taken into account when $U_f \gg t_{d1}$. However, we need to take into account the remaining auxiliary operators ($s^\dagger$, $b^\dagger$) where the single site fermionic (bosonic) creation operator is denoted by $s^\dagger$ ($b^\dagger$). The operator $s^\dagger$ ($b^\dagger$) corresponds to the electron's spin (charge). The link between these auxiliary operators ($s^\dagger$, $b^\dagger$) to the physical f -electron operator is $f_\zeta^\dagger = s_\zeta^\dagger b_\zeta$. In our SBT-MFT framework with $U_f \gg t_{d1}$, we make the further assumption that the slave boson field (b) at each lattice site can be replaced by a c -number. The crucial anti-commutation relation $\{f_\zeta, f_{\zeta'}^\dagger\} = \delta_{\zeta\zeta'}$ between the physical f -electron operators implies that the auxiliary operators will then satisfy the relation $\{s_\zeta, s_{\zeta'}^\dagger\} = b^{-2} \delta_{\zeta\zeta'}$. Furthermore, the restriction $\sum_\zeta s_\zeta^\dagger s_\zeta + b^\dagger b = 1$ or, $\sum_\zeta \langle s_\zeta^\dagger s_\zeta \rangle \cong 1 - b^2$ at a site

needs to be imposed to take care of the conservation of the auxiliary particle number. Thus, the complications associated with the large on-site repulsion ($U_f \gg t_{d1}$) between the f -electrons is conveniently circumvented in the SBT by imposing a constraint to remove the double occupancy. The signature of the assumption “large on-site repulsion ($U_f \gg t_{d1}$) between the f -electrons” is carried over by the parameters λ and b , which are present in Γ_2 (the defining equation could be found below (25)). The term Γ_2 is significant for the surface state energy spectrum given by (29). Thus, the outcome noted above, viz. surface band structure showing an odd number of crossings, is a consequence of the assumption. It will be interesting to reinvestigate the problem with $U_f > t_{d1}$ (i.e., the on-site repulsion between the f -electrons is moderately strong) where the double occupancy is permissible. The slave particle mean-field-theory is valid at very low values of temperature ($T \rightarrow 0$). Moreover, we neglected the dynamics of the boson field completely as the light slave boson creation and destruction operators were replaced by a c-number ‘ b ’. This approximation reduced the system to a non-interacting one with the bulk spectral gap dependent on the parameters (b, λ, ζ, V). Whereas the first two parameters took care of the strong correlation effect between the f -electrons, the hybridization parameter V is the harbinger of a topological dispensation.

In the expression of the momentum-dependent form-factor matrix Γ , we took into account only the lowest-order cubic harmonics [1,15,16]. In fact, our intention is to use more complicated odd-parity expressions for Γ and reinvestigate the present problem, bringing about some improvement in the surface Hamiltonian. This is expected to facilitate a more refined analysis of odd/even number crossing issues. We summarize below our progress for the benefit of the readers. Let us consider the momentum-dependent form-factor matrix involved in the third term in Equation (1). This term is actually given by

$$\sum_{k,m_j,\zeta=\uparrow,\downarrow} \left\{ \langle k, \zeta = \uparrow, \downarrow | V_0 | \Gamma^f : R = 0, m_j \rangle d_{k\zeta}^\dagger f_{m_j} + \text{H.C.} \right\}$$

where the fermionic operator $d_{k\zeta}^\dagger$ creates a Bloch state with k and $\zeta \in \{\uparrow, \downarrow\}$ being momentum and physical spin quantum numbers, respectively. The fermionic operator $f_{m_j}^\dagger$ creates a localized Kramers doublet state $| \Gamma^f : R = 0, m_j \rangle$ associated with the crystal field effect and spin-orbit coupling. In the case of SmB_6 , the lowest-lying Kramers doublet is $| \Gamma_8^{f(2)} \rangle = | m_j = \pm \frac{1}{2} \rangle$. Thus, $m_j \in \{\uparrow, \downarrow\}$ is a pseudospin quantum number, corresponding to the two possible values of the projection of the total angular momentum in the lowest-lying Kramers doublet. We assume that the hybridization operator has a spherical symmetry in the vicinity of the heavy atom. Moreover, we expand the Bloch wave of $s = 1/2$ fermion in terms of spherical harmonics and partial waves. Besides, the lowest-lying Kramers doublet state can be decomposed into radial and angular part. We further assume a constant hybridization amplitude (CHA). One can now rewrite the effective hybridization matrix elements by using these assumptions as a product of CHA, the Clebsch–Gordan coefficient for $s = \frac{1}{2}$ and the spherical harmonics. One can then calculate the hybridization matrix for two interesting cases, viz. (i) $l = 1, s = 1/2, j = 1/2$ and $m_j = \pm 1/2$ (ii) $l = 3, s = 1/2, j = 5/2$ and $m_j = \pm 1/2$. In the former case, we find the form factor is equal to a product of V_0 , an odd spin, and odd momentum operator. Therefore, it is time reversal invariant. In the latter case (which corresponds to SmB_6), it is of form $\{V_0 k^3 \det\}$ where ‘det’ is the determinant involving spherical harmonics. All of the matrix elements of the Hamiltonian (25) will now have to be correct up to $O(k^3)$, including the hopping terms for consistency. One then expects to find a better version of the surface state Hamiltonian to investigate the odd/even number of crossing issues. Furthermore, we will have a more accurate platform of investigating, theoretically, the mysterious behavior of bulk insulator SmB_6 displaying the metal-like Fermi surface, even though there is no long-range transport of charge.

The effect of the Bychkov–Rashba term on the present system is quite interesting. To show why, we proceed with the new surface state Hamiltonian $H^{\text{slab}}(k_x, k_y) = H_s(k_x, k_y) + \text{Bychkov–Rashba term}$, where the two-by-two matrix equivalent of the latter is $A_0 = [\lambda_R(k_x \sigma_y - k_y \sigma_x)]$ and λ_R is the strength of the interaction. It is imperative to assume

that there must be metals, such as Au(111), on the surface in close proximity or deposition of particles with considerably high Rashba spin–orbit (RSO) interaction strength on the surface of the material. Assuming that the Rashba interaction is between f -electrons only, we write the surface state Hamiltonian, in the basis $(d_{k,\uparrow}^\dagger s_{k,\uparrow}^\dagger s_{k,\downarrow}^\dagger d_{k,\downarrow}^\dagger)^T$, as

$$\mathbb{H}_{mn}^{slab}(k_x, k_y) = \begin{pmatrix} \Gamma_1 & -i A_1 & 0 & 0 \\ i A_1 & \Gamma_1 & A_3^* & 0 \\ 0 & A_3 & \Gamma_1 & -i A_2 \\ 0 & 0 & i A_2 & \Gamma_1 \end{pmatrix} \quad (31)$$

where $A_3(K) = \lambda_R(-ik_x - k_y)$, $A_1 = c_{\zeta=+1}$, and $A_2 = c_{\zeta=-1}$. The equation to find the eigenvalues of the Hamiltonian is a biquadratic. This yields the following roots

$$E_{\alpha, surface}^{(\zeta)}(K) = \Gamma_1(K) + \left(\frac{\alpha}{2}\right) \left(\left(A_1^2 + A_2^2 + |A_3(K)|^2 \right) + \zeta c_0(K) \right)^{1/2}, \quad (32)$$

where $c_0(K) = \left((A_1^2 + A_2^2 + |A_3(K)|^2)^2 - 4 A_1^2 A_2^2 \right)^{1/2}$, $\alpha = \pm 1$ is the band-index, and $\zeta = \pm 1$ is the spin-index. Plots of surface state single-particle excitation spectrum given by Equation (32) versus the dimensionless wave vector is shown in Figure 5. The parameter values are $b = 0.95$, $t_{d1} = 1$, $t_{f1} = -0.35$, $\varepsilon_f = -0.06$, $\mu = -0.50$, $V = 0.10$, $V_p = \left(\frac{V_{ab}}{d}\right) = 0.05$, $A_1 = 5.3333 \cdot V_p$, $A_2 = 13.7143 \cdot V_p$, and $\lambda_R = 0.81$. Since all four bands are partially empty, the surface state will be metallic. The hopping integral t_{f1} is negative and, therefore, the system corresponds to insulating bulk. In Figure 5, the two bands

$$\Gamma_1(K) + \left(\frac{1}{2}\right) \left(\left(A_1^2 + A_2^2 + |A_3(K)|^2 \right) - c_0(K) \right)^{1/2}, \quad (33)$$

and

$$\Gamma_1(K) - \left(\frac{1}{2}\right) \left(\left(A_1^2 + A_2^2 + |A_3(K)|^2 \right) + c_0(K) \right)^{1/2}, \quad (34)$$

appear to be degenerate. They are, in fact, not so, as that would demand fulfilment of the inadmissible condition $c_0(K) = 0$. Actually, they are too close to appear as resolved in Figure 5a. As we have noted, if there are an odd/even numbers of TRIM-related surface state crossings (SSC), the surface states are topologically non-trivial (trivial). We find that, with greater resolution, there are no TRIM involved SSCs (the apparent near-degeneracy of (33) and (34) may mislead us to believe that there is an even number of TRIM-linked SSCs) in Figure 5b. This means a disorder or correlations can remove pairs of such crossings by pushing the surface bands entirely above or below the Fermi energy E_F . Seemingly, the broken IS due to the Bychkov–Rashba term, ushers in the change from the strong topological insulator to a conventional one. A detailed investigation is required before we announce the final verdict.

Figure 5. Plots of surface state single-particle excitation spectrum given by Equation (32) versus dimensionless wave vector. The parameter values are $b = 0.95$, $t_{d1} = 1$, $t_{f1} = -0.35$, $\varepsilon_f = -0.06$, $\mu = -0.50$, $V = 0.10$, $V_p = \left(\frac{V_{ab}}{d}\right) = 0.05$, $A_1 = 5.3333 \cdot V_p$, $A_2 = 13.7143 \cdot V_p$, and $\lambda_R = 0.81$. Since all four bands are partially empty, the surface state will be metallic. The hopping integral t_{f1} is negative and, therefore, the system corresponds to insulating bulk. (a) This figure apparently shows an even number of TRIM involved surface state crossings (SSC). (b) This figure, with greater resolution, shows that only non-TRIM momenta are involved in the SSC.

In conclusion, we are aware of the fact that the investigation presented does not take into account the specific electronic structure of the real TKI system, such as SmB_6 . This makes the work less useful. In a follow-up to this paper, this issue will be addressed. Moreover, we recall that, in a slab geometry, the top and bottom of the slab interface with vacuum and hopping events between the surface states on the bottom and top, opens a finite gap at the Γ point ($k = 0$). Off-diagonal mass-like terms must be included in the surface Hamiltonian H_s , in a suitable basis, to characterize the opening of this finite gap. The point we wish to make is that, while in hopping, a particle has to have energy greater than or equal to that of the height of the potential barrier (in between atoms at the top and

bottom) in order to cross the barrier, in tunneling, the particle can cross the barrier, even with energy less than the height of the barrier. Besides, the former is classical, whereas the latter, which depends on the width of the barrier, is a quantum mechanical phenomenon. Thus, our assumption of the “occurrence of the hopping only” needs to be supplemented with an account of the tunneling. In fact, a full-proof description must account for all processes that make an electron cross from one atom to another.

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