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PAPER

Surface reconstruction in a tight-binding model for the topological Kondo insulator SmB_6

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Abstract

For the strongly correlated topological insulator SmB_6 we discuss the influence of a 2×1 reconstruction of the (001) surface on the topological surface states. Depending on microscopic details, the reconstruction can be a weak or a strong perturbation to the electronic states. While the former leads to a weak backfolding of the surface bands only, the latter can modify the surface-state dispersion and lead to a Lifshitz transition. We analyze the quasiparticle interference signal: while this tends to be weak in models for SmB_6 in the absence of surface reconstruction, we find that the 2×1 reconstruction can induce novel peaks. We discuss experimental implications.

1. Introduction

The material SmB_6 has attracted significant attention during recent years, as it has been proposed [1–3] to realize a three-dimensional (3D) topological Kondo insulator (TKI). In this fascinating class of materials, a topologically non-trivial band structure emerges at low energies and temperatures as a result of Kondo screening of strongly correlated f electrons [4]. Similar to weakly correlated topological insulators (TIs), the surfaces of 3D TKIs display topological surface states with Dirac dispersion and spin-momentum locking.

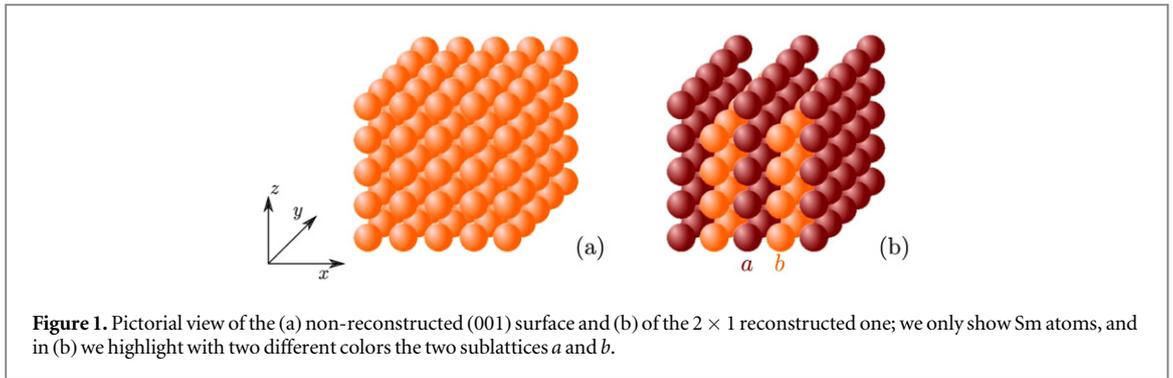
Recent theory [5–7] suggests SmB_6 to be also a topological crystalline insulator (TCI), its band structure being characterized by three non-zero mirror Chern numbers, $C_{k_z=0}^+$, $C_{k_z=\pi}^+$, $C_{k_x=k_y}^+$, defined on planes in the 3D Brillouin zone (BZ) which are invariant under mirror operations. This allows us to further classify topological surface states according to their mirror-symmetry eigenvalues.

On the experimental front, a number of results obtained on SmB_6 , e.g. from transport studies [8–10], quantum oscillation measurements [11], angle-resolved photoemission spectroscopy (ARPES) [12–16] and spin-resolved ARPES [17], appear to be consistent with the presence of Dirac-like surface states. However, doubts have been raised about the proper interpretation of ARPES data [18–20].

An important class of experiments, typically used to verify the topological nature of TI surface states, employ scanning tunneling spectroscopy (STS): the

surface-state quasiparticle interference (QPI) signal allows one to deduce characteristic wavevectors for spin-conserving elastic scattering due to defects and thus directly probes the spin-momentum locking of surface electrons. Unfortunately, to date, conclusive QPI results on SmB_6 are lacking. In fact, surface-sensitive probes such as STS face the problem that SmB_6 surfaces are hard to characterize experimentally: non-reconstructed (001) surfaces are polar, such that surfaces typically reconstruct. A frequent case is the 2×1 reconstructed (001) surface, as observed in large areas in STS experiments [21, 22]. Such a surface is non-polar, rendering it more favorable for the observation of topologically non-trivial surface states. This implies, however, that a proper theoretical modeling must take into account the surface reconstruction, i.e. the fact that one half of the top Sm rows are missing—this has not been done in the theory literature to date.

It is the purpose of this paper to fill this gap: we shall study the effects of surface reconstruction of the electronic states of SmB_6 on the level of tight-binding models. In particular, we shall focus on the fate of the topological surface states and on signatures in STS and QPI experiments. Our main results can be summarized as follows. Not unexpectedly, the importance of the surface reconstruction depends strongly on the effective strength of the electronic reconstruction potential. The latter depends on various microscopic details which cannot be reliably extracted from our simplified modeling, such that we rely on assumptions here. In the case that the reconstruction potential is



weak, its effects on QPI are minor despite the back-folding of the surface bands, i.e. the effect of reconstruction can—for most purposes—be ignored. If, however, the reconstruction potential is sufficiently strong, a Lifshitz transition—a change in the Fermi-surface topology as a function of the Fermi energy—of the surface states is expected. Its general properties can be described by appealing to the presence of a mirror plane which prevents band hybridization along certain high-symmetry directions. This is analogous to other TCI materials [23–25] (where a similar scenario applies to non-reconstructed surfaces). Importantly, such a 2×1 reconstruction can entirely modify the tunneling signal, and new QPI peaks with a unidirectional character may appear.

The remainder of the paper is organized as follows. We will start with an introductory discussion about SmB_6 and its surfaces in section 2. Section 3 will then qualitatively discuss the effect of surface reconstruction on the surface states. Concrete numerical results for band structures as well as tunneling and QPI spectra will be given in section 4. Section 5 summarizes the results of our work.

2. SmB_6 : general remarks

To set the stage, we summarize the key aspects of SmB_6 surfaces and the tight-binding modeling of both bulk and surface electronic states, and we also highlight general aspects of the surface reconstruction.

2.1. SmB_6 (001) surface

(001) Surface terminations. SmB_6 crystallizes into a simple cubic lattice, with the lattice constant $a_0 = 4.13\text{\AA}$. Crystals cleave preferentially along the (001) direction. This surface, however, presents many challenges from both experimental and theoretical points of view, since it can come with many different terminations (Sm [21, 22, 26], B_6 [21], Sm reconstructed [21, 22], single B [26], six or eight B donut-like [26], disordered [21, 22]). All of these have different electronic properties, and are both difficult to control experimentally and to describe in a coherent fashion theoretically.

In particular, simple Sm and B_6 terminated surfaces are polar, which has led to the suggestion that the observed surface conductance might be carried by non-topological surface states [18]. STS experiments [21, 22], however, show that, while these nominally polar surface regions can be observed, they are somewhat rare and small, being electrostatically unstable. The most common situation is instead the one of a reconstructed surface, in which, on average, one half of the terminating atoms are missing, restoring the electrostatic neutrality.

2×1 reconstructed (001) surface. Even though this reconstruction is most often disordered, large regions of ordered, Sm terminated, 2×1 reconstructed (001) surfaces can be observed [21, 22]. In these areas every second Sm row on the top layer is missing, as shown in figure 1. Due to the absence of macroscopic surface charges, this is the experimental scenario which most closely resembles the idealized (001) surface which is usually described by tight-binding-based theoretical models [1–3, 6, 27–29].

Impact of reconstruction on the surface states. The removal of one half of the atoms in the top layer cannot be considered a harmless process; this is especially true if we consider the surface states, which mostly live in the few top layers. Due to relaxation effects and the removal of neighboring atoms, even layers below the reconstructed one are expected to be influenced by the process. Here, the penetration depth λ of the surface states plays an important role: if $\lambda/a_0 \gg 1$, these states live on many planes, and a strong perturbation on one or a few of them has a weak impact; if instead $\lambda/a_0 \sim 1$, they live on just a few top layers, and a strong perturbation there can have a relevant effect. Using a simple model [30], it has been found that the penetration depth is of the order of a few atomic layers, suggesting the second possibility to be relevant.

2.2. Modeling

Even though it is generally agreed that the destruction of one or more of the top atomic layer(s) via disorder simply shifts the topological surface states deeper in the bulk [31, 32], not much is known about a strong but periodic perturbation, as in the 2×1 reconstruction that we consider here. It is therefore the aim of

this paper to discuss the effect of this scenario on the electronic surface states. To this end, we shall employ an eight-orbital tight-binding model, following [3, 6, 29] (see the appendix for details).

Bulk mean-field approach. We recall that SmB_6 is a strongly interacting material, in which local f moments are coherently screened by conduction d electrons to lead to a Kondo insulating phase. At low temperatures, this physics can be captured using a single-particle description with renormalized parameters [33]: in particular, the f kinetic energy is strongly suppressed, by a factor that the dynamical mean-field theory and the Gutzwiller approximation find to be ~ 10 [2, 27, 28]. Simpler theories such as mean-field slave bosons [33] can qualitatively reproduce this reduction, but with a smaller renormalization factor of ~ 2 [3, 29]. Instead of describing interaction-induced renormalizations explicitly, here we will work directly with renormalized parameters [34] that are designed to match qualitatively the computed band structure and the measured ARPES dispersion.

Role of surfaces and Kondo breakdown. In the presence of spatial inhomogeneities, the interaction-induced renormalizations will be position-dependent [35]. In particular, Kondo screening can be appreciably reduced on a surface, leading to an effective decrease of the Kondo temperature. This can generate a so-called ‘Kondo breakdown’ [36], in which surface moments are no longer Kondo screened: they can be free, order magnetically, or be possibly still screened but with a Kondo temperature smaller than the bulk one. Decoupled moments lead to an increase of the Dirac velocity, and to a displacement of the Dirac energy deep in the valence band, which resembles experimental results indicating ‘light’ rather than ‘heavy’ surface states. In [36] the Kondo temperature was estimated to drop by roughly a factor of 3, as a consequence of the surface Sm atoms having one first nearest neighbor (NN) Sm atom less than in the bulk. In the presence of a 2×1 reconstruction, atoms on the top row will have three neighbors less: in this case, the reduction of the hybridization, hence of the Kondo temperature, at the surface would be even larger.

However, an analysis [6, 29] of tight-binding models built to fit ab-initio calculations indicates that the bulk gap is mostly generated by second NN hybridization, and in [37] a model with third NN hybridization only seemed to well reproduce neutron-scattering data. This then leads to a more complex scenario, where the reduction of the hybridization of the surface atoms is less drastic. We summarize the count of different NNs in table 1. While we will not model Kondo breakdown explicitly, we will return to this aspect in the next paragraph.

Additional surface scattering potential. To formally eliminate half of the atoms on layer 1, we introduce a virtually infinite reconstruction potential V_{rec} acting on every second row (in practice we take $V_{\text{rec}} = 100$ eV). With V_{rec} being active, we need

Table 1. Number of Sm neighbors for Sm atoms (A) in the bulk, (B) on the (001) non-reconstructed surface, (C) in the first [(D, E): second] row on the 2×1 reconstructed (001) surface; different positions A–E are illustrated in figures 2(a)–(d).

Atom	1st NN	2nd NN	3rd NN
A (bulk)	6	12	8
B (non-rec. surface)	5	8	4
C (rec., top row)	3	4	4
D (rec., below the missing row)	5	10	8
E (rec., below the existing row)	6	10	4

to introduce an additional surface scattering potential $\Delta E = \Delta E_d = \Delta E_f$ of a few hundred meV, acting on the d and f orbitals of the remaining atoms in layer 1, in order to qualitatively reproduce the surface-state dispersion as seen by ARPES (large Dirac velocity, Dirac energy in the valence band). For f electrons, which have a bandwidth of a few meV, this value turns out to be very close to the infinite scattering potential of the Kondo breakdown scenario $\Delta E_f = \infty$, in which surface f electrons are no more part of the coherent Fermi liquid. Even though quantitative details might vary between our approach and the Kondo breakdown one, most of the features we are going to describe are general, and independent of microscopic details. We also remark that, while a large ΔE_f is needed to reproduce light surface states, ΔE_d is introduced to further adjust the position of the Dirac energy, hence the Fermi momentum k_F (that we try to obtain as close as possible to experiments), and may not be needed for some choices of the parameters (see section 4.3).

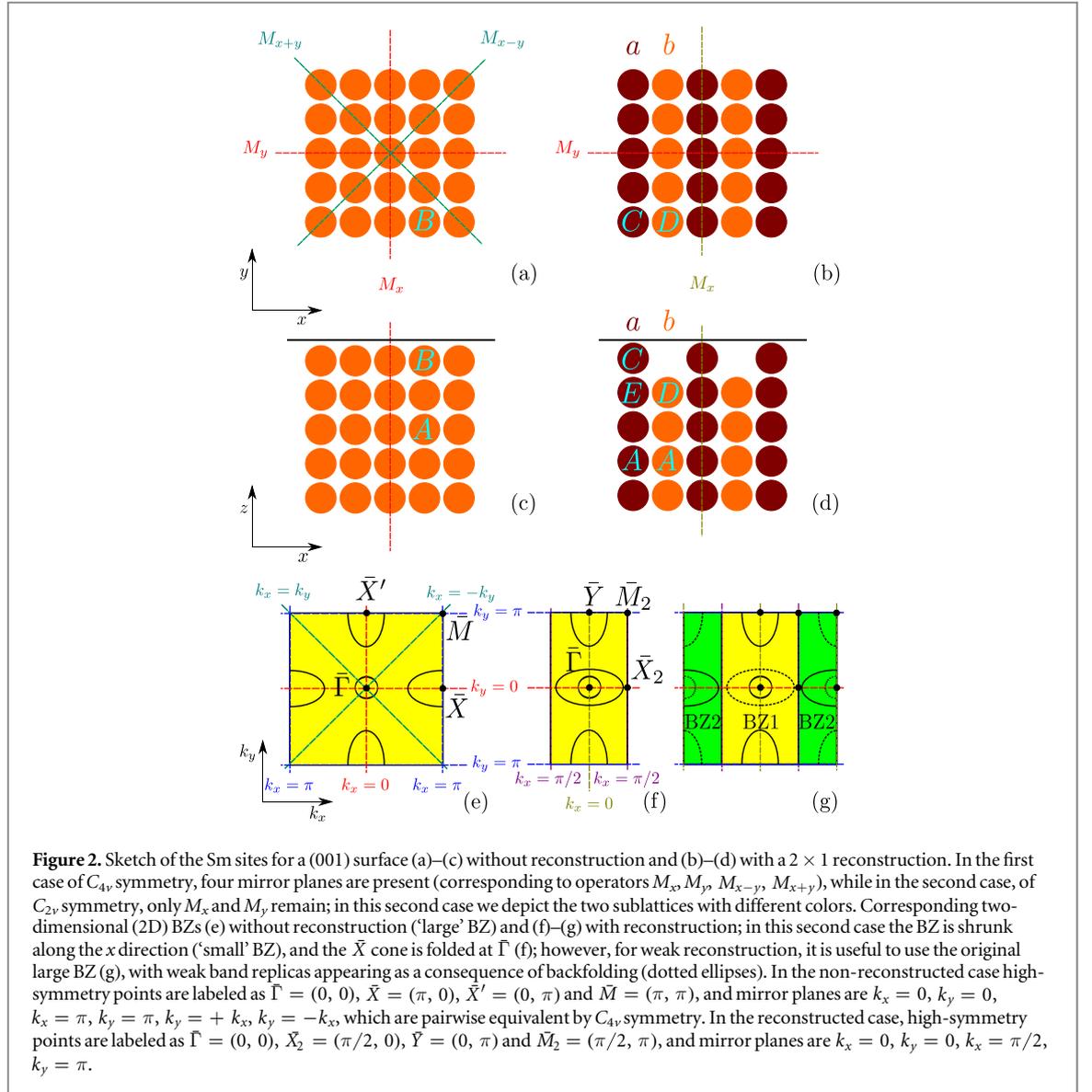
2.3. Qualitative effects of the reconstruction

In the following we choose a coordinate system as shown in figure 2, with \hat{z} being perpendicular to the surface and \hat{y} being parallel to the surface rows.

Surface BZ. A 2×1 reconstruction doubles the size of the primitive surface unit cell in the \hat{x} direction and introduces two sublattices, a and b with and without a top row, respectively, as shown in figures 2(a)–(d). The 2D surface BZ, originally a square for the (001) surface, shrinks by one half in the \hat{x} direction according to the reconstruction wavevector $\mathbf{Q} = (\pi, 0)$, as indicated in figures 2(e)–(f). Here we will use the term ‘2nd BZ’ for the difference between the original (‘large’) and the folded (‘small’) BZ.

Spectral weights. A (weak) reconstruction causes a backfolding of bands which leads to replicas (or shadow bands) shifted by \mathbf{Q} w.r.t. the original bands and with reduced spectral weight. Experimentally, a weak replica of the \bar{X} cone has been observed at $\bar{\Gamma}$ [13, 14] in ARPES, even though the origin of this signal is not totally clear (for example, having polycrystalline samples, one would expect to observe the replica of the \bar{X}' cone at $\bar{\Gamma}$, too).

Within our model calculations, we can quantitatively define the spectral weights in the following way.



The wavefunction $\psi_n(\mathbf{k}, z, \alpha, m)$ of a single-particle state with energy E_n for a system in slab geometry depends on the momentum $\mathbf{k} \equiv (k_x, k_y)$ in the small BZ ($-\pi/2 \leq k_x \leq \pi/2, -\pi \leq k_y \leq \pi$), on the layer index z , on the orbital index α , and on the sublattice index $m = 0(a), 1(b)$. Its spectral weight in the large BZ is given by:

$$w(n, \mathbf{K}, z, \alpha) = \left| \sum_{m=0,1} e^{i\mathbf{K}_x \cdot m} \psi_n(\mathbf{k}, z, \alpha, m) \right|^2, \quad (1)$$

with $\mathbf{K} \equiv (K_x, K_y)$ from the large BZ ($-\pi \leq K_x, K_y \leq \pi$), and \mathbf{k} its backfolded partner, $\mathbf{k} = \mathbf{K} \bmod \mathbf{Q}$. We can define a global (i.e. orbital-, layer-, and momentum-integrated) energy-resolved weight separately for the 1st or 2nd BZ:

$$w^{BZ1}(E) = \sum_{n, \mathbf{K}^{1st}, z, \alpha} w(n, \mathbf{K}^{1st}, z, \alpha) L(E - E_n), \quad (2)$$

$$w^{BZ2}(E) = \sum_{n, \mathbf{K}^{2nd}, z, \alpha} w(n, \mathbf{K}^{2nd}, z, \alpha) L(E - E_n), \quad (3)$$

where L is a Lorentzian kernel, and \mathbf{K}^{1st} means $|K_x| \leq \pi/2$, while \mathbf{K}^{2nd} means $|K_x| > \pi/2$. We can also define a layer-resolved weight w_z ,

$$w_z(E) = \sum_{n, \mathbf{K}, \alpha} w(n, \mathbf{K}, z, \alpha) L(E - E_n), \quad (4)$$

and decompose it into contribution from the 1st and 2nd BZ by limiting the sum over \mathbf{K} accordingly, to yield $w_z^{BZ1}(E)$ and $w_z^{BZ2}(E)$, with $w_z^{BZ1}(E) + w_z^{BZ2}(E) = w_z(E)$, and $\sum_z w_z(E) = \rho(E) = w^{BZ1}(E) + w^{BZ2}(E)$, where $\rho(E) = \sum_n L(E - E_n)$ is the density of states (DOS).

Effective reconstruction potential. To quantify the effect of the reconstruction on the surface states, we introduce the qualitative notion of ‘effective reconstruction potential’ (ERP) strength which is based on spectral weights. ERP is a dimensionless quantity

between 0, implying no effect, and 1, implying maximal effect.

We start from an idealized situation, in which the reconstruction potential only affects wavefunctions in the first layer $z = 1$. On this layer, the weight in the 1st and 2nd BZ are equal, $w(n, \mathbf{K}^{1st}, z = 1, \alpha) = w(n, \mathbf{K}^{2nd}, z = 1, \alpha) = w(n, \mathbf{K}, z = 1, \alpha)/2$, as only the $m = 0$ term in equation (1) survives. In all other layers, the weight (of a single state) will be totally either in the 1st or in the 2nd BZ, according to where it was without the reconstruction. Hence, the ratio of the layer-integrated weights in the 1st and 2nd BZ (i.e. the relative weight of replicas) can be used to infer the weight of the surface states on the top layer. Specifically, for a band located in the 2nd BZ without reconstruction (like the \bar{X} cone), with $w(n, \mathbf{K}^{1st}, z > 1, \alpha) = 0$, $w(n, \mathbf{K}^{2nd}, z > 1, \alpha) = w(n, \mathbf{K}, z > 1, \alpha) \neq 0$, the normalized weight on the first layer can be written as:

$$w_1' \equiv \frac{w_1}{\rho} = \frac{2w^{BZ1}}{w^{BZ1} + w^{BZ2}}, \quad 0 \leq w_1' \leq 1. \quad (5)$$

We note that the above assumption is not strictly valid: we found that the weight of the \bar{X} cone can be non-negligible in the 1st BZ even for deeper layers $z > 1$, even though no explicit reconstruction potential is present there, see section 4. Nevertheless, we shall use w_1' from equation (5), evaluated for a surface state at the Fermi level, as a measure of the ERP. We will see in section 4 that this value can also be cone-dependent.

How strong is the reconstruction? We now briefly discuss whether existing experimental or theoretical data are sufficient to infer the effective strength of the reconstruction potential.

Experimentally, ARPES data indicates that band replicas are weak and hence the ERP, as measured by equation (5), is small [13, 14]. This is, however, difficult to reconcile with our model calculations which, under essentially all circumstances, show that the removal of every second Sm atom in the surface layer is a strong perturbation to the surface states, with large ERP (see section 4 for details). Possible reasons for this discrepancy are: (i) only a fraction of the surface probed by ARPES features an ordered 2×1 surface reconstruction, thus reducing the ERP in the collected ARPES signal, or (ii) the surface states in the real material tend to be expelled from the first layer(s) by some other mechanism, such as Kondo breakdown, or (iii) the penetration length of the surface states is too small in the model calculations. Issue (i) may be investigated with small-spot ARPES experiments, and we will not discuss this further. For (ii), we found that the introduction of the surface scattering potential, ΔE_d and ΔE_f , to model this expulsion often enhances rather than decreases the ERP, but this is a model-dependent statement. We note that ARPES may not probe the full weight of the surface states if their penetration length is larger than that of the ARPES probe, but this is unlikely to explain the above discrepancy. The issue (iii) of

correctly modeling the surface-state penetration is delicate. The problem of the excessive reduction of the bulk gap using renormalized parameters (with respect to density-functional theory ones, noted for example in [38]) has a direct impact here: if one wants to match the experimental ARPES gap ~ 20 meV using renormalized parameters, one has to increase the value of the hybridization, effectively decreasing the penetration length of the surface states, and, as a consequence, enhancing the strength of the ERP. The problem is further complicated by Γ_7 states [6, 27–29], whose inclusion would reduce the value of the bulk gap (in our model, we will ignore these states, but a more detailed analysis would need to include them).

We conclude that we are not in the position to fully resolve this discrepancy, and further work—both theoretical and experimental—is needed to do so. Instead, we will take a pragmatic point of view and analyze the fate of the surface states provided that the ERP is sufficiently strong enough to generate observable effects.

3. Surface states with reconstruction

In this section we qualitatively analyze the effect of surface reconstruction on the in-gap surface states, based mainly on symmetry arguments. Numerical examples, taking into account details of microscopic modeling and testing these predictions, will be provided in section 4.

3.1. Symmetries and dispersion

Energies close to the Dirac point. If the Dirac energies were close to the Fermi level, the Fermi wavevector k_F of the cones was small, and essentially the only effect of reconstruction would be the folding of bands into the small BZ, as shown in figures 2(f)–(g) (the same applies at all energies for weak ERP).

Overlap of \bar{X} cone with its replica. Away from the Dirac energies, Dirac cones and their replicas will start to overlap with each other. ARPES data on SmB₆ shows that the only relevant overlap is the one of the \bar{X} cone with its replica: $2k_F$ of the \bar{X} cone along the $\bar{X} - \bar{\Gamma}$ direction is estimated to be [13] around 0.80 \AA^{-1} , while the original BZ has a halfwidth $\pi/a_0 = 0.76 \text{ \AA}^{-1}$. Thus, we expect that, due to the reconstruction, the \bar{X} cone should overlap and hybridize with its replica for energies close to the Fermi energy; we will ignore similar effects which might affect the \bar{X}' (now \bar{Y}) and $\bar{\Gamma}$ cones at higher energies.

Hybridization, the role of mirror symmetry, and the Lifshitz transition. We now discuss general aspects of the coupling between the \bar{X} cone and its replica which are largely independent of microscopic details; see figure 3. A key ingredient is the reflection symmetry with respect to the xz plane, described by operator M_y : states with $k_y = 0$ are invariant under M_y [5]. Along this direction the two cones have the smallest distance,

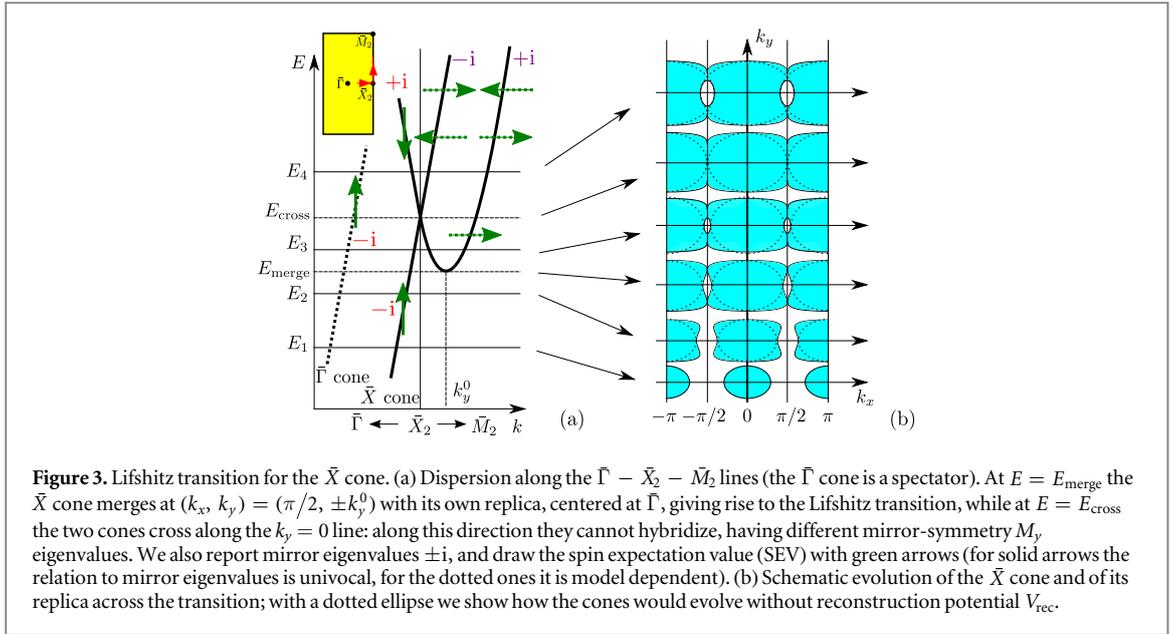


Figure 3. Lifshitz transition for the \bar{X} cone. (a) Dispersion along the $\bar{\Gamma} - \bar{X}_2 - \bar{M}_2$ lines (the $\bar{\Gamma}$ cone is a spectator). At $E = E_{\text{merge}}$ the \bar{X} cone merges at $(k_x, k_y) = (\pi/2, \pm k_y^0)$ with its own replica, centered at $\bar{\Gamma}$, giving rise to the Lifshitz transition, while at $E = E_{\text{cross}}$ the two cones cross along the $k_y = 0$ line: along this direction they cannot hybridize, having different mirror-symmetry M_y eigenvalues. We also report mirror eigenvalues $\pm i$, and draw the spin expectation value (SEV) with green arrows (for solid arrows the relation to mirror eigenvalues is univocal, for the dotted ones it is model dependent). (b) Schematic evolution of the \bar{X} cone and of its replica across the transition; with a dotted ellipse we show how the cones would evolve without reconstruction potential V_{rec} .

and the overlapping states have opposite mirror eigenvalues $\pm i$ (their exact value depends on the sign of the mirror Chern number $C_{k_z=0}^+$ but is irrelevant to the argument). Hence, the cones cannot hybridize for $k_y = 0$ (as long as mirror symmetry is preserved), instead they cross at $E = E_{\text{cross}}$.

In contrast, hybridization is allowed for $k_y \neq 0$. We observe that for energies $E_{\mathbf{k}}$ corresponding to momenta $k \lesssim \pi/2$, the \bar{X} cone deforms ($E = E_1$ in figure 3) along the $k_y = 0$ direction, until a Lifshitz transition at $E = E_{\text{merge}} < E_{\text{cross}}$ is achieved: the \bar{X} cone and its replica merge at $(\pi/2, k_y^0)$, where in general $k_y^0 \neq 0$. As a consequence, a pocket centered at $\bar{X}_2 = (\pi/2, 0)$ is created; we note that the minimum along $\bar{X}_2 - \bar{M}_2$ is actually a saddle point. When the two cones cross at $E = E_{\text{cross}}$ along the $k_y = 0$ direction, the \bar{X}_2 pocket area vanishes. At higher energies $E > E_{\text{cross}}$, the \bar{X}_2 pocket grows again, such that a new Dirac cone is created at the \bar{X}_2 pocket from the crossing of the two original Dirac cones. We note that for vanishing scattering potential, the two cones always cross without hybridizing: this yields $E_{\text{merge}} = E_{\text{cross}}$, and the two branches along the $\bar{X}_2 - \bar{M}_2$ direction ($k_x = \pi/2$) are degenerate. Finally, for the case with reconstruction and *broken* mirror symmetry, a gap is opened at \bar{X}_2 .

Analogy to TCIs. The hybridization behavior in figure 3 is similar to what happens on the (001) surface of face-centered cubic TCIs such as $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ [23], $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ [24], and SnTe [25]. For these materials, for which the standard \mathbb{Z}_2 indices are zero and which are not TIs in the usual sense, mirror Chern numbers are non-zero, and predict two pairs of Dirac cones along the $k_x = 0$ and $k_y = 0$ directions of the 2D BZ. These cones are at $(\pi \pm \delta_k, 0)$ and $(0, \pi \pm \delta_k)$, where the BZ is defined by $-\pi < k_x, k_y < \pi$. Each pair of cones merge around $(\pi, 0)$ or $(0, \pi)$ through the same

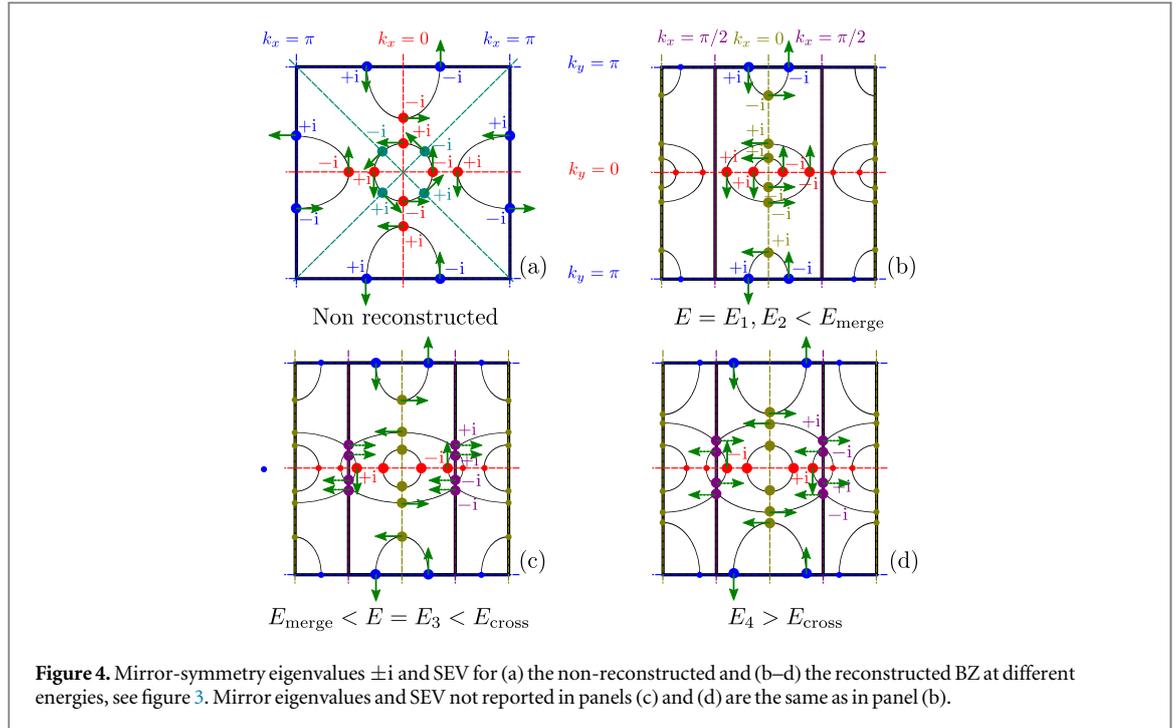
mechanism that we have described here, and which has been also predicted [5] for the (110) surface of SmB_6 . The similarity lies in the non-trivial topology of the band structure and the presence of mirror planes, which create states with different mirror eigenvalues which cannot hybridize along specific directions.

However, in the TCI case, no surface reconstruction is needed to generate the pair of cones. Also, the role of symmetries is reversed: in standard TCIs mirror symmetry protects cones at $(0, \pi \pm \delta_k)$, while parity invariants predict two Dirac cones at $(0, \pi)$. In our case we identify $(0, \pi)$ with \bar{X}_2 and $(0, \pi \pm \delta_k)$ with $\bar{\Gamma}$ and \bar{X} , but now mirror symmetry protects the cones at \bar{X}_2 , while parity invariants predict cones at $\bar{\Gamma}$ and \bar{X} .

ARPES experiments on TCIs have verified [23, 24, 39] the surface-state behavior as depicted in figure 3. While a similar verification might be possible in SmB_6 , we note a few caveats: visible hybridization effects require the ERP to be strong; as noted in the previous section its magnitude is unknown. Moreover, the features might be beyond the present ARPES energy and momentum resolution, and finally the cone crossing might occur above the Fermi energy, rendering ARPES ineffective.

3.2. Direction of spin

So far, the analysis of crossing Dirac cones was based on the presence of a mirror plane, but was otherwise independent of microscopic details. We now take a step further and compute the mirror-symmetry eigenvalues and the expectation value of the electronic spin operator. As shown in [6, 7, 40, 41], mirror-symmetry eigenvalues are determined by the sign of mirror Chern numbers (see appendix). While four TCI phases with $C_{k_z=0}^+ = \pm 2$, $C_{k_z=\pi}^+ = +1$, $C_{k_x=k_y}^+ = \pm 1$ are possible in principle, we restrict the analysis to the $C_{k_z=0}^+ = +2$, $C_{k_z=\pi}^+ = +1$, $C_{k_x=k_y}^+ = -1$ phase,



which—as we have argued in [6]—is the one which has experimental relevance for SmB_6 . In figure 4(a) we report the mirror-symmetry eigenvalues for the non-reconstructed surface [6].

Mirror-symmetry eigenvalues with reconstruction. In the reconstructed case, there are four distinct mirror planes in the 2D BZ, namely $k_x = 0, \pi/2$ and $k_y = 0, \pi$; the former commute with M_x , the latter with M_y (see figures 2(b), (d), and (f)). We can therefore assign mirror eigenvalues to the states crossing these planes. For planes $k_x = 0, k_y = 0, k_y = \pi$ everything is equivalent to the non-reconstructed case, and we can transfer the eigenvalues directly from figure 4(a) into figure 4(b). For energies below E_{merge} , no states cross $k_x = \pi/2$, and no further work is needed. Above E_{merge} , however, four states are crossing the $k_x = \pi/2$ plane, two for $k_y > 0$, and two for $k_y < 0$. Concentrating on $k_y > 0$ we find that below E_{cross} both states have the eigenvalue $-i$, see figure 4(c), simply because they belong to the same band, see figure 3(a). In contrast, above E_{cross} , figure 4(d), one of the $k_y > 0$ states has the eigenvalue $+i$, and the other $-i$, see figure 3(a), since they now belong to different bands; the same happens for $k_y < 0$, see figures 4(c) and (d).

SEV. Since mirror-symmetry eigenvalues are not directly measurable, we now concentrate on the SEV, which depend on these eigenvalues and is accessible in spin-resolved ARPES experiments. For atomic d and Γ_3 states, that we consider here, the relation between the mirror eigenvalues and the SEV is straightforward, and it is the same one as for free spins [6]: if the eigenvalue is $-i$, the SEV points along $+x$ for M_x and $+y$ for M_y , and vice versa for the eigenvalue $+i$.

This holds also for lattice states with a definite momentum, when symmetry operations act like they do in the non-reconstructed case. This applies to the states $k_x = 0, k_y = 0$, or $k_y = \pi$ —hence, on these planes, the SEV is identical to the non-reconstructed case—but not for the states at $k_x = \pi/2$ because this is not a BZ mirror plane in the absence of reconstruction.

Let us analyze the latter case of $k_x = \pi/2$ in more detail. For the two sublattices a and b we define the mirror eigenstates according to $M_x|a^+\rangle = +i|a^+\rangle$, $M_x|b^+\rangle = +i|b^+\rangle$, and we build Bloch states $|\mathbf{k}_a^+\rangle$ and $|\mathbf{k}_b^+\rangle$ with $\mathbf{k} = (\pi/2, k_y)$. When we act with the mirror operator M_x on $|\mathbf{k}_a^+\rangle$ we get $M_x|\mathbf{k}_a^+\rangle = +i|\mathbf{k}_a^+\rangle$, but for states on sublattice b we pick up a minus sign: $M_x|\mathbf{k}_b^+\rangle = -i|\mathbf{k}_b^+\rangle$ [the opposite would happen if we took a mirror operator M_x centered on b rather than on a in figures 2(b)–(d)]. This can be realized by observing that M_x , when centered on sublattice a , sends states a in the n primitive cell into states a in cell $(-n)$, while b states at n are sent into b states at $(-n - 1)$: so, the effect of M_x on $|\mathbf{k}_b^+\rangle$ states carries an additional e^{-2ik_x} factor, which is -1 for $k_x = \pi/2$. As a consequence, states $|\mathbf{k}\rangle$ with $M_x|\mathbf{k}\rangle = +i|\mathbf{k}\rangle$ and $\mathbf{k} = (\pi/2, k_y)$ are composed by states $|a^+\rangle$ on the sublattice a , and by states $|b^-\rangle$ on sublattice b , so there is no general rule for their SEV given the mirror eigenvalues. We can however state that, if we restrict the analysis to the top layer, where no b states are present, the eigenvalue $-i$ corresponds to a SEV pointing along $+\hat{x}$, and vice versa for states with $+i$. When including all layers, however, we have to resort to numerical diagonalization. In our model we find that, close to the Lifshitz transition, the total contribution from other layers is opposite to the one from layer 1, so

the SEV for $-i$ states points along $-\hat{x}$; at higher energies, however, we observe a transition to a situation where the SEV for $-i$ states points along $+\hat{x}$ (see figure 3(a)), in agreement with the results from layer 1.

4. Numerical examples and QPI

In this section we provide numerical examples, using explicit tight-binding calculations, of the scenario depicted in the previous section, together with simulated QPI patterns.

4.1. Introduction to QPI

Generalities. QPI can be used as a probe of the topological character of surface states [42–44], owing to their spin texture: non-magnetic impurities cannot induce transitions between states which are Kramers partners. Also, when mirror symmetries are present, impurities which do not break these symmetries cannot induce transitions between states with opposite mirror eigenvalues [45]. In the following, we will exclusively consider impurities which do not break time-reversal and mirror symmetries; more complicated impurities may induce additional QPI peaks [44, 45] which we will not discuss here.

In general, peaks in the QPI signal are expected for pairs of stationary states [46] (states which have the same tangent in the BZ to the isoenergy contour), for which no selection rule forbids an elastic scattering process. For TI surface states, no peaks are expected from intracone scattering as long as the dispersion is linear, since pairs of stationary points are time-reversal conjugates in the Dirac Hamiltonian [44]. Peaks can arise when the dispersion deviates from linear, as it is known to happen in TIs such as Bi_2Ti_3 due to hexagonal warping [42].

Intercone scattering and QPI on SmB_6 non-reconstructed (001) surfaces. Intercone scattering is less restricted by selection rules and may hence give rise to strong QPI peaks [35]. However, for the non-reconstructed (001) SmB_6 surface, we showed in [6, 29] that the experimental spin pattern, corresponding to the $C_{k_z=0}^+ = +2$, $C_{k_z=\pi}^+ = +1$, $C_{k_x=k_y}^+ = -1$ mirror Chern numbers and to a positive winding number $w \equiv \text{sgn}(C_{k_z=0}^+ C_{k_z=\pi}^+)$ on the \bar{X} cone, leads to a strong suppression of the intercone scattering, implying virtually no observable QPI peaks. This most likely explains why STS experiments on SmB_6 have not found noticeable QPI signals to date [26, 47].

QPI in SmB_6 with reconstruction. A key question is whether QPI peaks can appear as a consequence of surface reconstruction. As noted above, the question makes sense only for sufficiently strong ERP, otherwise the non-reconstructed picture, which shows no peaks, still holds to be a good approximation. We can expect new QPI scattering channels in the energy region around the Lifshitz transition: first, because for energies below the transition an appreciable warping

of the \bar{X} cone is achieved, second, because above the transition the topology of the Fermi surface changes, with the appearance of the new pocket at \bar{X}_2 . Concrete calculations are required to see whether these prerequisites yield a noticeable QPI signal—these will be presented in what follows.

4.2. Numerical results: significant warping

We employ the model described in the appendix, taken from [6, 29], which is designed to match as closely as possible the calculated bulk band structure, and to reproduce the experimentally observed surface-state dispersion and spin pattern. Without surface reconstruction it yields no sharp QPI peaks, and consequently the appearance of any QPI peaks can be traced to the reconstruction effects. For a specific set of parameters which produces significant warping near the cone crossing, we report the band dispersion for a slab geometry in figure 5, the corresponding DOS in figure 6, and constant energy cuts through the ARPES and QPI signals in figure 7. Here, we define the ARPES signal as the sum over the weights from all orbitals [34], and add the signal from layers 1 and 2,

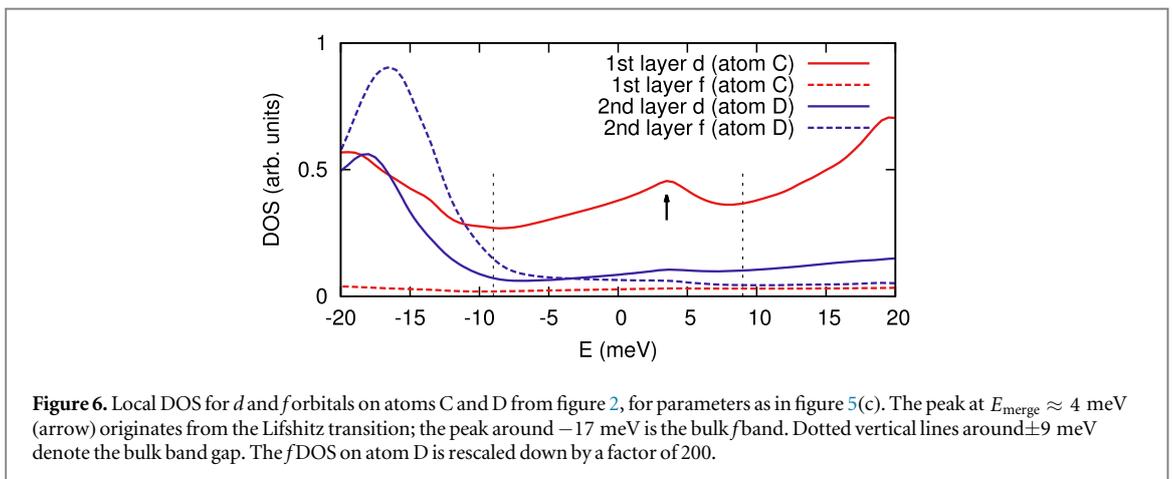
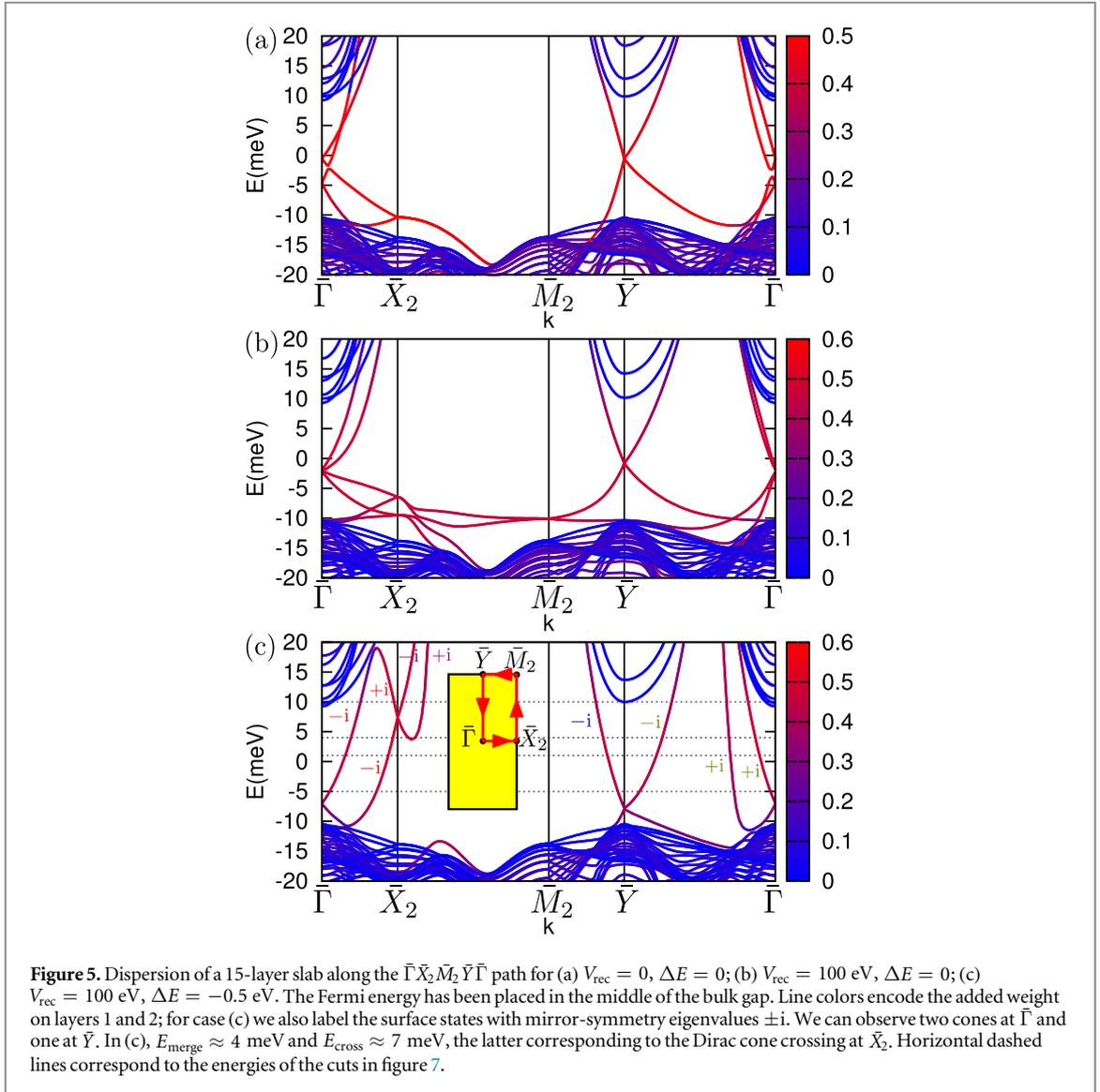
$$A(E, \mathbf{K}) = \sum_{n, \alpha} \sum_{z=1,2} w(n, \mathbf{K}, z, \alpha) L(E - E_n), \quad (6)$$

expressed using the weight defined in equation (1).

Dispersion and DOS. In the dispersion represented in figure 5, we can see two cones at $\bar{\Gamma}$, and one cone at \bar{Y} . For completeness, we present in figure 5(a) the case without reconstruction, $V_{\text{rec}} = 0$, and in figure 5(b) the case with reconstruction but no surface scattering potential, $\Delta E = 0$. In what follows we mainly concentrate on figure 5(c), which shows the case with both reconstruction and surface scattering potential.

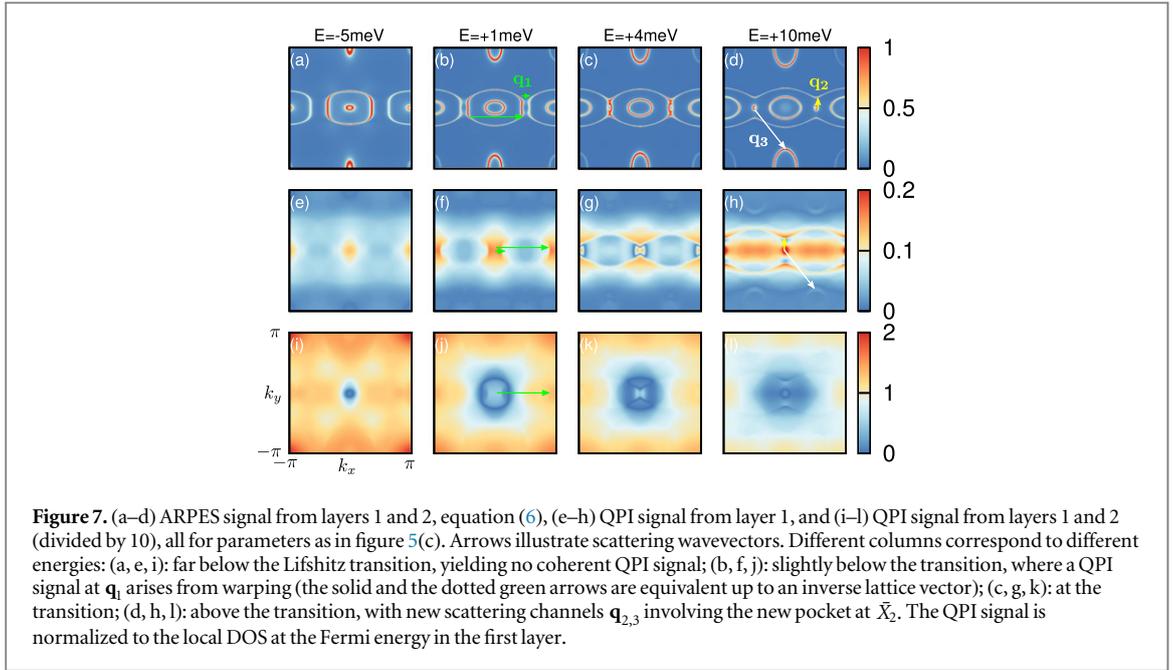
The weight distribution in figures 7(a)–(d) shows that the \bar{Y} cone is weakly affected by the reconstruction, and lives mostly in the 1st BZ: for this cone the ERP is weak. In contrast, the two cones present at $\bar{\Gamma}$ are strongly hybridized with each other, and have appreciable weight both in the 1st and in the 2nd BZ even when considering the signal from deeper layers: for these cones the ERP is strong. Their origin is from $\bar{\Gamma}$ and \bar{X} in the non-reconstructed BZ; in analogy to the experimental situation we identify as ‘ $\bar{\Gamma}$ ’ the cone with Dirac energy close to the top of the valence band and a smaller Fermi momentum, and as ‘ \bar{X} ’ the cone with lower Dirac energy and a larger Fermi momentum (see figure 3).

We can observe that the \bar{X} cone undergoes the Lifshitz transition that we described in the previous section, while the $\bar{\Gamma}$ cone remains inert. The saddle point at E_{merge} gives rise to a peak in the DOS (strictly speaking, a logarithmic divergence), as shown in figure 6. Parenthetically, we note that no cone crossing is observed inside the gap for significantly smaller values of the surface scattering potential ΔE (see for example figure 5(b)).



QPI. To illustrate the QPI effects, we consider a single impurity (corresponding to the dilute limit) and employ the standard T matrix technique to compute the Fourier-transformed local DOS in the presence of elastic scattering; for details see the appendix. We

report two sets of results: in figures 7(e)–(h) we show the QPI signal from layer 1, which has equal weight in the 1st and in the 2nd BZ due to the missing b atoms. In contrast, in figures 7(i)–(l) the signal is constructed from the sum of the local DOS in layers 1 and 2, the



latter scaled down by a factor of 10, to account for its larger distance from the tip. A more refined analysis might include interference contributions from the d and f channels [29, 48] as well as from layers 1 and 2, but would lead to the same qualitative results.

It can be observed that far from the Lifshitz transition no QPI signals, apart from an incoherent peak at $\bar{\Gamma}$, are present (figure 7(a)); this is the same result as without reconstruction. At higher energies, slightly below the Lifshitz transition a weak intracone scattering signal is generated as a consequence of cone warping (wavevector \mathbf{q}_1 in figure 7(b)), while above the transition two scattering channels appear to be active, both involving the newly formed \bar{X}_2 cone. In the first one the scattering is towards the newly formed band coming from the merging of the \bar{X} cone with its replica, denoted \mathbf{q}_2 in figure 7(d), and which involves states with the same mirror eigenvalue with respect to M_x on the $k_x = \pi/2$ plane; this is analogous with the results of [45] for $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$. The second one is towards the \bar{Y} cone (\mathbf{q}_3); in some cases we also observe a weak signal coming from the scattering to the $\bar{\Gamma}$ cone. We stress, however, that the intensities (both absolute and relative) of these new QPI peaks depend on the exact choice of the model parameters, as well as on the parameters used to simulate the tunneling process from the tip to the surface. We also note that these peaks arise primarily from the spectral weight in the first layer, which is mostly of d character. Since d states contribute a small fraction of the total weight of the surface states, their QPI peaks may—depending on details of the tunneling process—be masked by an incoherent background arising from f states. This is illustrated in figures 7(i)–(l) where we have included a contribution from the second layer (which does carry f weight); as a result, most QPI peaks dramatically lose

contrast. Even under these circumstances it is still possible to observe a weak signal from the \mathbf{q}_1 channel.

4.3. Numerical results: other cases

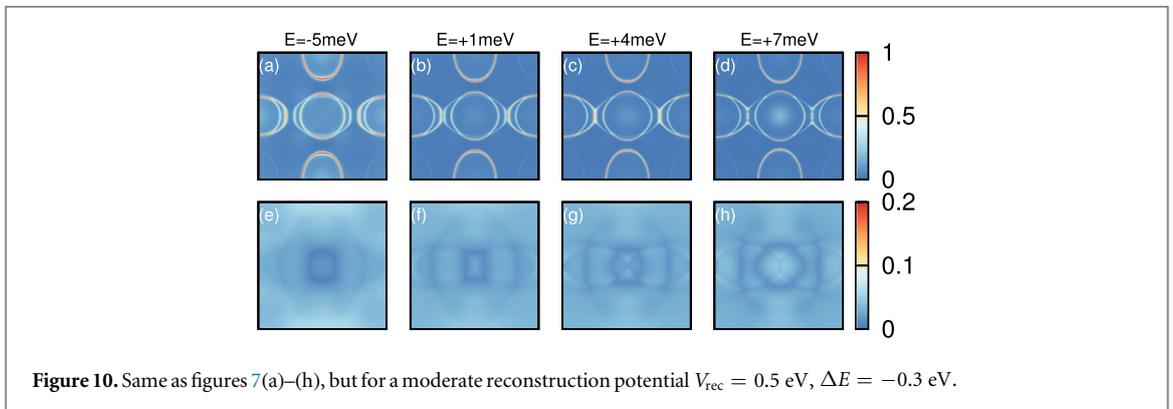
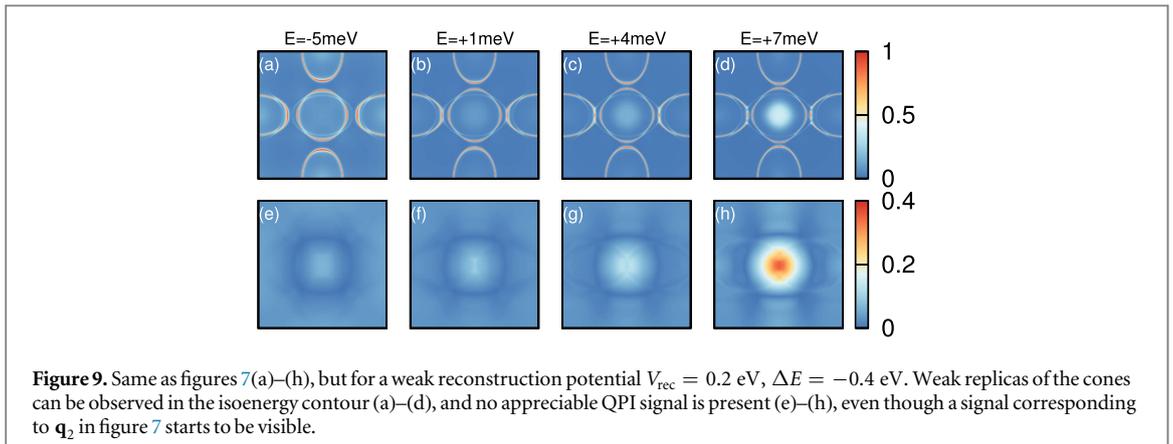
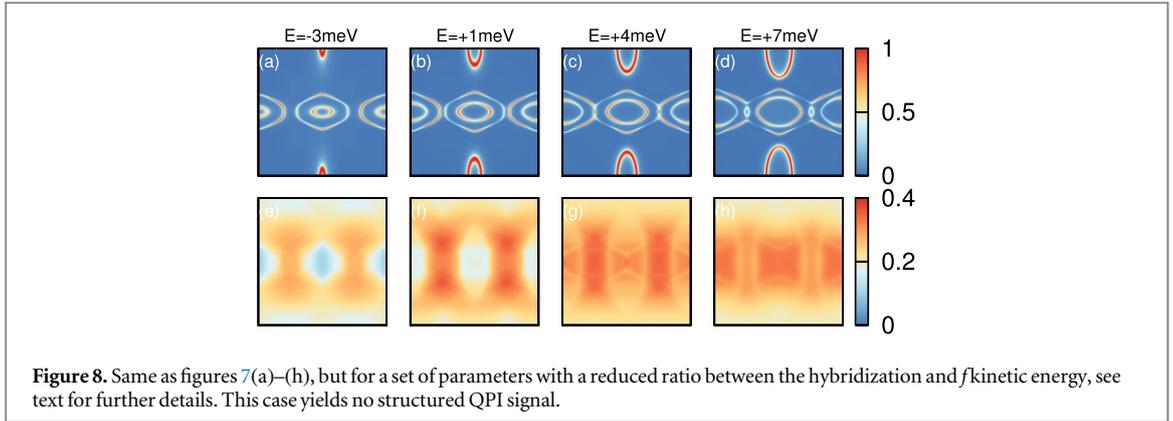
We have repeated the same calculations for various other sets of parameters, and we describe a few representative cases in what follows.

Kondo breakdown. To model the Kondo breakdown in the top layer, we take $\Delta E_f = 100$ eV, which is much larger than all other energy scales. Combined with the same $\Delta E_d = -0.5$ eV, we obtained numerical data (not shown) that is almost indistinguishable from the example shown before in figure 7. We remark that a finite ΔE_d is needed in our set of parameters to increase the k_F and allow for the Lifshitz transition, but is not needed for all sets of parameters (see below).

Reduced hybridization versus kinetic energy. If we reduce the hybridization with respect to the f kinetic energy, while keeping approximately the same gap ($tf \rightarrow 1.9tf$, $v \rightarrow 0.5v$), the QPI signal strength is strongly reduced, as shown in figure 8. In particular, for energies below the Lifshitz transition, we observe no sign of nesting. This can be reasonably linked to the slightly increased penetration length of the surface states, which makes reconstruction a weaker perturbation. In general, the appearance of QPI peaks and in particular their strength is found to be parameter-dependent.

Surface scattering potential $\Delta E_d = 0$. For a similar set of parameters (see appendix) we are able to get a k_F close to the experimental value and realize a Lifshitz transition with $\Delta E_f = 100$ eV and $\Delta E_d = 0$. The resulting QPI signal (not shown) is similar to that indicated in figure 8.

Small reconstruction potential. For a smaller reconstruction potential $V_{\text{rec}} = 0.2$ eV and $V_{\text{rec}} = 0.5$ eV, figures 9 and 10, the ARPES signal displays weak



replicas of the cones appearing translated at the reconstruction wavevector $\mathbf{Q} = (\pi, 0)$. In this case the QPI signal is very weak and is almost indistinguishable from the case $V_{\text{rec}} = 0$, which, as remarked, shows no peaks.

5. Conclusions

In this paper we have studied the role of a periodic 2×1 surface reconstruction on the topological surface states of SmB_6 using a simple tight-binding model. We qualitatively distinguish two cases, according to whether the ERP acting on the surface states is weak or strong. A weak ERP only produces a backfolding of surface bands, such that weak replicas of the original Dirac cones appear shifted by the reconstruction wavevector $\mathbf{Q} = (\pi, 0)$. In contrast, a strong ERP induces a particular crossing of

Dirac cones, accompanied by a Lifshitz transition of in-gap states and the formation of a new Dirac cone, protected by mirror symmetry, at the edge of the small BZ. We have provided a numerical example for the case of strong ERP, and shown that new QPI peaks can appear as a consequence of this transition.

The ERP itself depends mostly on the weight of the surface states on the first atomic layer(s), which in turn depends on microscopic details such as the penetration depth λ of the surface states, or the presence of a surface scattering potential. Our tight-binding approach cannot fully predict the strength of the ERP because detailed information on the structure of the reconstructed surface would be required. Ab-initio calculations could help, but to our knowledge no systematic studies have been conducted on reconstructed SmB_6

surfaces. Experimentally, existing ARPES data—showing weak replicas only—suggests a weak ERP which, however, is difficult to reconcile with our analysis: using reasonable model assumptions, we tend to generically obtain a strong ERP. Possibly, the ERP is stronger than what appears from the ARPES experiments, for example if the probed surface area contains large non-reconstructed (or disordered) regions which in turn do not contribute to band backfolding. We recall that some other correlated materials with strong periodic modulations also fail to display strong bandfolding effects in ARPES, presumably due to quenched disorder, one example being $\text{La}_{1.8-x}\text{Eu}_{0.2}\text{Sr}_x\text{CuO}_4$ [49].

Based on our results, we suggest that small-spot ARPES on 2×1 reconstructed surfaces as well as careful QPI studies, searching for additional peaks appearing above the Lifshitz transition, could clarify and further elucidate the surface-reconstruction effects in SmB_6 .

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Appendix A. Tight-binding modeling

A.1. Bulk model

To model SmB_6 , we only retain Sm atoms, and we build a tight-binding model out of the $d_{x^2-y^2}$ - d_z^2 quadruplet in the d shell, and of the Γ_8 quadruplet in the f shell, where $|\Gamma_8^{(1)} \pm \rangle = \sqrt{\frac{5}{6}} | \pm \frac{5}{2} \rangle + \sqrt{\frac{1}{6}} | \mp \frac{3}{2} \rangle$, $|\Gamma_8^{(2)} \pm \rangle = | \pm \frac{1}{2} \rangle$ [1, 3, 6, 29]. We use two kinetic energy terms for d states ($t_1^d = \langle d_z^2 | H | d_z^2 \rangle_{001}$, $t_2^d = \langle d_z^2 | H | d_z^2 \rangle_{110}$, where the suffix 001 or 110 denotes the direction along which the matrix element is considered), two kinetic energy terms for f states ($t_1^f = \langle \Gamma_8^{(2)} + | H | \Gamma_8^{(2)} + \rangle_{001}$,

$t_2^f = \langle \Gamma_8^{(2)} + | H | \Gamma_8^{(2)} + \rangle_{110}$), two hybridization terms ($v_1 = \langle d_z^2 \uparrow | H | \Gamma_8^{(2)} + \rangle_{001}$, $v_2 = \langle d_z^2 \uparrow | H | \Gamma_8^{(2)} + \rangle_{110}$), and one on-site energy difference between the d and f states $\epsilon_d - \epsilon_f$. The kinetic energy is fixed to give at the three $X = (0, 0, \pi) = (0, \pi, 0) = (\pi, 0, 0)$ points a minimum in the d shell, with $d_{x^2-y^2}$ symmetry at $(0, 0, \pi)$, and a maximum in the f shell; this leads to band inversion at the X points, and to the topological \mathbb{Z}_2 indices $(\nu_0, \nu_1, \nu_2, \nu_3) = (1, 1, 1, 1)$. The hybridization is chosen to be in the $C_{k_z=0}^+ = +2$, $C_{k_z=\pi}^+ = +1$, $C_{k_x=k_y}^+ = -1$ phase, where C^+ are mirror Chern numbers [5–7]:

$$C_{\overline{BZ}}^+ = \frac{i}{2\pi} \sum_{a,b=1}^2 \epsilon_{ab} \sum_{n=1}^N \int_{\overline{BZ}} d^2\mathbf{k} \times \langle \partial_a u_n^+(\mathbf{k}) | \partial_b u_n^+(\mathbf{k}) \rangle, \quad (\text{A.1})$$

where $M | u_n^+(\mathbf{k}) \rangle = +i | u_n^+(\mathbf{k}) \rangle$ and \mathbf{k} lying in the plane \overline{BZ} which is invariant under the symmetry operator M ($M = M_z$ when \overline{BZ} is $k_z = 0$ or $k_z = \pi$, $M = M_{x-y}$ when \overline{BZ} is $k_x = k_y$). This leads to a positive winding number on the \bar{X} cones [6] as observed experimentally [17], and is relevant for the QPI signal and the spin structure of the surface states, but not for their dispersion.

The Hamiltonian

$$H = H_{\text{kin}} + H_{\text{hybr}} \quad (\text{A.2})$$

is composed by the kinetic energy term:

$$H_{\text{kin}} = \begin{pmatrix} H_d & 0 \\ 0 & H_f \end{pmatrix}, \quad (\text{A.3})$$

and by the hybridization:

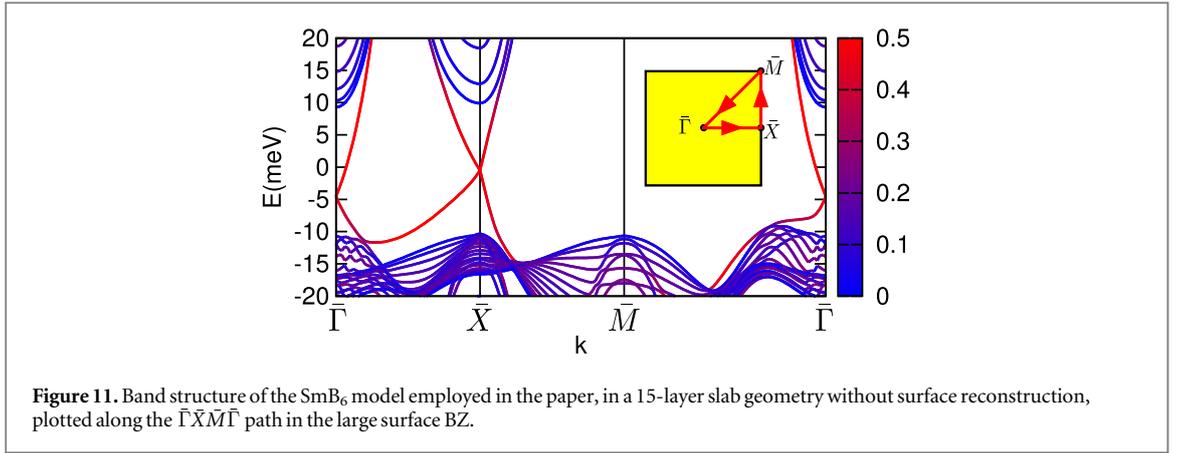
$$H_{\text{hybr}} = \begin{pmatrix} 0 & iH_{df} \\ -iH_{df}^\dagger & 0 \end{pmatrix}. \quad (\text{A.4})$$

The kinetic energy H_i , $i = d/f$, is diagonal in the (pseudo)spin index, with basis $d_{x^2-y^2}$ and d_z^2 when $i = d$, and $\Gamma_8^{(1)}$, $\Gamma_8^{(2)}$ when $i = f$; the hybridization H_{df} is nondiagonal in the (pseudo)spin index, with basis $d_{x^2-y^2} \uparrow$, $d_{x^2-y^2} \downarrow$, $d_z^2 \uparrow$ and $d_z^2 \downarrow$ for rows, and $\Gamma_8^{(1)} +$, $\Gamma_8^{(1)} -$, $\Gamma_8^{(2)} +$ and $\Gamma_8^{(2)} -$ for columns.

Their explicit form is as follows ($c_x = \cos k_x$, $c_y = \cos k_y$, $c_z = \cos k_z$, $s_x = \sin k_x$, $s_y = \sin k_y$, $s_z = \sin k_z$, $s_\pm = s_x \pm i s_y$, $cs_\pm = c_y s_x \pm i c_x s_y$):

$$H_i = \begin{pmatrix} \epsilon^i + 3(c_x + c_y)(t_1^i/2 + c_z t_2^i) & \sqrt{3}(c_x - c_y)(-t_1^i/2 + c_z t_2^i) \\ \sqrt{3}(c_x - c_y)(-t_1^i/2 + c_z t_2^i) & \epsilon^i + (c_x + c_y)(t_1^i/2 + c_z t_2^i) + 2c_z t_1^i + 4c_x c_y t_2^i \end{pmatrix}, \quad i = d/f, \quad (\text{A.5})$$

$$H_{df} = \begin{pmatrix} 3v_2(c_x + c_y)s_z & 3s_-(v_1/2 + c_z v_2) & \sqrt{3}(c_x - c_y)s_z v_2 & \sqrt{3}s_+(-v_1/2 + c_z v_2) \\ 3s_+(v_1/2 + c_z v_2) & -3v_2(c_x + c_y)s_z & \sqrt{3}s_-(-v_1/2 + c_z v_2) & -\sqrt{3}(c_x - c_y)s_z v_2 \\ \sqrt{3}(c_x - c_y)s_z v_2 & \sqrt{3}s_+(-v_1/2 + c_z v_2) & s_z[2v_1 + (c_x + c_y)v_2] & s_-(v_1/2 + c_z v_2) + 4v_2 cs_- \\ \sqrt{3}s_-(-v_1/2 + c_z v_2) & -\sqrt{3}(c_x - c_y)s_z v_2 & s_+(v_1/2 + c_z v_2) + 4v_2 cs_+ & -s_z[2v_1 + (c_x + c_y)v_2] \end{pmatrix}. \quad (\text{A.6})$$



Parameters are taken from the tight-binding calculations of [28, 29], with a slave-boson-like renormalization of the f kinetic energy by b^2 and of the hybridization by b , with $b^2 \sim 0.08$, and fine tuned to better match the ARPES experimental data. For figures 5–7 we increased the value of the hybridization by roughly 50% with respect to this estimation to better highlight the QPI features; this however does not appreciably affect the ERP, which would be in any case large. In particular we employ: $\epsilon^d - \epsilon^f = 1.8\text{ eV}$, $t_1^d = -0.76\text{ eV}$, $t_2^d = 0.2\text{ eV}$, $t_1^f = 3.2\text{ meV}$, $t_2^f = -1.6\text{ meV}$, $\nu_1 = -84\text{ meV}$, $\nu_2 = 24\text{ meV}$, which lead to a bulk gap $\Delta = 18\text{ meV}$, to $\epsilon^f = -10\text{ meV}$ with respect to the chemical potential, and to a level occupation $n_d = 0.51$, $n_f = 3.49$, which corresponds to a $\text{Sm}^{2.5+}$ valence; the chemical potential is set in the middle of the bulk gap. In figure 11 we show the dispersion for a slab without reconstruction; the same data is shown in figure 5(a) in the small BZ.

A.2. Surface reconstruction

We model the reconstruction by applying a large scattering potential $V_{\text{rec}} = 100\text{ eV}$ on sites on every second row of the top layer; we neglect any relaxation effect that the removal of these top atoms can cause. We also apply a surface scattering potential $\Delta E = \Delta E_d = \Delta E_f = -0.5\text{ eV}$, which is set to align the energies of the Dirac cones to approximately reproduce a situation close to the experimental one, allowing for the Lifshitz transition of the surface states. The penetration length λ at the Fermi energy is about two atomic layers for all cones.

In the Kondo breakdown scenario we set $\Delta E_f = 100\text{ eV}$ for the f states, but still retain a finite $\Delta E_d = -0.5\text{ eV}$ for the d states; in this case no appreciable modification of the dispersion or of the QPI signal is observed with respect to figures 5 and 7 of the main text.

In figure 8 we use $t_1^f = 6\text{ meV}$, $t_2^f = -3\text{ meV}$, $\nu_1 = -42\text{ meV}$, $\nu_2 = 12\text{ meV}$, $\Delta E = 0.1\text{ eV}$, and keep the other parameters fixed.

We are able to achieve the Lifshitz transition with $\Delta E_d = 0$, when $t_1^f = 4.8\text{ meV}$, $t_2^f = -1.8\text{ meV}$, $\nu_1 = -46\text{ meV}$, $\nu_2 = 13\text{ meV}$, and the other parameters are fixed. For this parameter set we do not show results, but the QPI patterns are very similar to those of figure 8.

A.3. QPI

The QPI figures are generated with a 400×400 mesh on a 15-layer slab, using the scattering matrix technique (see [35] for technical details) with an artificial broadening of $\delta = 1\text{ meV}$ (figures 9 and 10: $\delta = 2\text{ meV}$). We take a 30meV scatterer in both the d and the f channels in the first two layers in sublattice a , but results were found to be qualitatively independent of the choice of the scattering potential. As remarked earlier, the quantitative results depend on the exact choice of the parameters [34].

In the QPI figures, we only report the Fourier transform of the impurity-induced piece of the LDOS, i.e. the structural peaks at momenta $(0, 0)$ and $(\pi, 0)$ (the reconstruction wavevector) are not shown.

References

- [1] Takimoto T 2011 *J. Phys. Soc. Jpn.* **80** 123710
- [2] Lu F, Zhao J, Weng H, Fang Z and Dai X 2013 *Phys. Rev. Lett.* **110** 096401
- [3] Alexandrov V, Dzero M and Coleman P 2013 *Phys. Rev. Lett.* **111** 226403
- [4] Dzero M, Sun K, Galitski V and Coleman P 2010 *Phys. Rev. Lett.* **104** 106408
- [5] Ye M, Allen J W and Sun K 2013 arXiv:1307.7191
- [6] Baruselli P P and Vojta M 2015 *Phys. Rev. Lett.* **115** 156404
- [7] Legner M, Rüegg A and Sigrist M 2015 *Phys. Rev. Lett.* **115** 156405
- [8] Wolgast S, Kurdak C, Sun K, Allen J W, Kim D-J and Fisk Z 2013 *Phys. Rev. B* **88** 180405(R)
- [9] Kim D J, Xia J and Fisk Z 2014 *Nature Mat.* **13** 466
- [10] Zhang X, Butch N P, Syers P, Ziemak S, Greene R L and Paglione J 2013 *Phys. Rev. X* **3** 011011
- [11] Li G *et al* 2014 *Science* **346** 1208
- [12] Neupane M *et al* 2013 *Nature Comm.* **4** 2991
- [13] Xu N *et al* 2013 *Phys. Rev. B* **88** 121102
- [14] Jiang J *et al* 2013 *Nature Comm.* **4** 3010
- [15] Min C-H, Lutz P, Fiedler S, Kang B, Cho B, Kim H-D, Bentmann H and Reinert F 2014 *Phys. Rev. Lett.* **112** 226402
- [16] Denlinger J D, Allen J W, Kang J-S, Sun K, Min B-I, Kim D-J and Fisk Z 2013 arXiv:1312.6636

- [17] Xu N *et al* 2014 *Nature Comm.* **5** 4566
- [18] Zhu Z-H, Nicolaou A, Levy G, Butch N P, Syers P, Wang X F, Paglione J, Sawatzky G A, Elfimov I S and Damascelli A 2013 *Phys. Rev. Lett.* **111** 216402
- [19] Frantzeskakis E *et al* 2013 *Phys. Rev. X* **3** 041024
- [20] Hlawenka P *et al* 2015 arXiv:1502.01542
- [21] Rößler S, Jang T-H, Kim D-J, Tjeng L H, Fisk Z, Steglich F and Wirth S 2014 *Proc. Nat. Acad. Sci.* **111** 4798
- [22] Yee M M, He Y, Soumyanarayanan A, Kim D-J, Fisk Z and Hoffman J E 2013 arXiv:1308.1085
- [23] Dziawa P *et al* 2012 *Nature Mat.* **11** 1023
- [24] Xu S-Y *et al* 2012 *Nature Comm.* **3** 1192
- [25] Hsieh T, Lin H, Liu J, Duan W, Bansil A and Fu L 2012 *Nature Comm.* **3** 982
- [26] Ruan W, Ye C, Guo M, Chen F, Chen X, Zhang G-M and Wang Y 2014 *Phys. Rev. Lett.* **112** 136401
- [27] Kim J, Kim K, Kang C-J, Kim S, Choi H C, Kang J-S, Denlinger J D and Min B I 2014 *Phys. Rev. B* **90** 075131
- [28] Deng X, Haule K and Kotliar G 2013 *Phys. Rev. Lett.* **111** 176404
- [29] Baruselli P P and Vojta M 2014 *Phys. Rev. B* **90** 201106
- [30] Roy B, Sau J D, Dzero M and Galitski V 2014 *Phys. Rev. B* **90** 155314
- [31] Schubert G, Fehske H, Fritz L and Vojta M 2012 *Phys. Rev. B* **85** 201105(R)
- [32] Wakeham N, Wang Y Q, Fisk Z, Ronning F and Thompson J D 2015 *Phys. Rev. B* **91** 085107
- [33] Hewson A C 1993 *The Kondo Problem to Heavy Fermions* (Cambridge: Cambridge University Press)
- [34] Interaction-induced renormalizations typically also reduce the quasiparticle weight in both ARPES and QPI. This is not taken into account in our modelling.
- [35] Baruselli P P and Vojta M 2014 *Phys. Rev. B* **89** 205105
- [36] Alexandrov V, Coleman P and Erten O 2015 *Phys. Rev. Lett.* **114** 177202
- [37] Fuhrman W T *et al* 2015 *Phys. Rev. Lett.* **114** 036401
- [38] Denlinger J D, Allen J W, Kang J-S, Sun K, Kim J-W, Shim J, Min B I, Kim D J and Fisk F 2013 arXiv:1312.6637
- [39] Tanaka Y Y, Ren Z, Sato T, Nakayama K, Souma S, Takahashi T, Segawa K and Ando Y 2012 *Nat. Phys.* **8** 800
- [40] Teo J C Y, Fu L and Kane C L 2008 *Phys. Rev. B* **78** 045426
- [41] Legner M, Rüegg A and Sigrist M 2014 *Phys. Rev. B* **89** 085110
- [42] Zhang T *et al* 2009 *Phys. Rev. Lett.* **103** 266803
- [43] Roushan P, Seo J, Parker C V, Hor Y S, Hsieh D, Qian D, Richardella A and Hasan M Z 2009 *Nature* **460** 1106
- [44] Guo H-M and Franz M 2010 *Phys. Rev. B* **81** 041102
- [45] Fang C, Gilbert M J, Xu S-Y, Bernevig B A and Hasan M Z 2013 *Phys. Rev. B* **88** 125141
- [46] Liu Q, Qi X-L and Zhang S-C 2012 *Phys. Rev. B* **85** 125314
- [47] Hoffman J E private communication
- [48] Maltseva M, Dzero M and Coleman P 2009 *Phys. Rev. Lett.* **103** 206402
- [49] Zabolotnyy V B *et al* 2009 *EPL* **86** 47005