The handle http://hdl.handle.net/1887/37232 holds various files of this Leiden University dissertation.

Author: Slager, Robert-Jan
Title: The symmetry of crystals and the topology of electrons
Issue Date: 2016-01-12
Chapter 5

The $K$-$b$-$t$ rule

The existence of physical responses distinguishing different associated orders is of central importance for the description and verification of any form of matter. The intricate relation between the appearance of mid gap dislocation modes and the space group classification of topological band insulators (TBIs), as established in the previous Chapters, directly reveals the unique status of the dislocation as the universal observable of translationally-active topological phases in this regard. In three spatial dimensions (3D), however, these results in fact impose a paradoxical conundrum from a geometrical point of view, as the characterization of the topological entity of the bulk heuristically corresponds to its specific monopole configuration in the Brillouin zone whereas dislocations in this scenario entail line-like defects. In addition, the possibility of aligning the dislocation line direction vector along the Burgers vector similarly signals a more profound interplay of the lattice topology and the electronic-band structure.

On the other hand, due to the generality of the above mechanisms, it is evident that a dislocation with a Burgers vector along the direction of a non-$\Gamma$ band inversion in reciprocal space should still result in the formation of mid gap modes. Accordingly, it was demonstrated that dislocation lines in three-dimensional TBIs indeed support propagating helical modes that can probe the weak invariants [138, 39]. Nonetheless, as the weak invariants have been proven to be inadequate in the light of the general characterization of $\mathbb{Z}_2$ topological insulating states when the underlying crystal symmetries are taken into account, this raises the question whether the additional anticipated effects regarding the response to dislocations can emerge when the description of the accommodating TBI is appropriately generalized.
In this Chapter, we elucidate the general rule governing the response of dislocation lines in three-dimensional TBIs and uncover their role in the space group classification scheme. According to this \textbf{K-b-t} rule, the lattice topology, represented by dislocation lines oriented in the direction $\mathbf{t}$ having Burgers vector $\mathbf{b}$, conspires with the electronic-band topology, characterized by the band-inversion momentum $\mathbf{K}_{\text{inv}}$, to produce an explicit criterium for the formation of gapless propagating modes along these line defects. Due to the indicated correspondence between the dislocation modes and the classification procedure this in turn reconfirms the introduced framework. Most interestingly, the general principles also identify that, for sufficiently symmetric crystals, this conspiracy leads to topologically-protected metallic states bound to freely deformable dislocation channels, that can be arbitrarily embedded in the parent TBI. These findings are moreover experimentally consequential as dislocation defects are ubiquitous in any real crystal.

5.1 Formulation and general principles

Although early on it was identified that in three-dimensional TBIs dislocation lines support propagating helical modes [138, 139, 140, 141], the precise role of dislocations has not been explored thoroughly. In particular, the relation between the lattice symmetry and the electronic topology, as well as the characterization of these topological states through the response of the dislocation lines has not been addressed. We here fill this void by detailing the specific mechanism in the light of the space group classification.

Dislocations in three dimensions (3D) are defects with a far richer structure than their two-dimensional counterparts. They form lines $\mathbf{l}(\tau)$ characterized by a tangent vector $\mathbf{t} \equiv d\mathbf{l}/d\tau$, with the discontinuity introduced to the crystalline order described by the Burgers vector $\mathbf{b}$. Both these vectors can only be oriented along the principal axes of the crystal, and screw (edge) dislocations are obtained when $\mathbf{b} \parallel \mathbf{t}$ ($\mathbf{b} \perp \mathbf{t}$), see Fig. 5.1. Moreover, the Burgers vectors are additive, and in full generality we can thus consider only dislocations with the Burgers vectors equal to Bravais lattice vectors. The crucial fact that then reconnects these notions to the classification scheme is the observation that translational lattice symmetry is preserved along the defect line for any proper dislocation probing the specific crystal geometry. Therefore, the full lattice Hamiltonian in the presence of a dislocation oriented along, for instance, the $z$-axis
\[ (t = e_z) \text{ can be written as} \]
\[ H_{3D}(x,y,z) = \sum_{k_z} e^{ik_z z} H_{2D}^{\text{eff}}(x,y,k_z). \] (5.1)

Notice that the 2D lattice Hamiltonian \( H_{2D}^{\text{eff}} \) possesses the (wallpaper group) symmetry of the crystallographic plane orthogonal to the dislocation line, because the Burgers vector is a Bravais lattice vector. This directly confirms the universal status of the dislocation as the translational probe of the lattice topology and shows the compatibility of the above in the context of the full underlying space group.

Given the fundamental reduction procedure, we revert to the electronic topology of a TBI, which is characterized by the band-inversions at the time-reversal invariant (TRI) momenta \( K_{\text{inv}} \) in the Brillouin zone (BZ). As a dislocation disturbs the crystalline order only microscopically close to its core, we can use the continuum theory of elasticity to describe its effect at low energies. The elastic deformation of the continuous medium is encoded by a distortion field \( \varepsilon_i \) of the global Cartesian reference frame \( e_i, e_\alpha = \delta_\alpha i \), with \( i, \alpha = 1,2,3 \) [116, 115]. The momentum of the electronic excitations near the transition from a topologically trivial to a non-trivial phase with the bandgap closing at the momentum \( K_{\text{inv}} \) is accordingly given by \( k_i = (e_i + \varepsilon_i) \cdot (K_{\text{inv}} - q) \), with \( q \ll K_{\text{inv}} \sim 1/a, \varepsilon \sim a/r, a \) the lattice constant, and \( r \) being the distance from the defect core. Therefore the dislocation gives rise to a \( U(1) \) gauge field \( A_i = -\varepsilon_i \cdot K_{\text{inv}} \) that minimally couples to the electronic excitations, \( q \rightarrow q + A \). Moreover, the translational symmetry then implies that the resulting gauge field only has non-trivial components in the plane orthogonal to the dislocation line, consistent with Eq. (5.1), carrying an effective flux \( \Phi = K_{\text{inv}} \cdot b \), as we demonstrate below.

Consider for concreteness an edge and a screw dislocation both oriented along the \( z \)-axis. We use that for the edge dislocation with Burgers vector \( b = ae_x \), the dual basis in the tangent space at the point \( r \) is \( E^x = \left( 1 - \frac{ay}{2\pi r^2} \right) e^x + \frac{ax}{2\pi r^2} e^y, E^y = e^y, E^z = e^z \), while for the screw dislocation with \( b = ae_z \), we have \( E^x = e^x, E^y = e^y, E^z = \frac{b}{2\pi r^2} (ye^x + xe^y) + e^z \); \( r^2 \equiv x^2 + y^2 \) [116]. The corresponding distortions for both an edge and a screw dislocation are then readily verified to be \( \varepsilon_x = \frac{y}{2\pi r^2} b, \varepsilon_y = -\frac{x}{2\pi r^2} b \) to leading order in \( a/r \) (see Appendix 5.B). Consequently, the corresponding gauge potential \( A(r) \) has non-trivial components in the plane orthogonal to the dislocation line, \( A \cdot t = 0 \), and
\[
A = \frac{-ye_x + xe_y}{2\pi r^2} (K_{\text{inv}} \cdot b) \equiv \frac{-ye_x + xe_y}{2\pi r^2} \Phi. \] (5.2)
When this flux $\Phi (\text{mod } 2\pi)$ is nonzero, the dislocations host propagating helical modes provided that the 2D Hamiltonian in a TRI plane orthogonal to the dislocation line, $\hat{\mathbf{t}} \equiv \mathbf{t}/|\mathbf{t}|$, is topologically non-trivial in the exact sense of the space group classification. That is, only when the projected Hamiltonian $H^{2D}_{\text{eff}}(k)$ features an odd number of non-symmetry related translationally-active inversion momenta, mid gap states at that momentum $k$ are developed for non-zero $\Phi$. The full spectrum of modes, for each $k$, is then protected by the lattice symmetry that relates the gauged momenta $\mathbf{K}_{\text{inv}}$. This is what we refer to as the K-b-t rule (see Fig. 5.1).

Finally, we note that this rule and the following descendant construction together imply that the bound states for a given $\mathbf{k} \cdot \hat{\mathbf{t}}$ momentum combine into a spectrum of propagating helical modes along the dislocation line. For $\mathbf{k} \cdot \hat{\mathbf{t}} = \mathbf{K}_{\text{inv}} \cdot \hat{\mathbf{t}}$, the system develops a Kramers pair of true zero modes $\Psi_0 \equiv (\psi_0, T\psi_0)^\top$, with $T$ representing the time-reversal operator satisfying $T^2 = -1$. We should stress here that for this specific momentum the reduced system precisely reduces to a representative of the 2D problems considered in the previous Chapters and that the term zero mode should be interpreted in this manner. This is a consequence of the fact that by definition the $\mathbf{K}_{\text{inv}}$ point is a TRI point hosting a band inversion. Deviating from this 'parent' momentum by $\mathbf{q} \cdot \hat{\mathbf{t}}$, the effective low-energy Hamiltonian for the propagating modes then generally develops a linear gap $H^{\text{eff}} \sim \mathbf{q} \cdot \hat{\mathbf{t}}$, to lowest order. The gapped Kramers pair of descendant states are then present as long as $H^{\text{eff}}(q)$ remains in the topological non-trivial phase and may then be captured by $H^{\text{eff}} = v_t \Sigma_3 (\mathbf{q} \cdot \hat{\mathbf{t}}) + \mathcal{O}(q^2)$. Where, the Pauli matrix $\Sigma_3$ acts in the two-dimensional Hilbert space of the dislocation modes, which are of the form $\Psi_{q_0} \equiv (\psi_{0} e^{i(\mathbf{q} \cdot \hat{\mathbf{t}})(\mathbf{r} \cdot \hat{\mathbf{t}})}, (T \psi_0) e^{-i(\mathbf{q} \cdot \hat{\mathbf{t}})(\mathbf{r} \cdot \hat{\mathbf{t}})}^\top$, and $v_t$ is the characteristic velocity, which is set by the symmetries and details of the band structure.
Figure 5.1: Illustration of the K-b-t rule relating the electronic topology in the momentum space (top panels), and the effect of dislocations in real space (bottom panels). Panels A to D show the electronic-band topology of the T-p3(4)_R and T-p3(4)_M phases on a simple cubic lattice and the p4_{R,M} and p4_{X',R} weak phases on tetragonal lattices. A dislocation with Burgers vector $b = e_x$ acts on the encircled TRI momenta in the planes orthogonal to the dislocation line. As a result, the colored planes host an effective $\pi$ flux. The resulting number of Kramers pairs of helical modes along the edge and screw parts of the loop is indicated with the blue number. (A) The symmetric T-p3(4)_R phase has a topologically non-trivial plane hosting a $\pi$ flux orthogonal to any of the three crystallographic directions and hence any dislocation loop binds modes along the entire core, as shown for a loop in the $\hat{x} - \hat{z}$ plane, panel E. (B) In the T-p3(4)_M phase, translationally active phases in the TRI planes orthogonal to $k_z$ and a valley phase in $k_x = \pi$ plane host $\pi$ fluxes. Hence the dislocation loop binds two pairs of modes, as displayed in panel F. These modes are symmetry-protected against mixing. (C) In the p4_{M,R} phase, only the TRI planes normal to $k_z$ host an effective $\pi$-flux and hence the same dislocation loop binds modes only to the edge-dislocation parts, as displayed in panel G. These modes are not protected against mixing. (D) The p4_{X',R} phase all TRI planes orthogonal to the dislocations lines have a trivial flux, and, according to the K-b-t rule, neither the edge nor the screw dislocation of the loop binds modes, as illustrated in panel H.
5.2 Implications of the rule

The above formulated \( \mathbf{K} \cdot \mathbf{b} \cdot \mathbf{t} \) rule demonstrates how the dislocation line \( \mathbf{t} \), the Burgers vector \( \mathbf{b} \) and the TRI momenta \( \mathbf{K}_{\text{inv}} \) conspire into a precise condition determining the existence of the dislocation propagating modes in certain directions in a topologically-insulating phase, consistent with the space group classification (see Fig. 5.1). By varying \( \mathbf{t} \) and \( \mathbf{b} \) in all directions, the number of ”parent” zero modes in any projection plane is in one-to-one correspondence with the space group classification in terms of the \( \mathbf{K}_{\text{inv}} \) momenta. Specifically, for a translational active phase with a single \( \mathbf{K}_{\text{inv}} \) momentum, edge and screw dislocations bind a single Kramers pair of helical modes if \( \mathbf{K}_{\text{inv}} \cdot \mathbf{b} \neq 0 \). In case of a translationally active phase or a valley phase with multiple \( \mathbf{K}_{\text{inv}} \) momenta, a projected 2D system may also result in a double pair of modes if the effective system entails a 2D valley phase. The two pairs are then protected by the symmetries relating the \( \mathbf{K}_{\text{inv}} \) momenta. Most interestingly, there is the possibility that both edge and screw dislocations bind modes in any crystal direction resulting in propagating modes along the full dislocation loops. In particular, in a completely isotropic lattice with \( O_h \) crystal symmetry a strong variant of this effect can be realized: the gapless states in the dislocation loop that propagate in a way completely oblivious to the lattice directions.

In contrast, in a weak phase characterized by the weak topological invariant \( \mathbf{M} \), protected helical modes are argued to exists only when the product \( \mathbf{M} \cdot \mathbf{b} \) (mod\(2\pi\)) is non-trivial [138, 139, 140, 39]. This is consistent with the fact that double pairs of modes originating from two \( \mathbf{K}_{\text{inv}} \) not related by symmetry may be gapped out. However, according to the \( \mathbf{K} \cdot \mathbf{b} \cdot \mathbf{t} \) rule if the \( \mathbf{K}_{\text{inv}} \) are related by symmetry such pairs in fact enjoy protection. Moreover, the \( \mathbf{K} \cdot \mathbf{b} \cdot \mathbf{t} \) rule precisely reveals the condition for the formation of the mid gap modes in the case of a generic crystal group, whereas the definition of a weak invariant necessitates a layered structure. We thus observe that the appropriate generalization of the weak invariants to the general space group classification directly exposes the anticipated more elaborate dislocation response mechanism.
5.3 Exemplification

The above general statements can be illustrated by employing the familiar class of simple tight-binding models comprising two orbitals (Appendix 5.A) with different parity and two spin states \([45, 142]\) on a simple cubic lattice with space group \(pm\bar{3}m\)

\[
H_{nn} = A(\gamma_1 \sin k_x + \gamma_2 \sin k_y + \gamma_3 \sin k_z) + M_{nn} \gamma_0. \tag{5.3}
\]

Here \(k\) refers the electron momentum, the \(\gamma\)-matrices act in the orbital and the spin spaces, and we have used natural units (\(\hbar = c = a = 1\)). As usual, the topological phases of the model (5.3) can be tuned with the mass term \(M_{nn} = m - 2B(3 - \cos k_x - \cos k_y - \cos k_z)\). Let us assume that the system is in the \(T-p3(4)R\) phase with the band-inversion at momentum \((\pi, \pi, \pi)\) (Figures 5.1(A) and 5.2). If \(b = e_x\) and \(t = e_z\), the effective Hamiltonian in the \(k_z = \pi\) plane reduces to the \(\pi\) flux problem in the two-dimensional \(T-p4M\) phase, and hence possesses zero modes. For the family of Hamiltonians (5.1) any momentum \(k_z = \pi + q_z\) infinitesimally close to \(k_z = \pi\) then yields the would-be zero modes in the absence of the term \(\sim \gamma_3\). When included, this term gives rise to the anticipated linearly dispersing propagating modes along the dislocation line. Moreover, the \(K-b-t\) rule also directly conveys the number of descendent states in the spectrum, as the mass term \(M_{nn}(k_z)\) sets the topological condition for the existence of the dislocation mode (see Appendix 5.B). Furthermore, the same rule implies that an edge or a screw dislocation along any Bravais lattice vector in the simple cubic lattice effectively acts as a \(\pi\) flux. Henceforth, when these defects are joined in a loop in the \(x-z\)-plane with \(b = e_x\), we expect propagating modes, which are indeed found in the corroborating numerical computations as detailed in the Appendix and Fig. 5.2. We note that TRS together with the crystal symmetry evidently protects the modes from backscattering in this scenario.

As a next step, we consider the system in the \(T-p3(4)M\) phase with the band-inversion located at the momenta \(M \equiv (\pi, \pi, 0)\), \(X' \equiv (\pi, 0, \pi)\), \(Y' \equiv (0, \pi, \pi)\), which are related by the threefold rotational symmetry (Figs. 5.1(B), (5.7) and (5.12)). According to the \(K-b-t\) rule, for the edge-segment of the dislocation loop, both the \(k_z = 0\) and \(k_z = \pi\) planes host an effective \(\pi\)-flux, originating from the \(M\) and \(X'\) points. Additionally, the \(k_x = \pi\) plane hosts a valley phase, and thus the screw-dislocation parts also host two pairs of modes. Therefore, there is a total of two Kramers pairs of gapless dislocation modes along the loop, which are protected by symmetry. Note that their existence crucially
Figure 5.2: The effect of dislocation lines in 3D topological band insulators. Edge and screw dislocations with Burgers vector $\mathbf{b} = \mathbf{e}_z$ are treated simultaneously by considering dislocation loops of $8 \times 8$ sites within the tight-binding model (5.3) on the lattice with $16 \times 16 \times 16$ sites in case of periodic boundary conditions, see the Appendix for details. Panels A and C show the spectrum of the dislocation modes traversing the gap in case of the $T$-$p^3(4)_R$ and $p^4_{M,R}$ phases, with the corresponding electronic topological configurations shown in the insets on the upper left. The circles indicate the TRI momenta hosting band-inversions that yield effective $\pi$-fluxes. Additionally, the spectral density as function of the momentum $\mathbf{k}$, defined along the dislocation line, is displayed in the insets on the lower right. We find a single cone for the $T$-$p^3(4)_R$ phase, and a double cone for the $p^4_{M,R}$ phase, consistent with the K-b-t rule. The energy levels are now eight-fold degenerate as both $k_z = 0$ and $k_z = \pi$ planes are topologically non-trivial, and thus each yields propagating modes due to the effective $\pi$ flux introduced by the dislocations. Panels B and D display the real space localization of the modes, where the weight of the wavefunction is indicated by the size of the circles and the color coding indicates the corresponding phase. Most importantly, the $T$-$p^3(4)_R$ features topologically-protected propagating dislocation modes along the complete loop. In contrast, the $p^4_{M,R}$ phase binds modes only along the edge-dislocation parts. In particular, we find eight energy levels in correspondence with the number of allowed momenta along the dislocation.
5.4 Experimental consequences

depends on the fact that the \( M \) and \( X' \) momenta are symmetry-related. Were this not the case, the weak index of this \( T-p3(4)_M \) phase \( M_i = (0,0,0) \) would predict no dislocation modes at all.

In contrast, let us now break the cubic symmetry by considering the \( p4_{M,R} \) phase on a tetragonal lattice with \( a_x = a_y = a, \ a_z = a/\alpha \), where \( a_i \) is the lattice constant in the direction \( e_i \), and \( \alpha \neq 1 \) is the lattice deformation parameter (Figs. 5.1(C) and 5.2). We stipulate here the subtle difference between such a weak phase and a valley phase, which has an even number of band-inversions protected by a 3D space group symmetry. The usual strong and weak indices [39, 37, 138] in this phase are \((\nu;M_i) = (0;0,0,1)\), and thus \( \mathbf{M} \cdot \mathbf{b} = 0 \). Nonetheless, the \( k_z = 0 \) and \( k_z = \alpha \pi \) planes are topologically non-trivial therein (Fig. 5.1 and Appendix). As a result, for a dislocation loop with \( \mathbf{b} = e_x \), according to the \( \mathbf{K-b-t} \) rule, we find modes bound only to the edge-dislocation parts. As both these planes contribute the midgap states, we expect a double Kramers pair of the propagating metallic states, which our numerical computations indeed confirm. However, these modes can mix in the dislocation loop, since no symmetry relates the momenta \( M \) and \( R \) giving rise to them. Nevertheless, in terms of principle we thus observe that the richer \( \mathbf{K-b-t} \) rule consistently unveils the formation mechanism of the dislocation modes, whereas the the underlying symmetry directly conveys the stability.

Finally, we consider the tetragonal \( p4_{X',R} \) \((p4_{Y',R}) \) phase obtained by deforming the cubic lattice in the \( e_y \) (\( e_x \)) direction with the corresponding band-inversions at \((\pi,0,\pi) \) \([(0,\pi,\pi)]\) and \((\pi,\alpha \pi,\pi) \) \([(\alpha \pi,\pi,\pi)]\) momenta (Fig. 5.1(D)). In this case, we find that no dislocation modes appear in the \( p4_{X',R} \) phase, whereas in the \( p4_{Y',R} \) phase only the band-inversion at momentum \((\alpha \pi,\pi,\pi) \) contributes a \( \pi \) flux, thus yielding the modes for both types of dislocations. These results are therefore similar as in the \( T-p3(4)_R \) phase, as also confirmed by numerical computations showing modes propagating along the entire loop in the \( x-z \) plane. Notice, nonetheless, that due to the unequivalence in directions the velocities along the loop are now in general anisotropic.

5.4 Experimental consequences

The response to dislocations in TBIs is evidently consequential from an experimental point of view, as these defects are ubiquitous in any crystals. In particular, the electron-doped mixed-valent perovskite oxide BaBiO\(_3\) with a simple cubic crystal symmetry has
been recently predicted to be a $\mathbb{Z}_2$ topological band insulator \cite{143}. Most interestingly, the associated topological phase is believed to entail the symmetric $T$-$p3(4)_R$ phase, which should host propagating gapless modes along any dislocation loop, as demonstrated above. The effective tight-binding model (5.3) therefore describes this phase in terms of the explicit parameters $A = 2.5\text{eV}$·Å, $B = 9.0\text{eV}$·Å$^2$, $M = 5.08\text{eV}$, and the lattice constant $a = 4.35\text{Å}$\cite{143}, implying that the velocity of the dislocation modes is $v = A/h = 4.3 \times 10^5 \text{m/s}$, while the localization length $\lambda \sim \sqrt{B/(12Ba^{-2} - M)} \approx 4.8\text{Å}$. More generally, the enhanced density of states near the dislocation line in any non-\Gamma TBI \cite{42, 144, 126, 127} should be observable by local probes, such as scanning tunneling microscopy. Angle-resolved photoemission spectroscopy may finally also be useful for mapping out these states, since the surface irregularities should not affect this probe.

5.5 Conclusions

In conclusion, we have addressed the specific criteria underlying the formation of propagating modes bound to dislocation defects in 3D $\mathbb{Z}_2$ topological band insulators, culminating in the formulation of the \textbf{K-b-t} rule. As a general result, this rule directly signifies the consistency of the introduced space group classification framework from a physical response perspective and, in fact, exposes an intricate relation between the lattice topology and the electronic band topology. Specifically, dislocations are naturally associated with a fundamental reduction procedure, that is compatible with the relevant lattice symmetries and allows for a direct determination of the existence of dislocation modes for each subsystem of descendant momentum $k$ in any specific topological phase. These results, in addition, bear experimental relevance, as dislocations represent ever-present defects in any crystal and serve as the universal probes of translational topological order. In particular, a strong representing and striking variant of the detailed mechanism occurs in the $T$-$p3(4)_R$ phase of materials that feature an isotropic $O_h$ symmetric crystal structure, as in this case the modes propagate along arbitrarily oriented loops in a manner that is completely oblivious to the lattice directions.
5.A Model details

Although we have employed the $M - B$ class of models (Eqs. (2.7) and (2.8)) already extensively for verification purposes, we here present the details regarding the associated topological states realized on cubic and tetragonal lattices. We depart from the generic form comprising two spin degenerate orbitals as described by

$$H = \varepsilon(k)1 + \sum_{\alpha} d_\alpha(k) \gamma_\alpha + \sum_{\alpha\beta} d_{\alpha\beta} \gamma_{\alpha\beta}$$

(5.4)

where $\gamma_\alpha$ are the five Dirac matrices obeying the Clifford algebra $\{\gamma_\alpha, \gamma_\beta\} = 2\delta_{\alpha\beta}$ and $\gamma_{\alpha\beta}$ are the ten commutators $\gamma_{\alpha\beta} = \frac{1}{2i} [\gamma_\alpha, \gamma_\beta]$. Specifically, we take the following basis of $\gamma$-matrices

$$\gamma_0 = \sigma_0 \otimes \tau_3 \quad \gamma_1 = \sigma_1 \otimes \tau_1, \quad \gamma_2 = \sigma_2 \otimes \tau_1, \quad \gamma_3 = \sigma_3 \otimes \tau_1, \quad \gamma_5 = -\gamma_0 \gamma_1 \gamma_2$$

with $\sigma$ and $\tau$ being the standard Pauli matrices acting in the spin and orbital space, respectively; $1 = \sigma_0 \otimes \tau_0$ with $\sigma_0, \tau_0$ as the $2 \times 2$ unity matrices.

The explicit form of the Hamiltonian (5.4) is then determined by exploiting the symmetries. For simplicity we assume, in addition to time-reversal symmetry, a well-defined parity for the tight-binding model, as our interest lies in the topological aspects of the resulting phases. Concretely, time-reversal symmetry is represented by the operator $T = i\vartheta K$, with $\vartheta = i\sigma_2 \otimes \tau_0$ and $K$ as complex conjugation, whereas the parity operator is $P = \gamma_0$. As the commutators $\gamma_{\alpha\beta}$ transform under time-reversal and parity with the opposite sign, the assumption of having both these symmetries thus simply results in $d_{\alpha\beta} = 0$. The remaining functions $d_\alpha(k)$ of the effective model can then be obtained from the theory of invariants. Let us consider the space group $pm\bar{3}m$ with the point group $O_h$ in particular. This point group has two one-dimensional, one two-dimensional and two three-dimensional irreducible representations. The matrix $\gamma_0$ anticommutes with the $\gamma$-matrices $\{\gamma_1, \gamma_2, \gamma_3\}$ and therefore represents the mass term, which is by construction even under the parity. The corresponding mass term has to be rotationally-symmetric and therefore entails an even polynomial in the momentum, $k$. Using also that the $\gamma$-matrices $\{\gamma_1, \gamma_2, \gamma_3\}$ form a three-dimensional representation under rotations in $O_h$, we arrive at the following minimal continuum Hamiltonian that captures the topologically non-trivial phases of interest

$$H_{eff} = \Lambda(k_x \gamma_1 + k_y \gamma_2 + k_z \gamma_3) + M_{nn} \gamma_0 + O(k^3)$$

(5.5)
where \(M_{nn} = m - 2B(k_x^2 + k_y^2 + k_z^2)\) and we have dropped the term \(\sim 1\) not relevant for the topological analysis here. This Hamiltonian evidently generalizes the 2D model (3.1) to three dimensions (3D) and its different incarnations have already been used to describe topological states in Bismuth-based compounds [45, 142].

We can then readily determine the lattice-regularized version of the effective model (5.5) to arrive at the usual class of models. Considering a simple cubic lattice with nearest-neighbor (nn) hoppings, we obtain the following tight-binding Hamiltonian

\[
H_{nn} = A(\gamma_1 \sin k_x + \gamma_2 \sin k_y + \gamma_3 \sin k_z) + M_{nn} \gamma_0, \tag{5.6}
\]

with the effective mass parameter

\[
M_{nn} = m - 2B(3 - \cos k_x - \cos k_y - \cos k_z).
\]

In the above we have set the lattice constant \(a\) to unity and we note that the parameters \(A\) (\(B\)) represent the familiar hopping amplitudes between different (same) orbitals, while \(m\) is the difference of the onsite energies between the two orbitals. Furthermore, the hoppings in the Hamiltonian (5.6) are equal in the three orthogonal directions due to the rotational symmetry.

The above Hamiltonian reduces to the continuum Hamiltonian (5.5) when expanded around the \(\Gamma\) or the \(R\)-point located at the momentum \((\pi, \pi, \pi)\) in the Brillouin zone (BZ). However, in order to enrich the phase diagram, we concede the possibility of adding next-nearest-neighbor hopping terms of the same fashion as the nearest-neighbor ones to the Hamiltonian. Taking into account that on a cube each site has four next-nearest in each of the three mutually orthogonal crystallographic planes, these additional terms assume the form

\[
H_{nnn} = \frac{\tilde{A}}{2} \left[ \sin(k_x + k_y)(\gamma_1 + \gamma_2) + \sin(-k_x + k_y)(-\gamma_1 + \gamma_2) \right] \\
+ \frac{\tilde{A}}{2} \left[ \sin(k_x + k_z)(\gamma_1 + \gamma_3) + \sin(-k_x + k_z)(-\gamma_1 + \gamma_3) \right] \\
+ \frac{\tilde{A}}{2} \left[ \sin(k_y + k_z)(\gamma_2 + \gamma_3) + \sin(-k_y + k_z)(-\gamma_2 + \gamma_3) \right] \\
- 4\tilde{B} \left[ 3 - \cos(k_x) \cos(k_y) - \cos(k_x) \cos(k_z) - \cos(k_y) \cos(k_z) \right] \gamma_0. \tag{5.7}
\]

Hence, considering both contributions the total Hamiltonian is given by

\[
H_{TB} = H_{nn} + H_{nnn} \tag{5.8}
\]
The different topological phases are then obtained by varying the mass term multiplying the $\gamma_0$ matrix. The topological phase transitions occur when the mass term vanishes at the time-reversal invariant momenta in the BZ and the corresponding phases can be characterized by the mass term at these special momenta, as outlined in the previous Chapter. As a result, the phase diagram, with $A = 1$, is readily obtained as a function of $M/B$ and $\tilde{B}/B$, see Fig. 5.3.

Finally, note that by lowering the full rotational symmetry of the Hamiltonian (5.6) to in plane $C_4$ rotations, one directly obtains a minimal tight-binding Hamiltonian describing topological phases on a tetragonal lattice

$$H_{\text{tetragonal}}^{\text{nn}} = A_x \gamma_1 \sin k_x + A_y \gamma_2 \sin k_y + A_z \gamma_3 \sin k_z$$
$$+ [m - 2B_x (1 - \cos k_x) - 2B_y (1 - \cos k_y) - 2B_z (1 - \cos k_z)] \gamma_0,$$

which will be of use in the remainder.

Figure 5.3: The phase diagram of the outlined model (5.8), in case of $O_h$ symmetry or space group $\text{pm}3m$. As function of the mass parameter $M/B$ and the nearest neighbor coupling $\tilde{B}/B$, the mass parameters at the TRI momenta can be tuned to produce the different electronic topological configurations shown.
5.B Analytical and numerical evaluation of dislocations modes in three dimensional \( \mathbb{Z}_2 \) topological insulators

In this Appendix we elaborate on the details underlying the formation criteria of the dislocation modes in the context of the models of the previous section, illustrating the working of the \( \mathbf{K-b-t} \) rule in a concrete setting. Let us first examine the effect of dislocations in the coarse-grained continuum theory. In this instance the lattice defects are described within the elastic continuum theory using vielbeins, encoding the map from the perfect lattice to the distorted lattice \([114, 116]\). The resulting torsion \( T^i \) and curvature \( R^i_j \) are then generally related to the vielbeins \( E^i_\alpha \) and the spin connection \( \omega^j_i \) by the Einstein-Cartan structure equations

\[
T^i = dE^i + \omega^j_i \wedge E^j \\
R^i_j = d\omega^j_i + \omega^k_j \wedge \omega^j_k.
\] (5.10)

For a dislocation defect, the curvature vanishes while the torsion is singular. Specifically, \( T^i = b^i \delta(l) \) in terms of the Burgers vector \( b \) and the position \( l \) of the dislocation line. Since the curvature tensor vanishes for a dislocation, the corresponding spin-connection can therefore be set to zero, thereby resulting in an exclusive dependence of the above set of equations on the effective vielbeins.

5.B.1 Edge dislocations

Turning to the case of an edge dislocation oriented along the \( \hat{z} \)-direction, the vielbein takes the form

\[
\hat{E} = E^i_\alpha = \begin{pmatrix}
1 - \frac{by}{2\pi r^2} & \frac{bx}{2\pi r^2} & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix},
\] (A8)

where \( b \) is the magnitude of the Burgers vector \( b \), which is assumed to be along the \( \hat{x} \)-direction \( b = be_x \), and \( r^2 = x^2 + y^2 \). The inverse of the above vielbein is subsequently
5.B Analytical and numerical evaluation of dislocations modes in three dimensional $\mathbb{Z}_2$ topological insulators

readily computed, resulting in

$$\hat{E}^{-1} = E_i^\alpha = \begin{pmatrix} 
(1 - \frac{by}{2\pi r^2})^{-1} & -\frac{bx}{2\pi r^2} (1 - \frac{by}{2\pi r^2})^{-1} & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 
\end{pmatrix}. \quad (5.11)$$

As for an elementary dislocation $b = a$, with $a$ as the lattice constant, the distortion field $E_i = e_i + \epsilon$ to the leading order in $a/r$ is directly verified to be

$$\epsilon_x = \frac{ay}{2\pi r^2}b_x = \frac{y}{2\pi r^2}b, \quad \epsilon_y = -\frac{ax}{2\pi r^2}b_x = -\frac{x}{2\pi r^2}b.$$ The corresponding gauge potential $A = -\epsilon_i \cdot K_{\text{inv}}$, with $K_{\text{inv}}$ the band-inversion momentum, can then straightforwardly be obtained, reproducing Eq. (5.2) in the main text.

We can now consider the effect of an edge dislocation in a 3D topological insulator. We note that along the core of the dislocation translational symmetry is preserved. Henceforth, $k_z$ is a good quantum number and we obtain a family of two-dimensional Hamiltonians

$$H(x,y,z) = \sum_{k_z} e^{ik_z} H_{\text{eff}}(x,y,k_z). \quad (5.12)$$

The dimensionally-reduced Hamiltonian $H_{\text{eff}}(x,y,k_z)$ can then be treated using the methods of the previous Chapters, allowing for a direct evaluation of the spectrum of dislocation modes. Let us make this more concrete for the model with the Hamiltonian (5.8). We assume that the system is in the $T-p3(4)_R$ or $R$ phase (Fig. 5.4). Using $k \rightarrow k + A = k + \frac{1}{2\pi} e_{\phi}$, a straightforward calculation yields

$$H_{\text{eff}}(x,y,k_z) = i\gamma_r \partial_r + i\gamma_\phi (\frac{\partial_r}{r} + \frac{1}{2r}) + \gamma_0 [M - 2B(\triangle + \frac{i}{r^2} \partial_\phi - \frac{1}{4r^2})]\sin(k_z)\gamma_3, \quad (5.13)$$

where

$$M = m - 8B - 2B(1 - \cos k_z) = \hat{M} - 2B(1 - \cos k_z). \quad (5.14)$$

Here, the Laplacian $\triangle = \frac{\partial^2}{r^2} + \frac{1}{r^2} \frac{\partial^2}{\phi^2}$, and $(r, \phi)$ refer to the usual polar coordinates, relating to the Cartesian ones as $x = r \cos \phi, y = r \sin \phi$.

To analyze the propagating dislocation-bound midgap modes, let us first neglect the last $\gamma_3$ term in the Hamiltonian $\sim \sin k_z$. In this scenario we then exactly retrieve the familiar 2D $M - B$ Hamiltonian with effective mass term $M$. Therefore, this Hamiltonian hosts zero modes for the values of the parameters $m, B, k_z$ obeying $0 < M/B < 4$. Now, take $k_z = \pi$. Then, as $8 < m/B < 12$, it follows that $4 < \hat{M}/B < 8$, which is precisely
Figure 5.4: The left panel shows the schematic configuration of the $T$-$p3(4)_R$ or $R$ phase in the Brillouin zone with an edge dislocation with Burgers vector $\mathbf{b} = \mathbf{e}_z$ and is oriented along the $\hat{z}$ direction in the real space. The right panel displays the modes $k_z$ on the unit circle in the complex plane. The imaginary part then encodes for the mass gap of the dislocation mode with respect to the zero mode, whereas the real part relates to the shift $\Delta M(k_z) = -M/B + \hat{M}/B = 2(1 - \cos(k_z))$ of the effective mass parameter in the associated dimensionally reduced $M - B$ model.

the condition for a zero mode solution bound to the dislocation. This solution entails the one derived and discussed in detail in previous Chapters. More specifically, in this parameter range the system entails the $T$-$p4$ or $M$ phase in the reduced 2D Hamiltonian. Similarly, the next $k_z$ value in a finite system results in a dislocation mode if the effective mass $\hat{M}(k_z)$ still satisfies the topological condition $4 < \hat{M}/B < 8$. Moreover, we can exactly determine the corresponding spectrum by reintroducing the last term in the Hamiltonian (5.13), $\Delta_3 \equiv \sin(k_z)\gamma_3$. Since $k_z$ commutes with the Hamiltonian and $\gamma_3$ anticommutes with the other $\gamma$-matrices in the Hamiltonian, the term $\Delta_3$ acts as a mass term for the modes comprising zero-energy subspace in its absence. The corresponding gap is thus $\pm |\sin(k_z)|$ with respect to the zero energy, and in the thermodynamic limit these midgap modes are linearly dispersing along the dislocation line with the velocity set by the hopping in this direction, in agreement with the $\mathbf{K}$-$\mathbf{b}$-$\mathbf{t}$ rule. These conclusions are schematically shown in Fig. 5.4. By displaying the allowed values of $k_z$ in a finite system, $k_z = 2\pi n/L$, with $L \in \mathbb{Z}$ and $n = 0, 1, 2 \ldots L - 1$, on the unit circle in the imaginary plane, the real part characterizes the effective $\hat{M}/B$, while the imaginary part signals the anticipated energy of the dislocation mode. We note that the shift in $\hat{M}$ indeed ensures that the $T$-$p3(4)_R$ phase hosts no dislocation modes with $k_z = 0$ and in the thermodynamic limit all the propagating modes indeed descend from the zero modes at...
the band-inversion momentum \((\pi, \pi, \pi)\), as expected from the K-b-t rule.

The above analytical results can easily be verified by numerical computations, and the two show an excellent agreement. In Fig. 5.5 we show the spectrum of a \(12 \times 12 \times 12\) system on a torus (periodic boundary conditions) and the real space localization of the dislocation modes. We note that the modes are neatly localized and come as two Kramers pairs, one from the dislocation and one from the anti-dislocation. Moreover, since \(\exp(ik_z)\) takes values in the set comprising of the twelfth roots of unity, we can compare the energy gaps with the anticipated \(\sin(k_z)\) dependence and find agreement up to two decimals. In addition, we change the mass parameter \(m\) to confirm that modes can be added or removed from the spectrum consistent with the condition in Eq. (5.13), see Fig. 5.6. These results reproduce for various sizes of the system (ranging up to 16 sites in linear dimension), confirming the presence of the zero mode together with the descendant propagating states, as predicted by the K-b-t rule. Furthermore, when the next-nearest neighbor hoppings are included, the phase \(T - p4M\) protected by both TRS and crystal symmetries with the band inversions at the momenta \((0, \pi, \pi), (\pi, 0, \pi),\) and \((\pi, \pi, 0)\) can be realized, see Fig.5.3. In that case, a dislocation with Burgers vector \(b = ae_x\) and oriented along the \(z\) axis, \(\hat{t} = e_z\), in both planes \(k_z = 0\) and \(k_z = \pi\) acts as \(\pi\)-flux, and thus a double Kramers pair is expected. This is indeed what we find numerically, see Fig. 5.7.

It is straightforward to generalize the explained reasoning to other phases. Let us illustrate this with the primitive tetragonal system taking \(A_x = A_y = \frac{1}{2}A_z\) and \(B_x = B_y = \frac{1}{2}B_z\) in Eq. (5.9). For these parameters we obtain the weak \(p4M,R\) phase with band-inversions at \(M\) and \(R\) points. This phase is displayed in Fig. 5.8, and is not protected by either time-reversal symmetry or a 3D space group symmetry, as opposed to a valley phase. By inserting an edge dislocation with \(b = e_x\) and \(\hat{t} = e_z\) we deduce that both time-reversal invariant planes \((k_z = 0, \pi)\) orthogonal to \(\hat{t}\) are topologically non-trivial and host a \(\pi\)-flux, yielding zero modes at both momenta \(k_z = 0\) and \(k_z = \pi\). Therefore, one anticipates a doubled spectrum of descendant propagating modes along the dislocation, according to the K-b-t rule. We indeed find these propagating modes numerically and explicitly observe the doubling of the Dirac cones as detailed in Figs. (5.8) and (5.9).

We stress, however, that the modes at \(k_z = 0, \pi\) are in this case not protected by any symmetry and may therefore be gapped out trivially by relevant perturbations.
Figure 5.5: The spectrum of the $12 \times 12 \times 12$ system ($M/B = 10$) in the $T\cdot p3(4)_R$ phase with the edge dislocation with periodic boundary conditions. The dislocation modes come in degenerate Kramers pairs, originating from the dislocation and anti-dislocation (panel A). The inset displays the complete spectrum. We note that the energy levels of these modes in the gap are located at $E_n = 0$, $\pm E_N = 0.50$ and at $\pm E_N = 0.86$, in agreement with the theory. Panel B shows the real space localization of the dislocation modes for a fixed $e_z$ plane. The weight of the wavefunction is represented here by the radius of the circles, whereas the color indicates the phase following the same conventions as in Fig 2 in the main text. Due to the translational symmetry, the $e_z$ planes are identical. Finally, panel C shows the spectral density as function of the momentum $k = k_z$ along the dislocation line for a $12 \times 12 \times 28$ system. This spectral density is also plotted as circles, where the radius indicates the weight, in order to further emphasize the excellent agreement with numerics.
Figure 5.6: The spectra for two $12 \times 12 \times 12$ systems on a torus, with $M/B = 9.4$ and $M/B = 10.6$ in the presence of an edge dislocation with Burgers vector $b = e_x$. In this instance $A_z$ was taken to be 0.3, shifting the energy levels to assure that they lie in the gap. The energy levels again take values that match the evaluation outlined above. Moreover, we observe that the $M/B = 9.4$ has one extra level, which is consistent with the mass condition $4 < \hat{M} < 8$. 
Figure 5.7: Effect of an edge dislocation in the $T\cdot p3(4)_M$ phase. The right panel shows the topological configuration, with an edge dislocation oriented along the $\hat{z}$ direction and with $b = e_x$. The left shows the spectrum, and as expected both $k_z = 0$ and $k_z = \pi$ planes host a $\pi$ flux yielding two Kramers pairs of zero modes. The resultant energy levels of the descendant states at finite energy are then fourfold degenerate. The modes originating from the $k_z = \pi$ plane result from the corresponding two-dimensional $p^4$ phase, whereas the $k_z = 0$ plane is in the $T\cdot p4$ phase.
5.B Analytical and numerical evaluation of dislocations modes in three dimensional $\mathbb{Z}_2$ topological insulators

Figure 5.8: The spectra of the tetragonal system with $12 \times 12 \times 12$ (A and E) and a $10 \times 10 \times 10$ (D and E) sites on a torus in the $p4_{M,R}$ phase, with the topological configuration shown in panel C, and an edge dislocation with $b = e_x$. We note the eightfold degeneracy per level, consistent with the $\mathbf{K} \cdot \mathbf{b} \cdot \mathbf{t}$ rule. Namely as the $k_z = 0$ and $k_z = \pi$ planes host the effective $\pi$ fluxes, the modes denoted by 1 in panels A and E are indeed localized around the defect as anticipated. Modes 2-5 and 2-3 in the same panels descend from these zero-energy modes with the spectra matching the analytical results.
Figure 5.9: The spectral density of the $p^4_{M,R}$ phase as function of the momentum $k = k_z$, in case of $16 \times 16 \times 16$ system with periodic boundary conditions. We observe a double Dirac cone situated at $k_z = 0$ and $k_z = \pi$, consistent with the findings in Fig. 5.8. Conventions are identical as in Fig. 5.5.

5.2 Screw dislocations

Three spatial dimensions, in contrast to the two dimensional case, also allow for an orientation of the Burgers vector parallel to the dislocation line. In contrast to the edge dislocation, which is essentially a 2D defect pulled out in the third dimension, the resulting screw dislocation is an intrinsic 3D defect. For a screw dislocation with the Burgers vector oriented along the $\mathbf{\hat{z}}$-axis, $\mathbf{b} = b\mathbf{\hat{z}}$, the vielbeins are given by

$$\mathbf{\hat{E}} \equiv E^i_\alpha = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{by}{2\pi r^2} & -\frac{bx}{2\pi r^2} & 1 \end{pmatrix},$$  \hspace{1cm} (5.15)

and

$$\mathbf{\hat{E}}^{-1} \equiv E^i_\alpha = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{by}{2\pi r^2} & -\frac{bx}{2\pi r^2} & 1 \end{pmatrix}. \hspace{1cm} (5.16)$$

The corresponding distortion field, taking into account that for an elementary dislocation $b = a$, is therefore again given by

$$\mathbf{\varepsilon}_x = \frac{ay}{2\pi r^2} \mathbf{e}_z = \frac{y}{2\pi r^2} \mathbf{b} \hspace{1cm} \mathbf{\varepsilon}_y = -\frac{ax}{2\pi r^2} \mathbf{e}_x = -\frac{x}{2\pi r^2} \mathbf{b},$$  \hspace{1cm} (5.17)

resulting in the same gauge potential given by Eq. (5.2) in the main text.
We note nonetheless that for a screw dislocation, the gauge potential can only be finite if \( K_{\text{inv}, z} \neq 0 \). In the case of a screw dislocation, \( k_z \) is still a good quantum number, and henceforth we find the same equation for the zero-energy modes and the corresponding descendant states (5.13). In Figs. (5.10) and (5.11), we present the numerical analysis of the spectrum of the Hamiltonian in the \( T - p3(4)R \) phase in the presence of a screw dislocation. We obtain in essence the same spectrum as for the edge dislocation. For various system sizes, we find precisely the number of dislocation modes in the spectrum according to the topological condition below Eq. (5.13). Also, we find that the energy difference between the levels is proportional with the \( A_z \) coefficient. We do find however that the energy levels have shifted as compared with the ones obtained in the presence of an edge dislocation in the same phase. Tuning the mass parameter \( M/B \) deeper into the phase, (closer to the value of this parameter \( M/B = 12 \)) results in levels closer to the analytically calculated value, as expected from the finite-size effects, and the fact that the matrix elements are now twisted with a factor \( e^{ik_z} \) along the dislocation direction. We observe in addition that, in general, the form of the underlying metric \( ds^2 = dr^2 + r^2 d\vartheta^2 + (dz + \beta d\vartheta)^2 \) may be mapped with \( z \rightarrow z + \beta \vartheta \) to a flat space with non-trivial quasi-periodic boundary conditions, which indeed result in energy shifts, which we do not explicitly compute here but this in principle can be done using the outlined procedure.

In the translationally active \( T-p3(4)M \) phase, obtained from the Hamiltonian (5.8) and for the values of the parameters as shown in Fig. 5.3, a screw dislocation with the Burgers vector \( \mathbf{b} = \mathbf{e}_x \) produces \( \pi \) fluxes in the plane \( k_x = \pi \), which hosts a valley phase. Therefore, according to the \( \mathbf{K} - \mathbf{b} - \mathbf{t} \) rule, we expect two Kramers pairs of the dislocation modes originating from the band-inversion at the \( M \) and the \( X' \) points. Our numerical computations indeed confirm this prediction, as shown in Fig.5.12.
Figure 5.10: Numerical results concerning the effect of a screw dislocation, with $\mathbf{b} = \mathbf{e}_x$ oriented in the $\mathbf{e}_x$ direction. Panel A shows the spectrum of the modes on a $12 \times 12 \times 12$ system with periodic boundary conditions. The modes are not exactly at $\pm 0.50$ as expected from the continuum model. The deviation of the energy levels from the anticipated value as obtained from the analytical treatment becomes smaller for larger systems sizes. Panel B shows a $28 \times 12 \times 12$ system showing that the splitting of the energy levels converges to the result from the continuum model. Similarly the agreement with numerical results is also better in the $T - p4(3)_R$ phase when the system is closer to the transition point $M/B = 12$ (C). Finally panel D shows the real space localization of the mode with the color coding shown above.
Figure 5.11: The spectral density of a screw dislocation, with Burgers vector $e_x$, in the $T$-$p3(4)_R$ phase of a $28 \times 12 \times 12$ system with periodic boundary conditions. The presentation is similar to the above Figures. The horizontal axis shows the momentum $k = k_x$ along the dislocation line. Although the energy levels are shifted due to the finite size of the system, the spectrum displays again a zero mode at $k_x = \pi$ and the expected number of descendant states that form a Dirac cone, analogous to the case of an edge dislocation.
Figure 5.12: Numerical results concerning the effect of a screw dislocation in the $T\text{-}p3(4)_M$ phase. (A) The topological configuration of the $T\text{-}p3(4)_M$ phase. The screw dislocation, with Burgers vector $\mathbf{b} = e_x$, acts on the encircled TRI momenta in the $\hat{y} - \hat{z}$ planes. (B) The resulting spectrum of a $28 \times 12 \times 12$ system with periodic boundary condition in the $T\text{-}p3(4)_M$ phase. The resulting spectrum shows a double pair of 'parent' helical zero modes. These modes originate from the encircled momenta, which form a 2D valley phase in the plane $k_x = \pi$, since these momenta are related by a threefold rotation around the axis connecting the $\Gamma$ and the $R$ points.

Let us now consider a dislocation loop, which can be thought of as a connected channel of screw and edge dislocations. Although the Burgers vector $\mathbf{b}$ of any dislocation remains constant [114, 116], the planes orthogonal to the dislocation line are different for the edge and screw dislocation part of the circuit. In general one can consider the full scattering problem of an edge and screw dislocation [145, 146], which essentially pertains to matching the phases of the solutions of Eq. (5.13). Due to time-reversal symmetry, however, the helical modes are protect from backscattering, and we can thus conclude that dislocation loops have helical modes along the core when both the edge and the screw dislocation possess the propagating modes. We emphasize the implications of the $K\text{-}b\text{-}t$ rule in this regard, dictating the precise existence criteria of the dislocation modes in the loop. Accordingly, the $T\text{-}p3(4)_R$ phase with a dislocation loop, see Fig (5.4), has dislocation modes along the loop for any orientation of the Burgers vector $\mathbf{b}$. In contrast, inserting a dislocation loop in the $\hat{x} - \hat{z}$ plane, with $\mathbf{b} = e_x$, in the $p4_{M,R}$ phase only binds dislocation modes to the edge dislocation part of the circuit, resulting in the exact same spectrum shown in Fig. 5.8. Changing the orientation of the Burgers vector to $\mathbf{e}_z$ then does result in dislocation modes along the loop, as the gauge
potential $A$ is non-trivial in all the planes normal to the dislocation lines and these planes are topologically non-trivial. At last, changing the Burgers vector to the $e_y$ direction, it is evident that the effective systems in each plane either has no flux or acquires $2\pi$-flux. As a result we anticipate no modes, analogously to the case of a screw dislocation with $b = e_x$, which is confirmed by numerical computations, see Fig. 5.13.

Finally, we address the full compatibility of the outlined analysis with the underlying characterization of topological insulators with different space groups in terms of the band-inversions. Consider, for example, the composite phase $T\text{-}pm\bar{3}m \oplus T\text{-}4p3X$, which is equivalent to the $T\text{-}4p3M \oplus T\text{-}4p3R$ or $\Gamma \oplus XYZ = MX'Y' \oplus R$ phase with the dislocation loop in the $y-z$ plane, as previously described, see Fig. 5.13. We expect here the response of the dislocations to be the same with both choices of the band-inversions. We see that upon applying the $K$-$b$-$t$ rule to either set of the band inversions, one indeed obtains the same outcome in terms of the fluxes acting on the planes. Along the edge dislocation, the $k_z = 0$ plane hosts a $\pi$ flux, in contrast to the $k_z = \pi$ plane. Similarly, for the screw dislocation part, which has momentum in the $k_x$ direction, we see that the $k_x = \pi$ plane hosts a zero mode. Note that in the latter case, the screw dislocation acts as a $\pi$-flux in this phase, which with respect to the $k_x = \pi$ plane, may be thought of as the $T\text{-}p4mm$ or $\Gamma$ phase, since the $(\pi,0,0)$ momentum acts as a $\Gamma$ point in this plane. The descendant values of $k_x$ thus contribute dislocation modes to the spectrum as long as the effective $M/B$ parameter in the reduced model is in the range corresponding to the $T\text{-}p4mm$ in 2D. As result, we find that the complete dislocation loop has modes along the core.
Figure 5.13: Dislocation loop in the $\hat{x} - \hat{z}$ plane with Burgers vector $\mathbf{b} = e_x$. Panels A to C show the spectra corresponding to the dislocation loops in Fig. 5.1 in the main text. Namely, considering systems with periodic boundary conditions, we tune the system to the respective phases and get the anticipated dislocation modes in the spectrum. Panel D indicates the electronic topological configuration of the $T_{4p3M} \oplus T_{4p3R}$ phase. As each plane hosts an effective $\pi$-flux problem, inserting the same dislocation loops gives the anticipated spectrum (E), the modes of which show the familiar real space localization (F).