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Author: Slager, Robert-Jan
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Chapter 3

Universal bulk probes of the $\mathbb{Z}_2$ topological insulator

The salient physical feature of $\mathbb{Z}_2$ topological band insulators (TBI) is that they are fully gapped in the bulk while possessing gapless propagating modes protected by time reversal symmetry (TRS) on their boundary. Although the presence of TRS ultimately underlies the topological description, it nonetheless constrains, fundamentally and especially experimentally, the availability of robust probes of this bulk-boundary correspondence or anomalous responses. In particular, for $2+1$ dimensional TBIs the charge Hall response vanishes, and instead a much more involved TRS invariant quantum spin Hall (QSH) effect characterizes the topological phase. It has been shown, however, through numerical studies that a $\pi$-flux vortex, which actually preserves TRS, can play the role of a $\mathbb{Z}_2$ bulk-probe in a QSH insulator through the appearance of topologically protected mid-gap modes. \[99, 100, 101, 102\]

In this Chapter, we introduce the $\pi$-flux vortex as the bulk probe of the $2+1$ dimensional $\mathbb{Z}_2$ topological band insulator and show that such a vortex binds a single Kramers pair of modes. Specifically, we analytically study the formation of these mid-gap states and show that their existence is intimately related to the non-trivial background. This analysis reveals that such vortices resultantly indicate an alternative classification route for the non-trivial characterization of the QSH phase. Most interestingly, we then bring these results to life by linking them to response of dislocations. Namely, dislocations are shown to provide for an effective $\pi$-flux problem, but only in specific $\mathbb{Z}_2$ topological insulating phases. This latter condition is physically relevant as this distinction turns
out to be intricately tied to the lattice topology and ultimately implies the existence of additional classification beyond the ten fold way. Finally, we corroborate these results with numerical calculations, which confirm the anticipated robustness of these modes.

The general way by which we achieve these results is by employing the $M - B$ model (2.7), initially constructed to describe the HgTe quantum well QSH insulator [40, 41]. The striking and universal feature of the low-energy (continuum) version of this model is that it describes a topological phase transition between a trivial and non-trivial $\mathbb{Z}_2$ topological phase, through a massive Dirac-Schrödinger theory. This field theory, especially in the presence of a $U(1)$ vortex, has not been widely studied in its own right. A peculiar property of this theory is that the presence of both linear and quadratic kinetic terms together with the ordinary Dirac mass term allows for the gap-closing transition which changes the Chern number of the bands and the $\mathbb{Z}_2$ invariant. From a broader perspective, the relationship of the $\pi$-flux modes to the QSH phase and the question of their protection can therefore also be regarded in the general context of zero-energy fermionic modes bound to topological defects, which in fact comprises a rich literature [103, 104, 105, 90, 91, 106].

3.1 Zero-modes bound to a $\pi$-flux vortex

We here derive the analytic form of the zero-modes in the continuum version of the $M - B$ model (2.7). In particular, let us focus on the non-trivial regime $0 < M/B < 4$, meaning that the Dirac cone formed by the surface states is associated with the $\Gamma$ point in the Brillouin zone (Figure 2.3), and set the expansion parameter $A$ to unity. Taking the continuum, i.e. large wavelength limit ($|k| \ll 1$), we arrive at a Dirac Hamiltonian which besides the ordinary Dirac mass term $(M)$ contains a Schrödinger kinetic term $(B)$

$$H_{\text{eff}}(k) = i\gamma_0 \gamma_i k_i + (M - Bk^2)\gamma_0.$$  

(3.1)

Here, the four-dimensional $\gamma$-matrices satisfy the canonical anticommutation relations

$$\{\gamma_\alpha, \gamma_\beta\} = 2\delta_{\mu\nu}$$

and are given by $\gamma_0 = \tau_3 \otimes \sigma_0$, $\gamma_1 = \tau_2 \otimes \sigma_3$, $\gamma_2 = -\tau_1 \otimes \sigma_0$. Furthermore, the Pauli matrices $\{\sigma_0, \sigma_\mu\}$ act in the spin space, with $\tau_0, \sigma_0$ representing the $2 \times 2$ identity matrices.

Considering the effect of the magnetic $\pi$-flux, it is sufficient to focus on a single spin projection, since the two spin projections are related by the time-reversal operator $T = -i\sigma_2 K$, with $K$ being the complex conjugation. In the lattice model this $\pi$-flux can
then readily be incorporated using a Peierls substitution, which amounts to the minimal coupling \( k \rightarrow k + A \) in its continuum counterpart. As result, the Hamiltonian (3.1) for the spin up part assumes the form

\[
H_{\text{eff}}(k, A) = \tau_i (k_i + A_i) + [M - B(k + A)^2] \tau_3, \tag{3.2}
\]

where the vector potential

\[
A = \frac{-ye_x + xe_y}{2r^2} \tag{3.3}
\]

represents the magnetic vortex carrying the flux \( \Phi = \pi \).

The remainder of this section is dedicated to showing that the above Hamiltonian possesses precisely one bulk zero-energy state with spin up. Expressing the Hamiltonian (3.2) in polar coordinates \((r, \phi)\), taking into account that \( A = (1/2r)e_\phi \), we obtain

\[
H_{\text{eff}} = -ie^{-i\phi} \left[ \partial_r - i \frac{\tilde{\partial}_r}{r} \right] \tau_+ - ie^{i\phi} \left[ \partial_r + i \frac{\tilde{\partial}_r}{r} \right] \tau_-
+ \left[ M + B \left( \partial_r^2 + \frac{1}{r} \partial_r + \frac{1}{r^2} \tilde{\partial}_r^2 \right) \right] \tau_3, \tag{3.4}
\]

where \( \tilde{\partial}_r \equiv \partial_r + i/2 \), and \( \tau_\pm \equiv (\tau_1 \pm i\tau_2)/2 \). It is easy to see that in case of an arbitrary flux \( \Phi \), the Hamiltonian (3.2) also acquires the form (3.4), but with the operator \( \tilde{\partial}_r = \partial_r + i\Phi/2\pi \). In the presence of a vortex carrying a \( \pi \) flux, we can exploit the well-defined angular momentum and seek for solutions of the form

\[
\psi(r, \phi) = \sum_l c_l \psi_l(r, \phi), \tag{3.5}
\]

where

\[
\psi_l(r, \phi) = \begin{pmatrix} e^{il\phi} u_l(r) \\ e^{i(l+1)\phi} v_{l+1}(r) \end{pmatrix}, \quad l \in \mathbb{Z}. \tag{3.6}
\]

As a result, the functions \( u, v \) are subjected to the following equations

\[
\Delta_{l + \frac{3}{2}} u_l(r) - i \left( \partial_r + \frac{l + \frac{3}{2}}{r} \right) v_{l+1}(r) = 0 \tag{3.7}
\]
\[
i \left( \partial_r - \frac{l + \frac{3}{2}}{r} \right) u_l(r) + \Delta_{l + \frac{3}{2}} v_{l+1}(r) = 0. \tag{3.8}
\]

Here the operator \( \Delta_l \) is defined as

\[
\Delta_l \equiv M + B \left( \partial_r^2 + \frac{1}{r} \partial_r - \frac{l^2}{r^2} \right) \equiv M + BO_l. \tag{3.9}
\]
Acting on Eq. (3.7) with the operator \( \Delta_{l+\frac{1}{2}} \), and using the identity

\[
[\Delta_l, \partial_r + \frac{l}{r}] = -(2l-1) \frac{B}{r^2} \left( \partial_r + \frac{l}{r} \right),
\]  

we can eliminate the function \( v_{l+1}(r) \) from the same equation to obtain

\[
\left( \Delta_{l+\frac{1}{2}} \Delta_{l+\frac{1}{2}} - O_{l+\frac{1}{2}} + \frac{2B(l+1)}{r^2} \Delta_{l+\frac{1}{2}} \right) u_l(r) = 0.
\]  

(3.11)

After some algebra, the above equation can then be rewritten as

\[
\left[ M^2 + (2MB - 1)O_{l+\frac{1}{2}} + B^2O_{l+\frac{1}{2}}^2 \right] u_l(r) = 0.
\]  

(3.12)

This result may also be obtained by noting that if the spinor in Eq. (3.6) is an eigenstate with the zero eigenvalue of the Hamiltonian (3.2), then it is also an eigenstate with the same eigenvalue of the square of this Hamiltonian. Using Eq. (3.2), one then readily obtains

\[
H_{\text{eff}}(k, A)^2 = B^2(k^2)^2 + (1 - 2MB)k^2 + M^2,
\]  

(3.13)

with \( \tilde{k} \equiv k + A \), and the operator \( \tilde{k}^2 \) after acting on the angular part of the upper component of the spinor (3.6) yields Eq. (3.12). Similarly, it may be shown that the function \( v_l(r) \) in the spinor given by Eq. (3.6) obeys an equation of the same form as (3.12) with \( l \to l + 1 \). From Eq. (3.12) we conclude that the function \( u_l(r) \) is an eigenfunction of the operator \( O_{l+1/2} \) with a positive eigenvalue

\[
O_{l+\frac{1}{2}} u_l(r) = \lambda^2 u_l(r),
\]  

(3.14)

since the operator \( \tilde{k}^2 \) when acting on a function with the angular momentum \( l \) is equal to \(-O_{l+1/2} \), and the eigenstates of the operator \( \tilde{k}^2 \) with a negative eigenvalue are localized. Eqs. (3.12) and (3.14) therefore imply

\[
\lambda_{\pm} = \frac{1 \pm \sqrt{1 - 4MB}}{2B},
\]  

(3.15)

and, accordingly, solutions of the form \( u_l(r) \sim I_{l+\frac{1}{2}}(\lambda r) \), where \( I_l(x) \) is the modified Bessel function of the first kind. However, from the above solutions the only square-integrable ones are those associated with \( l - 1 \) since \( I_l(x) \sim x^{-|l|} \) as \( x \to 0 \). Furthermore, only the linear combination \( I_{1/2}(x) - I_{-1/2}(x) \sim x^{-1/2}e^{-x} \) has the asymptotic behavior at infinity consistent with a finite norm of the state.
As a result, we only find square-integrable zero-energy solutions in presence of the \( \pi \)-flux vortex. Indeed, there are no normalizable solutions in the absence of the vortex, due to the asymptotic behavior of the modified Bessel functions. However, introducing the \( \pi \)-flux shifts the angular momentum \( l \) of the solutions (3.6) by a half, resulting in two square integrable zero-energy solutions in the zero angular momentum channel, being the localized \( l = -1 \) solutions. In order to make these solutions more explicit, we should distinguish two regimes of parameters, \( 0 < MB < 1/4 \) and \( MB > 1/4 \), for which the argument of the square-root is positive and negative, respectively. For \( 0 < MB < 1/4 \), since the argument of the square-root in the above equation is positive, we obtain two zero-energy solutions

\[
\Psi_{\pm}(r) = \frac{e^{-\lambda_{\pm} r}}{\sqrt{2\pi \lambda_{\pm}^{-1} r}} \left( \begin{array}{c} e^{-i\varphi} \\ i \end{array} \right),
\]

with \( \lambda_{\pm} > 0 \) because of the square-integrability. On the other hand, when \( MB > 1/4 \), up to a normalization constant, the solutions have the form

\[
\Psi_{1}(r) = \frac{e^{-r \sqrt[4]{MB} \cos \theta}}{\sqrt{r}} \cos \left(r \sqrt[4]{MB} \cos \theta\right) \left( \begin{array}{c} e^{-i\varphi} \\ i \end{array} \right),
\]

\[
\Psi_{2}(r) = \frac{e^{-r \sqrt[4]{MB} \cos \theta}}{\sqrt{r}} \sin \left(r \sqrt[4]{MB} \cos \theta\right) \left( \begin{array}{c} e^{-i\varphi} \\ i \end{array} \right),
\]

where

\[
\theta = \frac{1}{2} \arctan \frac{\sqrt{1 - 4MB}}{1 - 2MB}.
\]

However, since the identity

\[
\sqrt{x} \cos \left(\frac{1}{2} \arctan \frac{\sqrt{1 - 4x}}{1 - 2x}\right) = \frac{1}{2}
\]

holds for \( 1/4 < x < 4 \), the localization length of the zero-modes for \( MB > 1/4 \) is actually just a constant independent of \( M, B \), namely Eq. (3.17) becomes

\[
\Psi_{1}(r) = \frac{e^{-r \sqrt[4]{MB} \cos \theta}}{\sqrt{r}} \cos \left(\frac{r}{2\sqrt{MB}}\right) \left( \begin{array}{c} e^{-i\varphi} \\ i \end{array} \right),
\]

\[
\Psi_{2}(r) = \frac{e^{-r \sqrt[4]{MB} \sin \theta}}{\sqrt{r}} \sin \left(\frac{r}{2\sqrt{MB}}\right) \left( \begin{array}{c} e^{-i\varphi} \\ i \end{array} \right).
\]
Therefore, we conclude that the Hamiltonian (3.2) possesses zero-energy modes in the entire range of parameters $M$ and $B$ for which the system is in the topologically non-trivially phase, $0 < M/B < 4$.

Notice also that in the regime when $0 < MB < 1/4$, there are two characteristic length scales associated with the midgap modes, $\xi_\pm \sim \lambda_\pm^{-1}$. Of course, after a short-distance regularization is imposed, only a linear combination of the two states survives. The physical interpretation of the two length scales depends on the form of the superposition of the state after the regularization has been imposed, as it may be easily seen from the form of the states (3.16). In the regime $MB > 1/4$, the zero-energy states are characterized by a single length-scale $\xi_\text{loc} \sim 2B$, which is at the same time the localization length and characterizes the oscillations of the exponentially decaying state.

Furthermore, although the bulk system does not feature normalizable zero-energy solutions, the edge states are closely related to the zero modes bound to the vortex. A derivation analogous to the one in subsection 2.2.3 reveals that by imposing open boundary conditions on the wave-functions at one of the edges of the system, for instance the one perpendicular to the $x$-axis, the obtained surface states for $k_y = 0$ feature a penetration depth given by exactly the same expression as the localization length for the zero-energy modes bound to the $\pi$-flux vortex. This signals that the bulk-boundary correspondence may thus be probed by inserting a $\pi$-flux vortex in the quantum spin Hall system.

We observe, nonetheless, that the zero-energy modes, given by Eqs. (3.16) and (3.20), form an overcomplete basis. This is a consequence of the fact that the Hamiltonian (3.2) is not self-adjoint due to the singularity of the vortex vector potential (3.3) at the origin. In order to overcome this apparent inconsistency, the gauge potential has to be regularized. Essentially, the regularization procedure then fixes the physical solution as a particular linear combination of the two basis states. This procedure is discussed in the subsequent subsection.

3.1.1 Self-adjoint extension

The simplest possible regularization is provided by considering the vortex with the flux concentrated in a thin annulus of a radius $R$. Let us first consider the Hamiltonian in the range of parameters $0 < MB < 1/4$. The zero-energy state of the Hamiltonian outside the annulus is then a linear combination of the modes $\Psi_\pm$ given by Eq. (3.16). Inside
3.1 Zero-modes bound to a π-flux vortex

In the annulus the vector potential \( \mathbf{A} = 0 \), and hence the zero-energy modes are

\[
\Psi_c(r) = C_1 \left( e^{-i\phi} I_{-1}(\lambda_+ r) \right) + C_2 \left( e^{-i\phi} I_{-1}(\lambda_- r) \right), \tag{3.21}
\]

with \( \lambda_{\pm} \) given by Eq. (3.15), and \( C_{1,2} \) being complex constants. By matching these solutions at \( r = R \), and taking \( R \to 0 \), we obtain, up to a normalization constant, the zero-energy state

\[
\Psi(r) = \frac{e^{-\lambda_+ r} - e^{-\lambda_- r}}{\sqrt{r}} \left( e^{-i\phi} i \right).
\tag{3.22}
\]

Notice that this zero-energy state is regular at the origin which is a consequence of the regularity at the origin of the solutions (3.21) of the vortex-free problem. Similarly, one can readily show that when \( MB > 1/4 \) the zero-energy mode is given by the spinor \( \Psi_2 \) in Eq. (3.17) which is resultantly also regular at the origin and behaving \( \sim r^{1/2} \) when \( r \to 0 \). Finally, an identical evaluation for the trivial regime \( MB < 0 \) shows that there are no square integrable combinations, that are also regular at the origin. This confirms that the modes are also intricately related to the non-trivial \( \mathbb{Z}_2 \) nature of the bulk system.

Although the above regularization results in concrete solutions, we should consider the self-adjoint extension of the corresponding Hamiltonian (3.2) in a more general manner by specifying the proper Hilbert space. Specifically, the application of the standard theory of self-adjoint extensions (SAE) [107, 108, 109, 110] prescribes that we need to ensure that the massive Dirac Hamiltonian (a differential operator) becomes Hermitian (self-adjoint) only after choosing the proper Hilbert space (i.e. domain of functions) on which it is allowed to act. Using von Neumann’s construction by looking directly at the conditions under which the Hamiltonian is Hermitian when acted on arbitrary square integrable functions, we can then obtain the coefficients of the linear combination \( C_1 \Psi_+ + C_2 \Psi_- \) unambiguously.

Rescaling the eigenfunctions (3.6) by \( \psi_l(r, \phi) = \frac{1}{\sqrt{r}} \psi_l(r, \phi) \), the radial part of the Hamiltonian containing the singularity assumes the form

\[
\tilde{H}_l(r) = \begin{pmatrix}
  m + B \left[ \partial_r^2 + \frac{l(l+1)}{r^2} \right] & -i \left( \partial_r + \frac{l+1}{r} \right) \\
  -i \left( \partial_r - \frac{l+1}{r} \right) & -m - B \left[ \partial_r^2 + \frac{(l+1)(l+2)}{r^2} \right]
\end{pmatrix}.
\tag{3.23}
\]
In particular, we may choose the following explicit form

$$\Gamma$$

is the image of some wavefunction under showing that the boundary space indeed becomes

$$H$$

The hermiticity requirement then imposes the following condition

$$42 \text{ Chapter 3. Universal bulk probes of the } \mathbb{Z}_2 \text{ topological insulator}$$

on the arbitrary wave functions $$\chi_i(r, \varphi)$$ and $$\psi_j(r, \varphi)$$, which vanish at infinity and take the form defined in Eq.(3.6) in terms of the radial components

$$\chi_i(r) \equiv \begin{pmatrix} w_i(r) \\ x_{l+1}(r) \end{pmatrix} \equiv \alpha(r) \quad \text{and} \quad \psi_j(r) \equiv \begin{pmatrix} u_j(r) \\ v_{l+1}(r) \end{pmatrix} \equiv \beta(r). \quad (3.25)$$

The above requirement (3.24) results in a continuous family of restrictions on the behavior of square-integrable functions at the origin, the corresponding parametrization of which is obtained by exploiting its linearity. Namely, we can define two linear surjective maps $$\Gamma_1, \Gamma_2$$ from the domain $$\mathcal{D}(\tilde{H}^\dagger)$$, being arbitrary functions, onto their value at the boundary. These operators are defined by Eq. (3.24)

$$\left[ B(\tilde{\alpha}^* \sigma_3 \partial_r \tilde{\beta} - (\partial_r \tilde{\alpha}^*) \sigma_3 \tilde{\beta}) - i \tilde{\alpha}^* \sigma_1 \tilde{\beta} \right] (0) \equiv \langle \Gamma_2 \tilde{\alpha}, \Gamma_1 \tilde{\beta} \rangle - \langle \Gamma_1 \tilde{\alpha}, \Gamma_2 \tilde{\beta} \rangle. \quad (3.26)$$

In particular, we may choose the following explicit form

$$\Gamma_1 \tilde{\beta} = B \sigma_3 \partial_r \tilde{\beta}(0) - i \frac{\sigma_1}{2} \tilde{\beta}(0), \quad (3.27)$$

$$\Gamma_2 \tilde{\beta} = \tilde{\beta}(0),$$

showing that the boundary space indeed becomes $$\mathcal{H}_b = \mathbb{C}^2$$, as any vector in this space is the image of some wavefunction under $$\Gamma_i$$.

The most general relation that has to be satisfied by a wavefunction such that (3.24) holds is now parametrized by unitary mappings $$U$$ in $$\mathcal{H}_b$$:

$$\mathcal{D}(\tilde{H}_U) = \{ \psi | (U - \sigma_0)\Gamma_1 \psi + i(U + \sigma_0)\Gamma_2 \psi = 0 \}, \quad (3.28)$$

with $$\sigma_0$$ the 2x2 identity matrix, and $$\mathcal{D}$$ denoting the domain of operator. One can directly understand from (3.26) that forcing arbitrary linear combinations of a general $$\tilde{\beta}(0)$$ and $$\partial_r \tilde{\beta}(0)$$ to zero will still preserve the condition (3.24), due to the linearity and the anti-symmetric nature of the form of this expression. Eq. (3.28) thus gives us a precise recipe
and parametrization of the fact that this is the most general restriction that needs to be made on the wavefunctions $\tilde{\mathbf{\beta}}(r)$, i.e. on the $\psi(r)$.

The form of $\Gamma_i$ can now directly be used to explore the allowed boundary conditions on the wavefunctions and, in particular, to determine whether there is a self-adjoint extension $\tilde{H}_U$ with the previously found zero energy states in its domain. For concreteness we will concentrate on the case that $MB < 1/4$, although the procedure is completely general. Since $\mathcal{H}_0$ is $\mathbb{C}^2$, the relevant mappings $U \in U(2)$ can be parametrized as

$$U = \frac{1}{d} \sum_{\mu} m_\mu q_\mu, \quad m_\mu \in \mathbb{R}, \quad \sum_\mu m_\mu^2 = 1, \quad d \equiv \begin{pmatrix} e^{i\eta} & 0 \\ 0 & 1 \end{pmatrix}, \quad \eta \in [0, 2\pi),$$

(3.29)

relative to the quaternion basis $q_\mu = (\sigma_0, i\vec{\sigma})$. Focussing first on the case $\eta = 0$, the condition (3.28) results in

$$\{ B \sum_\mu \xi_\mu q_\mu \} \partial_r(\sqrt{r}\psi_0) \bigg|_{r=0} = \{ \sum_\mu \eta_\mu q_\mu \} \sqrt{r}\psi_0 \bigg|_{r=0},$$

(3.30)

where

$$\xi_\mu^\top = (-im_3, -im_2, im_1, i(m_0 - 1)), \quad \eta_\mu^\top = \left( \frac{m_1}{2} + i(1 + m_0), \frac{1 - m_0}{2} + im_1, \frac{m_3}{2} + im_2, -\frac{m_2}{2} + im_3 \right).$$

(3.31)

Moreover, since

$$\sqrt{r}\psi_0 \bigg|_{r=0} = \begin{pmatrix} C_1 + C_2 \\ i(C_1 + C_2) \end{pmatrix} \quad \text{and} \quad \partial_r(\sqrt{r}\psi_0) \bigg|_{r=0} = -\begin{pmatrix} C_1 \lambda_- + C_2 \lambda_+ \\ i(C_1 \lambda_- + C_2 \lambda_+) \end{pmatrix},$$

(3.32)

with $\lambda_{\pm}$ the positive solutions of Eq. (3.15), we obtain a relation between $C_1$ and $C_2$ as function of the particular self-adjoint extension $m_\mu$. In this case, $m_\mu$ parameterizes the hypersphere $S^3$ and can correspondingly be rewritten in terms of angular coordinates

$$m_\mu = (\cos \psi, \sin \psi \cos \theta, \sin \psi \sin \theta \cos \varphi, \sin \psi \sin \theta \sin \varphi),$$

(3.33)

where $\psi \in [0, \pi]$, $\theta \in [0, \pi]$, and $\varphi \in [0, 2\pi)$. Given the parameters $M$ and $B$, Eq. (3.30) thus results in a parameterized family of restrictions on the solutions, specifying the self-adjoint domain.

We notice that $\det(\sum_\mu \xi_\mu q_\mu) = \sum_\mu \xi_\mu^2 = 2(m_0 - 1)$. Let us therefore consider the case $m_0 = 1$ explicitly. Setting $m_0$ to unity immediately implies $m_\mu \neq 0 = 0$ and hence results in $0 = i\sigma_0 \tilde{\psi}(0) = i\sigma_0 \sqrt{r}\psi(0)$. This then yields $C_1 = -C_2$ and thus pertains to
the zero energy solution (3.22) found with the thin solenoid regularization. In fact, a detailed analysis [111] shows that this self adjoint extension, determined by \( \eta = \psi = 0 \), is the only possible extension which allows for the existence of a zero energy state that is both localized and regular (vanishing) at the origin. Moreover, the SAE procedure similarly applies to the other regime, thereby reconfirming the above intuitive approach. This then finally concludes the proof that the spin projected Hamiltonian (3.2) hosts a single zero-energy mode in the topological regime \( 0 < M/B < 4 \).

3.2 Quantum numbers of the zero-energy modes

The above derived zero-energy modes can be associated with the same spin-charge separated quantum numbers appertaining to the Jackiw-Rebbi solitons in the Su-Schieffer-Heeger model. To make this concrete, we consider the continuum \( 4 \times 4 \) Hamiltonian (3.1) coupled to the \( U(1) \) vector potential

\[
H = i\gamma_0 \gamma_i (k_i + A_i) + (M - B(k + A)^2) \gamma_0
\]

(3.34)

where the vector potential \( A \) given by Eq. (3.3). We note that the unitary matrices \( \gamma_3 = \sigma_2 \otimes \tau_2 \) and \( \gamma_5 = \sigma_2 \otimes \tau_1 \) anticommute with the gamma-matrices \( \gamma_\alpha, \alpha = 0, 1, 2 \). Therefore, the Hamiltonian anticommutes with the matrices \( \Gamma_3 \equiv i\gamma_0 \gamma_3 \) and \( \Gamma_5 \equiv i\gamma_0 \gamma_5 \) which then generate chiral (spectral) symmetry relating states with positive and negative energies, i.e., if \( H|E\rangle = E|E\rangle \), then, for instance, \( \Gamma_5|E\rangle = |−E\rangle \), and the matrix \( \Gamma_5 \) reduces in the zero-energy subspace of the Hamiltonian. As a result, we can straightforwardly apply Eq. (2.14),

\[
\langle Q \rangle = \frac{1}{2} \left( \sum_{\text{occupied}} \Psi_E^\top Q \Psi_E - \sum_{\text{unoccupied}} \Psi_E^\top Q \Psi_E \right),
\]

(3.35)

to obtain the same ground state quantum numbers \( \langle Q \rangle \) characterizing the polyacetylene case. Namely, when both states are occupied or empty the charge is \( +e \) or \( −e \) and the spin quantum number is zero, whereas single occupied modes are characterized by a spin quantum number \(-1/2\) or \(1/2\) and a net charge zero. These results can additionally be understood from a physical perspective [99]. Since a \( \pi \)-flux is equivalent to a \( −\pi \)-flux, there are four different adiabatic processes that result in the same final flux configuration. That is, for each spin projection \( \uparrow \) (\( \downarrow \)) the flux can adiabatically be increased from 0 to \( \pm \pi \). Considering a loop around the vortex, Faraday’s law of induction then implies that
during such an adiabatic process a tangential electric field is induced along the loop. Accordingly, the quantized Hall conductivity per sub block thus results in a net charge transfer per spin component along the loop that simply amounts to \( \Delta Q_{\uparrow(\downarrow)} = \mp e/2 \) for the \( \pm \pi \)-flux process. Combining the four different scenarios \( \phi_{\uparrow, \downarrow} = \pm \pi \), we then readily obtain the net relative charge \( \Delta Q = Q_\uparrow + Q_\downarrow \) and spin \( \Delta S_z = Q_\uparrow - Q_\downarrow \) for each case, culminating in the outlined quantum numbers.

3.3 \( \pi \)-fluxes as a bulk classification tool

Although the discrepancy in spatial dimensions allows for the spin-charge separated quantum numbers of the vortex zero-modes, we notice that the characterization of the modes is nevertheless rather reminiscent of the edge state description. Of topical interest in this regard is the question to what extent the above indicated relation between the existence of the zero-modes and the non-trivial topological characterization of the bulk system, formalized by the bulk-boundary correspondence in the case of the surface states, translates to a profound entity. Interestingly, it turns out that the \( \pi \)-flux modes are indeed intricately tied to the \( \mathbb{Z}_2 \) topological nature of the quantum spin Hall phase [99, 100], making them versatile probes of the non-trivial order. Let us now make this somewhat more concrete.

Concerning the topological stability of the mid gap states, being the stability under continuous deformations of the vector potential, it is well-known that both the Dirac and Schrödinger Hamiltonian are characterized by an index theorem [103, 104]. However, as the continuum theory (3.1) entails a combination of the two, a definite index theorem mathematically relating the number of zero-modes to the non-triviality of the defining differential operator is yet to be established. Moreover, it is evident that in the above treatment the description of the zero-modes coincides with the manifest chiral symmetry of the \( M - B \) model (2.7), which in the generic context amounts to an artifact rather than a fundamental symmetry. Fortunately, the generality of the Laughlin argument allows nonetheless for an explicit verification of the intricate relation between the \( \pi \)-flux modes and the QSH phase also in absence of the additional spin \( U(1)_s \) symmetry.

As a first step it is important to realize that actually only TRS is needed to define spin-charge separated modes, as the time reversal operator \( T \) acts differently on integer and half-integer spin states. Specifically, denoting the electron number operator...
as \( N \), one can generalize the concept of spinons to arbitrary quantum states satisfying \((-1)^N|\psi_s\rangle = |\psi_s\rangle\) and \(T^2|\psi_s\rangle = -|\psi_s\rangle\). Correspondingly, states transforming as \((-1)^N|\psi_c\rangle = -|\psi_c\rangle\), \(T^2|\psi_c\rangle = |\psi_c\rangle\) define chargeons and holons. These concepts subsequently allow for the construction of an explicit invariant that quantifies the non-trivial \(\mathbb{Z}_2\) order of the assumed unique ground state. Namely, consider the adiabatic process of \(\pi\)-flux treading represented by the matrix \(\Gamma\), as function of the interpolating parameter \(\theta \in [0, \pi]\). In the case of a lattice model the hoppings along some cut ending on the vortex are then altered as \(t_{ab} \rightarrow t_{ab}e^{i\theta(i)\Gamma}\), whereas in the continuum setting this amounts to an evident redefinition of the gauge potential. Crucially, for any time reversal odd matrix \(\Gamma\), satisfying \((-1)^{i\pi\Gamma} = -1\), one can then show that such an adiabatic process results in the pumping of an integer \(N\) amount of charge to the flux tube, proving that \((-1)^N\Gamma\) defines a \(\mathbb{Z}_2\) invariant \([99, 112]\).

The arguments underlying these facts find their foundation in the Laughlin argument. In particular, as the resulting state after spin flux threading can similarly be obtained by charge flux threading we can consider the closed path \(l = l_c^{-1}l_{\Gamma}\) in parameter space \([112]\). Here \(l_c, l_{\Gamma}\) refer to adiabatic paths associated with charge and spin flux threading, respectively. As the ground state is unique and the response during the charge threading process equates to zero by virtue of time reversal symmetry, we immediately conclude that an integer amount of charge is pumped to the flux tube by the spin flux threading process. Moreover, for two different adiabatic processes \(\Gamma_1\) and \(\Gamma_2\), the closed path \(l_{\Gamma_2}^{-1}l_{\Gamma_1}\) has to result in the transport of an even multiple of charge, as it must map the unique ground state (e.g. a Kramers singlet) to itself (again a Kramers singlet). This shows that the invariant \((-1)^N\Gamma_1\) is independent of \(\Gamma_1\).

As a result, we see that the adiabatic \(\pi\)-flux threading is thus directly related to a concrete invariant characterizing the \(\mathbb{Z}_2\) phase. Only in the case of a non-trivial \(\mathbb{Z}_2\) invariant, an odd multiple of charge is transported to the flux tube for the appropriate \(\Gamma\). Moreover, using the explicit occupation relation between the chargeons/holons and spinons in conjunction with Kramers theorem, we conclude that the formation of the mid gap modes bound to the \(\pi\)-flux vortex is in direct correspondence with the topological non-triviality of the bulk system. In the specific context of the previous subsection, we may, for example, consider the process associated with \(\phi_\uparrow = -\phi_\downarrow = \pi\) represented by the matrix \(\Gamma = \sigma_z \otimes \tau_0\), creating the chargeon state in the non-trivial regime. Due to the outlined arguments the associated mid gap modes are then stable to perturbations that do not close the gap, although in the absence of spectral symmetry they are no longer
pinned to zero-energy.

From a heuristic point of view, the transition maps of the vector bundle structure associated with the non-trivial $\mathbb{Z}_2$ phase imply that during a full Laughlin cycle the many body energy levels cross an odd number of times. As noted before, insertion of half a quantum flux, i.e. a $\pi$-flux, thus results in a change in degeneracy for the edges of the system, characterizing the physical significance of the $\mathbb{Z}_2$ invariant (Figure 1.3). Accordingly, we see that a similar mechanism lies at heart of the appearance of a single Kramers pair of mid-gap modes at the $\pi$-flux vortex, the formation of which then mimics the usual bulk-boundary correspondence. Notice in this regard that in case of periodic boundary conditions the effective spin transfer is then associated with the two time reversed Kramers pairs of mid gap modes at the two different defects. Similarly, for a single defect in an open boundary system this process has to be identified with a spectral flow on the edge due to charge neutrality, conforming the intricate relation between the defect modes and the surface states.

3.4 Dislocations as probes of the physics beyond the tenfold way

As shown, the $\pi$-flux modes represent universal topological observables that intricately relate to the $\mathbb{Z}_2$ topological status of the bulk. However, the derived notions come to live in the context of dislocations. In particular, as the piercing of $\pi$-fluxes through elementary plaquettes of the size of the lattice constant is far from experimentally viable, experimental ubiquitous defects that effectively amount to flux probes are obviously consequential in this regard. Numerical simulations have already hinted that dislocations can act as pseudo-magnetic fluxes [113], and we will exploit their prominent role in detail in the remainder.
Most importantly, as dislocations are the unique topological defects associated with the transitional symmetry breaking of the underlying lattice, these results in turn expose a route to an additional classification scheme that incorporates the lattice symmetries. Namely, the tenfold way, based on time-reversal symmetry and particle-hole symmetry, relies on the spatial continuum limit while TBIs actually necessitate a crystal lattice that breaks the translational symmetry. The simple $M-B$ model (2.7),

$$H(k_x, k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(-k) \end{pmatrix} = A \sin(k_x) \gamma_x + A \sin(k_y) \gamma_y + M(k) \gamma_0,$$

(3.36)

already gives away a generic wisdom in this regard. Depending on its parameters, this model describes topological phases which are in a thermodynamic sense distinguishable: their topological nature is characterized by a Berry phase skyrmion lattice (SL) in the extended Brillouin zone (BZ), where the sites of this lattice coincide with the reciprocal lattice vectors (“Γ-phase”) or with the TRS points $(\pi, \pi)$ (“M-phase”).

Concretely, rewriting the spin projected sub blocks of the simple M-B model (2.7) in the compact form of Eq. (2.4),

$$H(k_x, k_y) = d(k) \cdot \tau,$$

(3.37)

we observe (Figure 3.1) that in the topologically non-trivial Γ-phase the band-structure vector field $\hat{d}(k) = d(k) / |d(k)|$ forms a skyrmion centered around the Γ-point in the BZ, with corresponding skyrmion density $s(k) = \partial_{k_x} \hat{d}(k) \times \partial_{k_y} \hat{d}(k)$. Here $s(k)$ tracks the position of minimal bandgap in the BZ, coinciding with it where $\hat{d}(k) || \partial_{k_x} \hat{d}(k) \times \partial_{k_y} \hat{d}(k)$. In the 2D extended BZ, this skyrmion structure forms a lattice which respects point group symmetry of the original square lattice. Moreover, in the $M$-phase, the skyrmion is centered at the $M$ point in the BZ. The position of the corresponding skyrmion lattice relative to the extended BZ is therefore different than in the Γ-phase, although the skyrmion lattice still respects the point group symmetry of the square lattice. On the other hand, in the topologically trivial phase, the vector field $d$ forms no skyrmion in the BZ, consistent with the vanishing of topologically invariant spin Hall conductance $\sigma_{xy}^S = (4\pi)^{-1} \int_{BZ} d^2k \ s(k)$. The position of the skyrmion lattice relative to the extended BZ thus encodes translationally active topological order which, as we now show, is probed by the lattice dislocations.
Let us first analytically motivate, using the elastic continuum theory, that a lattice dislocation effectively amounts to the above magnetic $\pi$-flux problem in the $M$ phase. We consider a dislocation with Burgers vector $b$, and expand the Hamiltonian (3.37) around the $M$-point in the BZ. As a next step, the dislocation introduces an elastic deformation of the medium described by the distortion \{\(e_i(r)\)\} of the (global) Cartesian basis \{\(e_i\), \(i = x, y\)\} in the tangent space at the point \(r\) [114]. Consequently, the momentum in the vicinity of the $M$-point reads
\[
k_i = E_i \cdot (k_M - q) = (e_i + e_i) \cdot (k_M - q),
\] (3.38)
where $k_M = (\pi, \pi)/a$, $q$ is the momentum of the low-energy excitations, $|q| \ll |k_M|$, and we have restored the lattice constant $a$. The corresponding continuum Hamiltonian after this coarse graining [115] then assumes the form
\[
H_{\text{eff}}(k, A) = \tau_i(k_i + A_i) + [\tilde{M} - \tilde{B}(k + A)^2] \tau_3,
\] (3.39)
in terms of the redefinitions $q \to k$, $\tilde{M} \equiv M - 8B$, $\tilde{B} \equiv -B$, and $A_i \equiv -e_i \cdot k_M$. The form of the distortion $e_i$ is determined from the dual basis in the tangent space at the point $r$ which in the case of a dislocation with $b = ae_x$ entails $E_x = (1 - \frac{ay}{2\pi r^2})e_x + \frac{ax}{2\pi r^2}e_y$, $E_y = e_y$ [116]. Using that $E_i \cdot E' = \delta^j_i$, we obtain the distortion field to the leading order in $a/r$, $e_x = \frac{ay}{2\pi r^2}e_x$, $e_y = -\frac{ax}{2\pi r^2}e_y$. This form of the distortion yields the vector potential
\[
A = \frac{-ye_x + xe_y}{2r^2}
\] (3.40)
in Eq. (3.39), demonstrating that the dislocation in the $M$-phase acts as a magnetic $\pi$-flux. On the other hand, in the $\Gamma$-phase, the continuum Hamiltonian has the generic form (3.39), with $\tilde{M} = M$ and $\tilde{B} = B$. However, the action of the dislocation in this case is trivial, since the bandgap is located at zero momentum rendering $A = 0$. Applying the above results, we conclude that a dislocation must bind a Kramers pair mid gap modes in the $M$-phase, while having no effect in the $\Gamma$-phase.

These notions can readily be corroborated by numerical means. We find that a dislocation only binds a Kramers pair of zero-energy states in the $M$-phase, confirming that the dislocation acts as a $\pi$-flux in this phase. Moreover, we can show the robustness of these modes in the bulk gap when we introduce a random chemical potential, and thus break PHS. To this end we perform a numerical analysis on the tight-binding $M - B$
Figure 3.1: Model of Eq. (3.36) in the BZ: (a) Band-structure $\hat{d}(\mathbf{k})$. (b) Skyrmion density $s(\mathbf{k})$. Mid-bulkgap localized dislocation states in 33x30 unit-cell $M - B$ tight-binding lattice with disorder. The Kramers degenerate pair states are omitted. (c) Dislocation in the center. Offset disks represent the amplitude of $s \uparrow, p \uparrow$ states, and the color their phase. (d) Total wavefunction amplitude in a periodic system (necessitating two dislocations), with Rashba coupling ($R_0$) mixing spins.

model in real space

$$H_{TB} = \sum_{\mathbf{R}, \mathbf{\delta}} \left( \Psi^\dagger_{\mathbf{R}} \left[ T_{\mathbf{\delta}, \uparrow\uparrow} i R_0/2 (\tau_0 + \tau_3) \mathbf{e}_z \cdot (\mathbf{\sigma} \times \mathbf{\delta}) \right] \Psi_{\mathbf{R}+\mathbf{\delta}} + \Psi^\dagger_{\mathbf{R}} \epsilon R_0/2 \Psi_{\mathbf{R}} + H.c. \right), \quad (3.41)$$

where $\Psi_{\mathbf{R}} = (s_{\uparrow}(\mathbf{R}), p_{\uparrow}(\mathbf{R}), s_{\downarrow}(\mathbf{R}), p^*_\downarrow(\mathbf{R}))$ annihilates the $\sim |s\rangle$ type, and $\sim |p_x + ip_y\rangle$ type orbitals at site $\mathbf{R}$ and nearest neighbors $\mathbf{\delta} \in \{\mathbf{e}_x, \mathbf{e}_y\}$. Furthermore, we set

$$T_{\mathbf{\delta}, \uparrow\uparrow} = \begin{pmatrix} \Delta_s & \mathbf{t}_\delta/2 \\ \mathbf{t}_\delta'/2 & \Delta_p \end{pmatrix}$$

and $T_{\mathbf{\delta}, \downarrow\downarrow} = T_{\mathbf{\delta}, \uparrow\uparrow}^\dagger$, with $t_x = t'_x = -i, t_y = -t'_y = -1, \Delta_{s/p} = \pm B + D$ and on-site energies $\epsilon = [(C - 4D)\tau_0 + (M - 4B)\tau_3] \otimes \sigma_0$. This reproduces Eq. (3.37) when $C = D = 0$, implying vanishing chemical potential. Finally, the $R_0$ term is the nearest neighbor Rashba spin-orbit coupling [117] which is induces a breaking of the $z \rightarrow -z$ reflection symmetry and resultantly the PHS symmetry.

Our numerical analysis of $H_{TB}$ pertains to various system shapes and sizes, with varying disorder strengths given by multiplication of the parameters for each $\mathbf{R}, \mathbf{\delta}$ by
3.4 Dislocations as probes of the physics beyond the tenfold way

Figure 3.2: Comparison of $\Gamma$ (a-d) and $M$ (e-h) phases. The density of states of 21x18 lattice (100 disorder realizations averages), with $C \equiv 0.2|\tau|$, $D \equiv 0.3|\tau|$ setting the chemical potential, and $R_0$ the Rashba coupling. (a) and (e) In absence of dislocation. (b,f) Robust midgap dislocation modes are present only in $M$-phase; (c,g) Same is true upon spin mixing through $R_0$. (d,h) Strong Rashba coupling closes the topological bulk gap.

Gaussian random variables of width $w$, while preserving TRS. Fig. 3.1(c) demonstrates the spectrum and the wavefunction at $w = 10\%$ disorder. Localization (even by weak disorder) decouples dislocation states from edges and possible edge roughness effects.

In the presence of the Rashba coupling ($R_0 \neq 0$, but not large enough to close the topological bulk gap [32]), the spins are mixed, but the Kramers pairs remain localized (Fig. 3.1(d)). Fig. 3.2 demonstrates the robustness of dislocation modes within the topological bulk gap, through the Rashba coupling perturbed and disorder averaged density of states (DOS) of $H_{TB}$ in a periodic lattice, contrasted between the $\Gamma$ and the $M$ phase.

These findings are obviously consequential in the view of experimental verification. Dislocations are ubiquitous in any real crystal, for instance in the form of small angle grain boundaries, and we thus predict that their cores should carry zero modes, which should be easy to detect with scanning tunneling spectroscopy. As a matter of fact, the real experimental challenge lies in the realization of non-$\Gamma$ TIs that are also easily accessible to spectroscopic measurements.

Moreover, we note that although the above considerations pertain to a simple toy model, that should be regarded in that sense, the characterization of the $\pi$-fluxes is completely general, as is the reminiscent principle concerning the dislocations. Hence, on a fundamental level the above results indicate the existence of a further subclassification, besides the “translationally trivial” $\Gamma$-type TBIs that are completely classified by
the tenfold way. In this specific case this characterization corresponds to the locus of the Berry phase skyrmion lattice in the extended BZ, however a more general classification method is highly desirable. This forms the subject of the next Chapter.

3.5 Conclusions

In conclusion, we have shown that the appearance of a pair of zero-modes bound to a magnetic $\pi$-flux is a generic feature of the $M - B$ model in the topologically non-trivial phase. In the continuum setting, these modes can analytically be derived and directly be related to the a particular self-adjoint extension of the continuum Hamiltonian. More generally, the existence of these mid gap states results in profound physical consequences. In particular, they provide for a two-dimensional realization of spin-charge separated quantum numbers. Of topical interest, however, is the deep relation between these special mid gap modes and the $\mathbb{Z}_2$ topological characterization of the bulk. Namely, the modes bound to the $\pi$-flux can directly be used to classify $\mathbb{Z}_2$ topological band insulators. These notions become physically profound in the context of dislocations. Specifically, dislocations act as $\pi$-fluxes, thereby binding similar mid gap modes, but only in certain $\mathbb{Z}_2$ topological insulators. This signals that there is a further subclassification, within the tenfold way.