Master Thesis on
The Bulk-Edge Correspondence
in Quantum Hall and Topological Insulator Systems

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ABSTRACT. This text documents work done towards a master thesis in mathematical physics at the ETH Zurich physics department from October 2014 until April 2015. We study two-band and four-band systems and present proofs for the bulk-edge correspondence of the topological invariants of these systems. We conclude by showing how some of the preceding mathematical analysis is relevant to physical systems.

Contents

List of Symbols

(1) $n \in \mathbb{N}\backslash\{0\}$ will always be a positive integer.
(2) $S^1 \equiv \frac{\mathbb{R}}{2\pi\mathbb{Z}}$ is the circle.
(3) $\mathbb{T}^2 \equiv S^1 \times S^1$ is the 2-torus.
(4) $\mathbb{Z}_n \equiv \frac{\mathbb{Z}}{n\mathbb{Z}} \equiv \{0, 1, \dots, n-1\}$.
(5) $J_n := \mathbb{Z}_n + 1 \equiv \{1, 2, \dots, n\}$.
(6) $M_n(\mathbb{F})$ is the set of all $n \times n$ matrices over a field $\mathbb{F}$.
(7) $\overline{\alpha}$ denotes the image under involution of an element $\alpha \in \mathbb{F}$, if an involution is defined on $\mathbb{F}$.
(8) If $A \in M_n(\mathbb{F})$ then $\overline{A}$ denotes the matrix with entries involuted.
(9) For a linear map A between two vector spaces, A^* denotes the adjoint of A.
(10) $\mathrm{Herm}(n)$ is the set of all Hermitian $n \times n$ matrices over $\mathbb{C}$.
(11) If S is a set and F is an ambient set ($F \supseteq S$), then $S^c \equiv F\backslash S$. Sometimes the ambient set will be implicit.
(12) $\chi_S(x) \equiv \begin{cases} 1 & x \in S \\ 0 & x \notin S \end{cases}$ is the characteristic function of S at x.
(13) $l^2(\mathbb{Z}; \mathbb{C}^n)$ or $l^2(\mathbb{N}; \mathbb{C}^n)$ is the set of all square-summable sequences in $\mathbb{Z}$ or $\mathbb{N}$ of vectors in $\mathbb{C}^n$, that is, $\sum_{j\in\mathbb{Z}} |\psi_j|^2 < \infty$ or $\sum_{j\in\mathbb{N}} |\psi_j|^2 < \infty$ for elements $\psi \in l^2(\mathbb{Z}; \mathbb{C}^n)$ or $\psi \in l^2(\mathbb{N}; \mathbb{C}^n)$.
(14) σ_j is the jth 2×2 Pauli matrix, defined $\forall j \in J_3$ as:
$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ and $\sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$.
We also use $\sigma_0 \equiv \mathbb{1}_{2\times 2}$.
(15) If X and Y are Banach spaces, $\mathcal{B}(X, Y)$ is the set of bounded linear operators from X to Y, and $\mathcal{B}(X) \equiv \mathcal{B}(X, X)$.
(16) $\sigma(H)$ is the spectrum of the bounded linear operator H over a complex Banach space:

$$\sigma(H) \equiv \{\lambda \in \mathbb{C} \mid (H - \lambda\mathbb{1}) \text{ is not invertible}\}$$

(17) $E_F \in \mathbb{R}$ is the Fermi energy.
(18) $\|v\| \equiv \sqrt{\sum_{i=1}^n \langle v, \hat{e}_i\rangle^2}$ for all $v \in \mathbb{R}^n$ where $\{\hat{e}_i\}_{i=1}^n$ is the standard basis of $\mathbb{R}^n$.
(19) Time-Reversal-Invariant Momenta on $\mathbb{T}^2$:

$$\mathrm{TRIM} \equiv \left\{ k \in \mathbb{T}^2 \,\middle|\, k = -k \right\} = \left\{ \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \pi \end{bmatrix}, \begin{bmatrix} \pi \\ 0 \end{bmatrix}, \begin{bmatrix} \pi \\ \pi \end{bmatrix} \right\}$$

(20) TRI stands for time-reversal invariance (to be defined in Eq. (3)).
(21) $\mathrm{Pf}[A]$ is the Pfaffian of an anti-symmetric $2n \times 2n$ matrix, given by

$$\mathrm{Pf}[A] = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \mathrm{sgn}(\sigma) \prod_{i=1}^{n} (A)_{\sigma(2i-1),\, \sigma(2i)}$$

where S_{2n} is the symmetric group and sgn is the signature of a permutation.

Part 1

The Bulk-Edge Correspondence

The Bulk-Edge correspondence refers to the equivalence of certain physical quantities computed for two *different* but related physical systems, one called "bulk" and the other "edge". For us, these physical quantities are the Hall electric charge conductance in the case of quantum Hall systems, or in the case of topological insulators, it is "time-reversal polarization" as in [Fu06]: "a $\mathbb{Z}_2$ quantity that signals whether a time reversal invariant one-dimensional system has a Kramers degeneracy associated with its ends." What defines the bulk system is that it has no boundaries, whereas the edge system (for us) usually has one boundary. Except for the employment of these boundary conditions, we assume the two systems are the same (in a sense made precise later). It is a striking fact that the two different mechanisms, happening in two different localizations of the system, give rise to the same physical quantities. In real world physical systems (which, of course, have boundaries) both both bulk and edge transport mechanisms take place in proportions that depend on the actual system's capture potential.

That the equivalence should exist is a surprising fact, yet, it has been proven already to various degrees of mathematical rigor and in rising levels of generality. For instance, [Ha93] was probably the first and least general, [Ke02] uses twisted equivariant K-theory, [Es11] uses Green's functions, [Gr13] presents two proofs, one using frame bundles and the other using Levinson's theorem in scattering theory, and [Ta12] uses the Atiyah-Singer index theorem.

In this work our task at hand was rather to find the *simplest* possible proofs, and so for each type of index, or topological invariant, we went to the simplest yet non trivial systems: a two-band model for the quantum-Hall system (because a gap is necessary), and a four-band model for the topological-insulator model (because of Kramer's degeneracy and a gap).

After setting the stage, we begin by recounting the results of [Mo11] regarding "Dirac" systems. This will allow us to characterize the existence of edge states easily. Next we present two different proofs for the quantum-Hall correspondence: one simpler and more restricted in generality, the other more general, relying on [Mo11]. This latter proof is heavily inspired by the one presented originally in [Mo11]. While the main tool to analyze the bulk system is algebraic topology and for the edge system functional analysis, we make use of this machinery sparingly, as our goal is indeed to make the most simple presentation possible.

In the last chapter, we present a new formula for the $\mathbb{Z}_2$ topological invariant for "Dirac" four-band systems, which is justified by two proofs: one a generalization of [Fu07] and the other new but inspired by [Mo07]. This formula, together with [Mo11], allows us to show the correspondence in a very short proof.

CHAPTER 1

Analysis of Nearest Neighbor Lattice Models

1.1. Setting

Let $N \in 2\mathbb{N}\backslash\{0\}$ be given. Following [Gr13], we study families of self-adjoint operators on the Hilbert space $l^2(\mathbb{Z};\mathbb{C}^N)$ parametrized on S^1 by the variable k_2 and denoted $H(k_2)$, called Hamiltonians, which have the form given by matrix elements

$$H_{(n,n')}(k_2) = V(k_2)\delta_{n,n'} + A(k_2)\delta_{n,n'+1} + A^*(k_2)\delta_{n,n'-1} \tag{1}$$

for all $(n, n') \in \mathbb{Z}^2$, where $\forall k_2 \in S^1$, $V(k_2) \in \mathrm{Herm}(N)$ and $A(k_2) \in M_N(\mathbb{C})$. Such families will be called "bulk" systems, because here $H(k_2)$ operates on maps $\mathbb{Z} \to \mathbb{C}^N$, and $\mathbb{Z}$ has no edge. From such systems, "edge" systems are derived, defined by the Hamiltonians $H^\sharp(k_2)$ with matrix elements

$$H^\sharp_{(n,n')}(k_2) = H_{(n,n')}(k_2) \quad \forall (n, n') \in \mathbb{N}^2 \tag{2}$$

and undefined elsewhere. So $H^\sharp(k_2)$ acts on $l^2(\mathbb{N};\mathbb{C}^N)$. Because $\mathbb{N}$ has a left edge (at 0), we call this system the edge system.

In what follows we shall often omit the explicit k_2 dependence and write merely H or $H^\sharp$ for the sake of brevity.

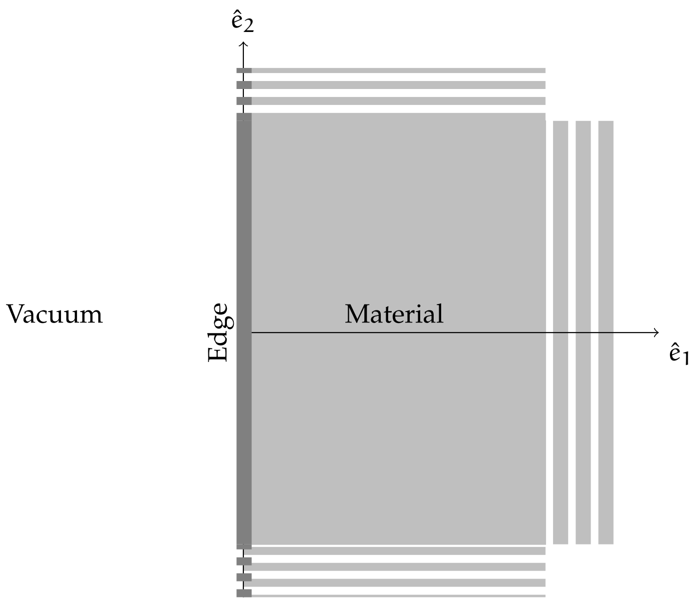

FIGURE 1.1.1. The orientation of the edge throughout this work.

1.1.1. REMARK. The form of H given in Eq. (1) is a nearest neighbor approximation of a one dimensional chain (or a family of chains parameterized by k_2). However, this system should be viewed as a two-dimensional lattice where on the $\hat{e}_2$ direction, we allow for arbitrary-length correlations, as we never use the explicit form of the k_2 dependence.

1.1.2. DEFINITION. A bulk Hamiltonian $H : S^1 \to \mathcal{B}\left(l^2\left(\mathbb{Z};\mathbb{C}^N\right)\right)$ is called gapped iff

$$E_F \notin \sigma\left(H\left(k_2\right)\right) \forall k_2 \in S^1$$

1.2. Time-Reversal

1.2.1. DEFINITION. Define a map on $C : \mathbb{C}^N \to \mathbb{C}^N$ called "complex conjugation" by

$$v_j \overset{C}{\mapsto} \overline{v_j} \qquad \forall j \in J_N$$

where v_j is the jth component of $v \in \mathbb{C}^N$.

1.2.2. DEFINITION. Define a block diagonal $N \times N$ matrix, ε, given by $\frac{1}{2}N$ blocks, each of which is $-i\sigma_2$, and denote the corresponding linear map $\mathbb{C}^N \to \mathbb{C}^N$ given by

$$v \mapsto \varepsilon v \quad \forall v \in \mathbb{C}^N$$

with ε as well.

1.2.3. DEFINITION. Define a map $\Theta : \mathbb{C}^N \to \mathbb{C}^N$ by

$$\Theta := \varepsilon \circ C$$

called "time-reversal". From this map, a map (still denoted by Θ) on the Hilbert space $l^2\left(\mathbb{Z};\mathbb{C}^N\right)$ or $l^2\left(\mathbb{N};\mathbb{C}^N\right)$ is induced by

$$\psi_n \mapsto \Theta\psi_n \quad \forall n \in \mathbb{N} \text{ or } \mathbb{Z}$$

where ψ_n is the nth component of $\psi \in l^2\left(\mathbb{Z};\mathbb{C}^N\right)$ or $\psi \in l^2\left(\mathbb{N};\mathbb{C}^N\right)$.

1.2.4. CLAIM. Θ is anti-linear and $\Theta^2 = -1$.

PROOF. That Θ is anti-linear follows directly from its definition as matrix multiplication (which is linear) together with complex conjugation.

$$\begin{aligned}(\Theta)^2 &= \varepsilon \circ C \circ \varepsilon \circ C \\ &\overset{\varepsilon \in M_N(\mathbb{R})}{=} \varepsilon^2 \\ &= -\mathbb{1}\end{aligned}$$

where the last step follows by direct computation. □

1.2.5. CLAIM. $\Theta^*\Theta = \mathbb{1}$.

PROOF. We have

$$\begin{aligned}\Theta^* \circ \Theta &= (\varepsilon \circ C)^* \circ \varepsilon \circ C \\ &= C^* \circ \underbrace{\varepsilon^* \circ \varepsilon}_{\mathbb{1}} \circ C \\ &= C^* \circ C \\ &= \mathbb{1}\end{aligned}$$

□

1.2.6. DEFINITION. Define a property of bulk Hamiltonians called "time-reversal invariant" by the following condition

$$H\left(-k_2\right) = \Theta \circ H\left(k_2\right) \circ \Theta^{-1} \;\; \forall k_2 \in S^1 \tag{3}$$

1.2.7. CLAIM. If a bulk Hamiltonian $H : S^1 \to \mathcal{B}\left(l^2\left(\mathbb{Z};\mathbb{C}^N\right)\right)$ is time-reversal invariant then the induced edge Hamiltonian $H^\# : S^1 \to \mathcal{B}\left(l^2\left(\mathbb{N};\mathbb{C}^N\right)\right)$ obeys:

$$H^\sharp\left(-k_2\right) = \Theta \circ H\left(k_2\right)^\sharp \circ \Theta^{-1} \;\; \forall k_2 \in S^1$$

PROOF. The claim follows immediately because Eq. (3) is equivalent to

$$H_{(n,n')}(-k_2) = \Theta H_{(n,n')}(k_2)\Theta^{-1} \ \ \forall (n,\ n',\ k_2) \in \mathbb{Z}^2 \times S^1$$

which implies

$$H_{(n,n')}(-k_2) = \Theta H_{(n,n')}(k_2)\Theta^{-1} \ \ \forall (n,\ n',\ k_2) \in \mathbb{N}^2 \times S^1$$

which is equivalent to

$$H^\sharp_{(n,n')}(-k_2) = \Theta H^\sharp_{(n,n')}(k_2)\Theta^{-1} \ \ \forall (n,\ n',\ k_2) \in \mathbb{N}^2 \times S^1$$

due to Eq. (2), and this is equivalent to the claim. □

1.2.8. CLAIM. If H is time-reversal symmetric then $\sigma(H(k_2)) = \sigma(H(-k_2))$ for all $k_2 \in S^1$.

PROOF. If $z \in \sigma(H(k_2))$ then $\ker(H(k_2) - \mathbb{1}z) \neq 0$ and so $[H(k_2) - z]\psi = 0$ holds for some $\psi \neq 0$.

- Multiply this equation by Θ from the left to get:

$$\begin{aligned}
(\Theta H(k_2) - \Theta z)\psi &= 0\\
(\Theta H(k_2) - \Theta z)\underbrace{\Theta^{-1}\Theta}_{\mathbb{1}}\psi &= 0\\
\left[\underbrace{\Theta H(k_2)\Theta^{-1}}_{H(-k_2)} - \underbrace{\Theta z\Theta^{-1}}_{\overline{z}}\right]\Theta\psi &= 0\\
[H(-k_2) - \overline{z}]\,\Theta\psi &= 0
\end{aligned}$$

- As a result we see that if $z \in \mathbb{R}$ then $z \in \sigma(H(-k_2))$. A symmetric argument shows the other direction of inclusion.

□

1.2.9. CLAIM. (Kramers theorem) At special points on S^1 where $k_2 = -k_2$, given by $\{0, \pi\}$, the eigenstates of $H(k_2)$ are at least two-fold degenerate.

PROOF. Because at these special points, Eq. (3) implies $[H(k_2), \Theta] = 0$, we have that if ψ is an eigenstate of the HamiltonianâĂŞ$H(k_2)\psi = E\psi$âĂŞthen $\Theta\psi$ is also an eigenstate of $H(k_2)$ with the same eigenvalue E:

$$\begin{aligned}
H(k_2)\Theta\psi &= ([H(k_2), \Theta] + \Theta H(k_2))\psi\\
&= \Theta H(k_2)\psi\\
&= \Theta E\psi\\
&= E\Theta\psi
\end{aligned}$$

Now, if ψ and $\Theta\psi$ are the same up to a phase, then there would be no degeneracy. However, this is impossible. To see this, assume otherwise, that is, assume that

$$\Theta\psi = c\psi$$

for some $c \in \mathbb{C}$. Multiplying this equation by Θ from the left we get

$$\begin{aligned}
\Theta^2\psi &= \Theta c\psi\\
&= \overline{c}\Theta\psi\\
&= \overline{c}c\psi\\
&= |c|^2\psi
\end{aligned}$$

which is of course nonsense as 1.2.4 would imply that $|c|^2 = -1$. We conclude that ψ and $\Theta\psi$ are two linearly-independent vectors. □

1.3. Bloch Reduction

The "bulk" Hamiltonian (which acts on $l^2(\mathbb{Z}; \mathbb{C}^N)$) possesses translational symmetry in the sense of

$$H_{(n,n')}(k_2) = H_{(n+m,n'+m)}(k_2) \ \ \forall (n, n', m) \in \mathbb{Z}^3$$

and as such, we may choose to work with a continuous parameter $k_1 \in S^1$ instead of the parameter $n \in \mathbb{Z}$.

To this end, we employ Bloch's theorem, which states that because of the periodicity of H in n, the eigenstates of H are simultaneously also eigenvectors of the translation operator $T : \psi_n \mapsto \psi_{n+1}$, and may be written as

$$\psi_{n,k_1} = e^{ik_1 n} u_{n,k_1}$$

where $k_1 \in S^1$ is a new quantum number labelling the eigenvalues of the translation operator, $e^{ik_1 n}$; u_{n,k_1} has the same periodicity of the Hamiltonian, $u_{n,k_1} = u_{n+1,k_1}$ and so we might as well drop its n index and write

$$\begin{aligned} \psi_{n,k_1} &= e^{ik_1 n} u_{k_1} \\ &= e^{ik_1 n} \psi_{0,k_1} \end{aligned}$$

We plug this into the eigenvalue equation to obtain:

$$\begin{aligned} \sum_{n' \in \mathbb{Z}} H_{(n,n')} \psi_{n',k_1} &= E_{k_1} \psi_{n,k_1} \\ \sum_{n' \in \mathbb{Z}} H_{(n,n')} e^{ik_1 n'} \psi_{0,k_1} &= E_{k_1} e^{ik_1 n} \psi_{0,k_1} \\ \sum_{n' \in \mathbb{Z}} H_{(n,n')} e^{ik_1 (n'-n)} \psi_{0,k_1} &= E_{k_1} \psi_{0,k_1} \\ \sum_{n' \in \mathbb{Z}} H_{(0,n'-n)} e^{ik_1 (n'-n)} \psi_{0,k_1} &\overset{*}{=} E_{k_1} \psi_{0,k_1} \\ \underbrace{\sum_{m \in \mathbb{Z}} H_{(0,m)} e^{ik_1 m}}_{H^B(k_1)} \psi_{0,k_1} &= E_{k_1} \psi_{0,k_1} \\ H^B(k_1) \psi_{0,k_1} &= E_{k_1} \psi_{0,k_1} \end{aligned}$$

where in $*$ we have used the translational symmetry of H and we have defined

$$H^B(k_1, k_2) := \sum_{m \in \mathbb{Z}} H_{(0,m)}(k_2) e^{ik_1 m} \qquad \forall (k_1, k_2) \in \mathbb{T}^2 \tag{4}$$

B stands for Bloch. Let us compute $H^B(k)$ where $k \in \mathbb{T}^2$ explicitly:

$$\begin{aligned} H^B(k) &\equiv \sum_{m \in \mathbb{Z}} H_{(0,m)}(k_2) e^{ik_1 m} \qquad (5) \\ &= H_{(0,0)}(k_2) + H_{(0,1)}(k_2) e^{ik_1} + H_{(0,-1)}(k_2) e^{-ik_1} + (\text{all other summands are zero}) \\ &= V(k_2) + [A(k_2)]^* e^{ik_1} + A(k_2) e^{-ik_1} \\ &= V(k_2) + \left\{[A(k_2)]^* + A(k_2)\right\} \cos(k_1) + i \left\{[A(k_2)]^* - A(k_2)\right\} \sin(k_1) \end{aligned}$$

This special form of $H^B(k)$ is a manifestation of the nearest-neighbor approximation.

1.3.1. CLAIM. If H is time-reversal invariant as in Eq. (3) then H^B obeys

$$H^B(-k) = \Theta H^B(k) \Theta^{-1} \qquad \forall k \in \mathbb{T}^2 \tag{6}$$

PROOF. We start by assuming Eq. (3) and using our formula for $H^B(k)$ given by Eq. (4):

$$\begin{aligned} H^B(-k) &\equiv \sum_{m \in \mathbb{Z}} H_{(0,m)}(-k_2) e^{-ik_1 m} \\ &= \sum_{m \in \mathbb{Z}} \Theta H_{(0,m)}(k_2) \Theta^{-1} e^{-ik_1 m} \\ &= \Theta \left[\sum_{m \in \mathbb{Z}} H_{(0,m)}(k_2) e^{+ik_1 m} \right] \Theta^{-1} \\ &= \Theta H^B(k) \Theta^{-1} \end{aligned}$$

□

1.4. Edge Systems

To get the spectrum and eigenstates of the bulk system, the preceding section showed we merely need to solve the eigenvalue problem for an $N \times N$ Hermitian matrix $H^B(k)$, the problem being parametrized by the parameter $k \in \mathbb{T}^2$. This is the result of employing the Bloch theorem, which saves us the trouble of having to solve the eigenvalue problem for an infinite chain on $\mathbb{Z}$.

For the edge system, we still have a half-infinite problem on $\mathbb{N}$, which is just as hard to solve as the infinite problem, yet now we may not employ Bloch's theorem as there is no translation symmetry.

1.4.1. CLAIM. If ψ solves the eigenvalue problem for the bulk system, and it obeys the condition $\psi_0 = 0$ then it solves the edge system as well.

PROOF. We assume that

$$\begin{aligned} \sum_{n' \in \mathbb{Z}} H_{(n,n')}\psi_{n'} &= E\psi_n \\ V(k_2)\psi_n + A(k_2)\psi_{n-1} + A^*(k_2)\psi_{n+1} &= E\psi_n \end{aligned}$$

which means that ψ is a solution for the bulk problem.

- At $n = 1$ the equation reads

$$\begin{aligned} V(k_2)\psi_1 + A(k_2)\underbrace{\psi_0}_{0} + A^*(k_2)\psi_2 &= E\psi_1 \\ V(k_2)\psi_1 + A^*(k_2)\psi_2 &= E\psi_1 \end{aligned}$$

- However, this is exactly the edge eigenvalue equation at $n = 1$, and so ψ solves the edge eigenvalue equation at $n = 1$. For $n > 1$, the edge and bulk eigenvalue equations are identical, and so, ψ solves the edge problem.

□

To produce bulk solutions ψ obeying $\psi_0 = 0$ we cannot simply take Bloch-decomposed bulk solutions, $\psi_{n,k_1} = e^{ink_1}\psi_{0,k_1}$ and enforce $\psi_0 = 0$ because that would mean that $\psi_{n,k_1} = 0 \forall n \in \mathbb{Z}$, giving us only zero solutions.

Instead we must take linear combinations

$$\psi_n = \sum_j c_j \psi^{(j)}_{n,k_1^{(j)}}$$

of such bulk solutions $\psi^{(j)}_{n,k_1^{(j)}}$ so that $\sum_j c_j \psi^{(j)}_{0,k_1^{(j)}} \overset{!}{=} 0$.

In addition we must also make sure that the edge solution decays into the bulk (so that it is indeed localized near $n = 0$). Indeed, in general (as in [Gr13])

$$\sigma_{ess}\left(H^\sharp(k_2)\right) \subset \sigma_{ess}(H(k_2)) \qquad \forall k_2 \in S^1$$

and so we would want to avoid finding solutions of $H^\sharp$ which resemble those of H. What is unique about solutions which are *only* of $H^\sharp$ is that htey are localized near the edge of $\mathbb{N}$.

The way to make sure that we have such a solution is to take solutions which have $\Im\left(k_1^{(j)}\right) > 0$ for all j. That way,

$$\exp\left[in\left(\Re\left(k_1^{(j)}\right) + i\Im\left(k_1^{(j)}\right)\right)\right]\psi^{(j)}_{0,k_1^{(j)}} \overset{n\to\infty}{\longrightarrow} 0$$

This is thus a generalization to the Bloch scheme where the eigenvalues of the translation operator T are taken to be on the unit circle in the complex plane: $\left|e^{ik_1}\right| = 1$. For localized edge solutions they need to be taken inside or within the unit circle: $\left|e^{ik_1}\right| \leqslant 1$.

1.4.2. REMARK. Thus our "recipe" to find the edge discrete spectrum from a given bulk, Bloch-decomposed problem is as such:

(1) Solve the Bloch problem, and fix some energy value E within a bulk gap and some arbitrary $k_2 \in S^1$.
(2) Find (at least) two values of $k_1 \in S^1 + i[0,\infty)$, $k_1^{(1)}$ and $k_1^{(2)}$ which solve the Bloch eigenvalue equation with corresponding eigenstates $\psi^{(1)}_{0,k_1^{(1)}}$ and $\psi^{(2)}_{0,k_1^{(2)}}$.
(3) Impose the boundary condition, from which another equation emerges. This last equation should allow one to find the edge energy E.

1.5. Dirac Hamiltonians

In this section we recount the analysis of [Mo11] for solving the edge spectrum of "Dirac Hamiltonians". The results in this section will be crucial to showing the bulk-edge correspondence later.

1.5.1. DEFINITION. Dirac Hamiltonians are Hamiltonians (after Bloch reduction, thus specified with $H^B(k)$ for all $k \in \mathbb{T}^2$) given by

$$H^B(k) = \sum_{j=1}^{m} h_j(k)\Gamma_j \tag{7}$$

where $\{\Gamma_j\}_{j=1}^m$ is a traceless set of Hermitian $N \times N$ matrices obeying the Clifford algebra

$$\{\Gamma_i, \Gamma_j\} = 2\delta_{ij}\mathbb{1}_{N\times N}$$

and $h(k) \equiv \sum_{i=1}^m h_i(k)\hat{e}_i$ is a map $\mathbb{T}^2 \to \mathbb{R}^m$. Note that summation convention on repeating subscript latin indices (such as j) will be assumed in what follows.

1.5.2. CLAIM. $\sigma(H^B(k)) = \{\|h(k)\|, -\|h(k)\|\}$.

PROOF. The eigenvalue equation is given by

$$h_j(k)\Gamma_j\psi = E^B(k)\psi$$

Multiply this equation from the left by $h_j(k)\Gamma_j$ to obtain:

$$\begin{aligned}(h_j(k)\Gamma_j)^2\psi &= h_i(k)h_j(k)\Gamma_i\Gamma_j\psi \\ &= \left[\sum_i (h_i(k))^2 \underbrace{(\Gamma_i)^2}_{\mathbb{1}_{N\times N}} + \underbrace{\sum_{j\neq i} h_i(k)h_j(k)\underbrace{\{\Gamma_i,\Gamma_j\}}_{2\delta_{ij}}}_{0}\right]\psi \\ &= \|h(k)\|^2\psi\end{aligned}$$

yet we also know that $(h_j(k)\Gamma_j)^2\psi = (E^B(k))^2\psi$ so that the result follows. □

1.5.3. COROLLARY. *The gapped Hamiltonian condition 1.1.2 then translates to the assumption that* $h(k) \neq 0 \forall k \in \mathbb{T}^2$.

1.5.4. CLAIM. $h(k)$ is of the form

$$h(k) = b^0 + be^{-ik_1} + \bar{b}e^{ik_1}$$

where $b^0 \in \mathbb{R}^m$ is given by the components

$$\left\langle b^0, \hat{e}_i\right\rangle = \frac{1}{N}\mathrm{Tr}[V(k_2)\Gamma_i]$$

and $b \in \mathbb{C}^m$ is given by

$$\langle b, \hat{e}_i\rangle = \frac{1}{N}\mathrm{Tr}[A(k_2)\Gamma_i]$$

PROOF. We have the two simultaneous assumptions, namely Eq. (5) and Eq. (7), from which we get the equality

$$h_j(k)\Gamma_j = V(k_2) + [A(k_2)]^* e^{ik_1} + A(k_2)e^{-ik_1}$$

Multiply this equation by Γ_i from the right, take the trace, and divide by $\frac{1}{N}$ to get:

$$h_j(k)\frac{1}{N}\mathrm{Tr}[\Gamma_j\Gamma_i] = \frac{1}{N}\mathrm{Tr}[V(k_2)\Gamma_i] + \frac{1}{N}\mathrm{Tr}\left[[A(k_2)]^*\Gamma_i\right]e^{ik_1} + \frac{1}{N}\mathrm{Tr}[A(k_2)\Gamma_i]e^{-ik_1}$$

But using the fact that the trace is cyclic, we have

$$\begin{aligned}\frac{1}{N}\mathrm{Tr}[\Gamma_j\Gamma_i] &= \frac{1}{2}\left(\frac{1}{N}\mathrm{Tr}[\Gamma_j\Gamma_i] + \frac{1}{N}\mathrm{Tr}[\Gamma_i\Gamma_j]\right) \\ &= \frac{1}{2}\frac{1}{N}\mathrm{Tr}[\{\Gamma_j,\Gamma_i\}] \\ &= \delta_{ij}\end{aligned}$$

so that we get

$$h_i(k) = \frac{1}{N}\operatorname{Tr}\left[V(k_2)\Gamma_i\right] + \frac{1}{N}\operatorname{Tr}\left[\left[A(k_2)\right]^*\Gamma_i\right]e^{ik_1} + \frac{1}{N}\operatorname{Tr}\left[A(k_2)\Gamma_i\right]e^{-ik_1}$$

Now use the fact that the $\operatorname{Tr}[A^*] = \overline{\operatorname{Tr}[A]}$ to obtain that $\frac{1}{N}\operatorname{Tr}[V(k_2)\Gamma_i] \in \mathbb{R}$ due to the Hermiticity of Γ_i and $V(k_2)$ whereas $\frac{1}{N}\operatorname{Tr}[A(k_2)\Gamma_i]$ is generally complex, as $A(k_2)$ is not necessarily Hermitian. □

1.5.5. REMARK. Observe that for a fixed k_2 and varying k_1 we have

$$\begin{aligned} h(k) &= b^0(k_2) + b(k_2)e^{-ik_1} + \overline{b(k_2)}e^{ik_1} \\ &= b^0(k_2) + 2\underbrace{\Re\{b(k_2)\}}_{b^r(k_2)}\cos(k_1) + 2\underbrace{\Im\{b(k_2)\}}_{b^i(k_2)}\sin(k_1) \end{aligned}$$

and so at fixed k_2, $h(k)|_{k_2}$ traces an ellipse in $\mathbb{R}^m$ as k_1 is varied on S^1. Note that this is a feature of the nearest neighbor approximation. This ellipse lives on the plane spanned by the two vectors $b^r(k_2)$ and $b^i(k_2)$ (and so in particular at different values of k_2 this plane changes, but it is independent of k_1) and is offset from the origin by the vector b^0.

1.5.6. DEFINITION. Define the following vectors and matrices, most of which are functions of k_2 alone unless otherwise noted:

$$\hat{e}^r := \frac{\Re\{b\}}{\|\Re\{b\}\|}$$

$$\hat{e}^i := \frac{\Im\{b\} - \langle\Im\{b\}, \hat{e}^r\rangle\hat{e}^r}{\|\Im\{b\} - \langle\Im\{b\}, \hat{e}^r\rangle\hat{e}^r\|}$$

$$\hat{e}^\nu := \pm\hat{e}^i$$

(the sign is unspecified for now)

$$b^{0\|} := \left\langle b^0, \hat{e}^r\right\rangle\hat{e}^r + \left\langle b^0, \hat{e}^i\right\rangle\hat{e}^i$$

$$b^{0\perp} := b^0 - b^{0\|}$$

$$\hat{e}^\perp := \frac{b^{0\perp}}{\|b^{0\perp}\|}$$

$$h^{\|}(k) := b^{0\|}(k_2) + b(k_2)e^{-ik_1} + \overline{b(k_2)}e^{ik_1}$$

$$\Gamma^\alpha := e^\alpha_j\Gamma_j \qquad \forall\alpha\in\{r, i, \perp, \nu\}$$

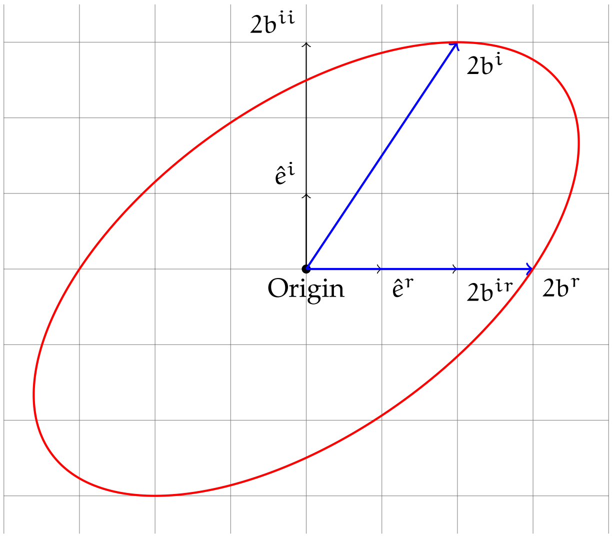

FIGURE 1.5.1. The ellipse spanned by $b^r(k_2)$ and $b^i(k_2)$, before the shift by $b^{0\|}(k_2)$.

$$\Gamma^{\pm} := \frac{1}{2}\left(\Gamma^{r} \pm i\Gamma^{\nu}\right)$$

$$h^{\alpha}(k) := \langle h(k), \hat{e}^{\alpha}\rangle \qquad \forall \alpha \in \{r, i, \perp, \nu\}$$

$$h^{\pm}(k) := h^{r}(k) \mp i h^{\nu}(k)$$

1.5.7. REMARK. Note that $\hat{e}^{\nu}$ is chosen so that it is orthogonal to $\hat{e}^{r}$ and $\hat{e}^{\perp}$. The reason we don't simply work with $\hat{e}^{i}$ instead is that we want to work in a generality in which the orientation of the system $(\hat{e}^{r}, \hat{e}^{\nu}, \hat{e}^{\perp})$ is not yet fully specified. This will be then used later in 1.5.21.

1.5.8. CLAIM. The Hamiltonian Eq. (7) may be written as

$$H^{B}(k) = \left\|b^{0\perp}(k_2)\right\|\Gamma^{\perp} + h^{+}(k)\Gamma^{+} + h^{-}(k)\Gamma^{-}$$

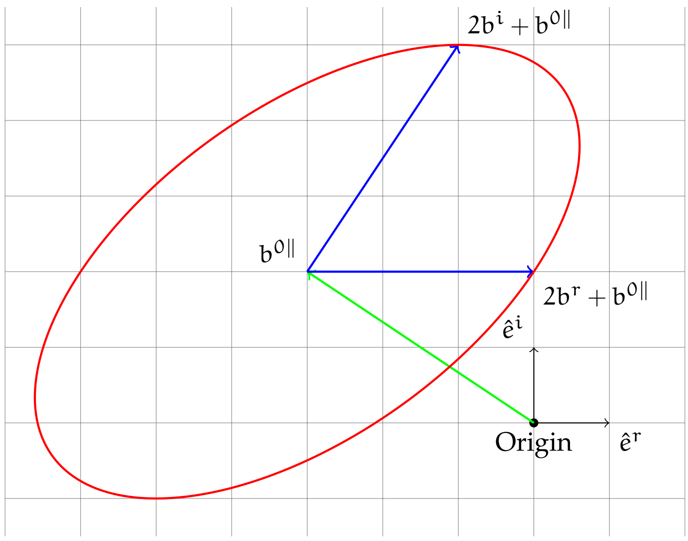

FIGURE 1.5.2. The ellipse spanned by $b^{r}(k_2)$ and $b^{i}(k_2)$, after the shift by $b^{0\|}(k_2)$. In this particular configuration there is no edge state because the origin is outside of the ellipse.

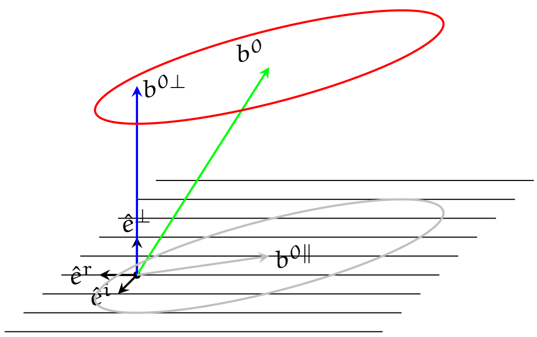

FIGURE 1.5.3. The ellipse embedded in $\mathbb{R}^3$. In this configuration, there *is* an edge state because the projection onto the ellipse's plane (in grey) contains the origin. The state's energy magnitude is given by the length of the blue vector and its sign is positive because $\hat{e}^{r}$, $\hat{e}^{i}$ and $\hat{e}^{\perp}$ form a right-handed system.

PROOF. Note that as $h(k)$ is spanned by only three vectors, we may write it as a sum of these components:

$$\begin{aligned} H^B(k) &= h_j(k)\Gamma_j \\ &= \left[h^\perp(k)e_j^\perp + h^r(k)e_j^r + h^\nu(k)e_j^\nu\right]\Gamma_j \\ &= h^\perp(k)\Gamma^\perp + h^r(k)\Gamma^r + h^\nu(k)\Gamma^\nu \\ &= h^\perp(k)\Gamma^\perp + \frac{1}{2}\left[h^+(k)+h^-(k)\right]\Gamma^r + i\frac{1}{2}\left[h^+(k)-h^-(k)\right]\Gamma^\nu \\ &= h^\perp(k)\Gamma^\perp + \frac{1}{2}h^+(k)(\Gamma^r+i\Gamma^\nu) + \frac{1}{2}h^-(k)(\Gamma^r-i\Gamma^\nu) \\ &= h^\perp(k)\Gamma^\perp + h^+(k)\Gamma^+ + h^-(k)\Gamma^- \end{aligned}$$

The last step is to recognize that $h^\perp$ in fact does not depend on k_1, as a result of the fact that it is defined as

$$\begin{aligned} h^\perp(k) &\equiv \left\langle h(k), \hat{e}^\perp(k_2)\right\rangle \\ &= \left\langle b^0(k_2) + 2\Re\{b(k_2)\}\cos(k_1) + 2\Im\{b(k_2)\}\sin(k_1), \hat{e}^\perp(k_2)\right\rangle \\ &= \left\langle b^0(k_2), \hat{e}^\perp(k_2)\right\rangle \\ &= \left\|b^{0\perp}(k_2)\right\| \end{aligned}$$

using $\hat{e}^\perp(k_2) \perp \Re\{b(k_2)\}$ and $\hat{e}^\perp(k_2) \perp \Im\{b(k_2)\}$. □

1.5.9. CLAIM. $\left\{\Gamma^\perp, \Gamma^\pm\right\} = 0$.

PROOF.

$$\begin{aligned} \left\{\Gamma^\perp, \Gamma^\pm\right\} &= \left\{e_j^\perp\Gamma_j, \frac{1}{2}(e_i^r\Gamma_i \pm ie_i^\nu\Gamma_i)\right\} \\ &= \frac{1}{2}e_j^\perp\left(e_i^r\{\Gamma_j, \Gamma_i\} \pm ie_i^\nu\{\Gamma_j, \Gamma_i\}\right) \\ &= \frac{1}{2}e_j^\perp(e_i^r \pm ie_i^\nu)2\delta_{ji}\mathbb{1} \\ &= \left(\hat{e}^\perp\cdot\hat{e}^r \pm i\hat{e}^\perp\cdot\hat{e}^\nu\right)\mathbb{1} \\ &= 0 \end{aligned}$$

□

1.5.10. CLAIM. $\{\Gamma^+, \Gamma^-\} = \mathbb{1}$.

PROOF.

$$\begin{aligned} \{\Gamma^+, \Gamma^-\} &= \left\{\frac{1}{2}(e_i^r\Gamma_i + ie_i^\nu\Gamma_i), \frac{1}{2}\left(e_j^r\Gamma_j - ie_j^\nu\Gamma_j\right)\right\} \\ &= \frac{1}{4}\left(e_i^re_j^r2\delta_{ij} + e_i^\nu e_j^\nu 2\delta_{ij} + 2e_i^re_j^\nu 2\delta_{ij}\right)\mathbb{1} \\ &= \mathbb{1} \end{aligned}$$

□

1.5.11. CLAIM. $(\Gamma^\alpha)^2 = \mathbb{1}\forall\alpha \in \{r, i, \perp, \nu\}$.

PROOF. Here there is no summation implied over the repeated index α, but only over latin indices:

$$\begin{aligned}(\Gamma^\alpha)^2 &= e_i^\alpha e_j^\alpha \Gamma_i\Gamma_j \\ &= \frac{1}{2}\left(e_i^\alpha e_j^\alpha \Gamma_i\Gamma_j + e_j^\alpha e_i^\alpha \Gamma_i\Gamma_j\right) \\ &= \frac{1}{2}e_i^\alpha e_j^\alpha \{\Gamma_i, \Gamma_j\} \\ &= \frac{1}{2}e_i^\alpha e_j^\alpha 2\delta_{ij}\mathbb{1} \\ &= \hat{e}^\alpha\cdot\hat{e}^\alpha\mathbb{1} \\ &= \mathbb{1}\end{aligned}$$

□

1.5.12. CLAIM. $\left(\Gamma^\pm\right)^2 = 0$.

PROOF.

$$\begin{aligned}(\Gamma^\pm)^2 &= \frac{1}{2}\left(e_i^r\Gamma_i \pm i e_i^\nu \Gamma_i\right)\frac{1}{2}\left(e_j^r\Gamma_j \pm i e_j^\nu\Gamma_j\right) \\ &= \frac{1}{4}\left(e_i^r e_j^r \Gamma_i\Gamma_j - e_i^\nu e_j^\nu \Gamma_i\Gamma_j \pm i e_i^r e_j^\nu \Gamma_i\Gamma_j \pm i e_i^\nu e_j^r \Gamma_i\Gamma_j\right) \\ &= \frac{1}{4}\Big[\underbrace{(\Gamma^r)^2 - (\Gamma^\nu)^2}_{0} \pm i e_i^r e_j^\nu \Gamma_i\Gamma_j \pm i e_i^\nu e_j^r \Gamma_i\Gamma_j\Big] \\ &= \pm\frac{1}{2} i e_i^r e_j^\nu \{\Gamma_i, \Gamma_j\} \\ &= \pm i\hat{e}^r\cdot\hat{e}^i\mathbb{1} \\ &= 0\end{aligned}$$

□

1.5.13. REMARK. It is assumed that all maps $\mathbb{T}^2 \to \mathbb{R}$ introduced so far ($h_j(k)$ for instance) can be analytically continued in such a way that k_1 takes on complex values:

$$\eta(\lambda, k_2) := b^0(k_2) + b(k_2)\lambda^{-1} + \overline{b}(k_2)\lambda \qquad \forall\lambda\in\mathbb{C}$$

when a map is analytically continued we denote it by the corresponding Greek letter:

$$\eta(\exp(ik_1), k_2) \equiv h(k) \qquad \forall k \in \mathbb{T}^2$$

1.5.14. CLAIM. Let $E\in\mathbb{R}$, $\eta^\perp\in\mathbb{R}$ and $u\in\mathbb{C}^N\setminus\{0\}$ be given.
If $E\neq\pm\eta^\perp$, then the equation

$$\left(\eta^\perp\Gamma^\perp + \eta^+\Gamma^+ + \eta^-\Gamma^-\right)u = Eu \tag{8}$$

where (η^+, η^-) are unknown variables is satisfied for *at most* a single pair (η^+, η^-).

PROOF. Applying $(\eta^\perp\Gamma^\perp + \eta^+\Gamma^+ + \eta^-\Gamma^-)$ on Eq. (8) from the left results in

$$\left(\eta^\perp\Gamma^\perp + \eta^+\Gamma^+ + \eta^-\Gamma^-\right)^2 u = E^2 u \tag{9}$$

yet

$$\begin{aligned}\left(\eta^\perp\Gamma^\perp + \eta^+\Gamma^+ + \eta^-\Gamma^-\right)^2 &= \sum_{(\alpha,\beta)\in\{\perp,\pm\}^2}\eta^\alpha\eta^\beta\Gamma^\alpha\Gamma^\beta \\ &= \sum_{(\alpha,\beta)\in\{\perp,\pm\}^2}\eta^\alpha\eta^\beta\frac{1}{2}\left\{\Gamma^\alpha, \Gamma^\beta\right\} \\ &= \left[\left(\eta^\perp\right)^2 + \eta^+\eta^-\right]\mathbb{1}\end{aligned}$$

so that Eq. (9) becomes

$$\eta^+\eta^- u = \left[E^2 - \left(\eta^\perp\right)^2\right] u$$

But as $u \neq 0$ it follows that

$$\eta^+\eta^- = E^2 - \left(\eta^\perp\right)^2 \tag{10}$$

Now assume that $\exists$ two pairs (η^+, η^-) and $(\tilde\eta^+, \tilde\eta^-)$ such that Eq. (8) is satisfied (observe that the assumption that $E^2 \neq (\eta^\perp)^2$ implies $0 \notin \{\eta^+, \eta^-, \tilde\eta^+, \tilde\eta^-\}$). Then from Eq. (10) we have

$$\eta^+\eta^- = \tilde\eta^+\tilde\eta^- \tag{11}$$

as well as

$$\begin{cases} \left(\eta^\perp\Gamma^\perp + \eta^+\Gamma^+ + \eta^-\Gamma^-\right) u &= Eu \\ \left(\eta^\perp\Gamma^\perp + \tilde\eta^+\Gamma^+ + \tilde\eta^-\Gamma^-\right) u &= Eu \end{cases}$$

directly from Eq. (8). Taking the difference of these two equations gives

$$\left[\left(\eta^+ - \tilde\eta^+\right)\Gamma^+ + \left(\eta^- - \tilde\eta^-\right)\Gamma^+\right] u = 0 \tag{12}$$

But observe that

$$\left[\left(\eta^+ - \tilde\eta^+\right)\Gamma^+ + \left(\eta^- - \tilde\eta^-\right)\Gamma^+\right]^2 = \left(\eta^+ - \tilde\eta^+\right)\left(\eta^- - \tilde\eta^-\right)\mathbb{1}$$

so that Eq. (12) implies, after acting on it from the left with $[(\eta^+ - \tilde\eta^+)\Gamma^+ + (\eta^- - \tilde\eta^-)\Gamma^+]$:

$$\left(\eta^+ - \tilde\eta^+\right)\left(\eta^- - \tilde\eta^-\right) = 0$$

which in turn implies that $\eta^+ = \tilde\eta^+$ *or* $\eta^- = \tilde\eta^-$. We will show that in fact *both* must hold.

Assume that $\eta^+ = \tilde\eta^+$ holds. Then Eq. (11) implies

$$\eta^+\eta^- = \eta^+\tilde\eta^-$$

and as $\eta^+ \neq 0$ we have that $\eta^- = \tilde\eta^-$. The other way around works similarly and so we conclude that

$$\left(\eta^+, \eta^-\right) = \left(\tilde\eta^+, \tilde\eta^-\right)$$

so that really there is only one pair. □

1.5.15. CLAIM. If for given $E \in \mathbb{R}$, $k_2 \in S^1$ and $u \in \mathbb{C}^N \setminus \{0\}$ the equation

$$\left(\left\|b^{0\perp}(k_2)\right\|\Gamma^\perp + \eta^+(\lambda, k_2)\Gamma^+ + \eta^-(\lambda, k_2)\Gamma^-\right) u = Eu \tag{13}$$

has *two* solutions (λ_1, λ_2) such that $|\lambda_1| < 1$ and $|\lambda_2| < 1$ then it must be that $E = \pm\left\|b^{0\perp}(k_2)\right\|$.

PROOF. Assume $E \neq \pm\left\|b^{0\perp}(k_2)\right\|$. Then using 1.5.14 it follows that there is a *single* pair (η^+, η^-) such that Eq. (13) holds, which we label as (ξ^+, ξ^-):

$$\left(\left\|b^{0\perp}(k_2)\right\|\Gamma^\perp + \xi^+\Gamma^+ + \xi^-\Gamma^-\right) u = Eu$$

and we label ξ_j the corresponding vector defined by (ξ^+, ξ^-):

$$\begin{aligned}
\xi_j &= \frac{1}{N}\mathrm{Tr}\left\{\left[\left\|b^{0\perp}(k_2)\right\|\Gamma^\perp + \xi^+\Gamma^+ + \xi^-\Gamma^-\right]\Gamma_j\right\} \\
&= \left\|b^{0\perp}(k_2)\right\|\frac{1}{N}\mathrm{Tr}\left[\Gamma^\perp\Gamma_j\right] + \xi^+\frac{1}{N}\mathrm{Tr}\left[\Gamma^+\Gamma_j\right] + \xi^-\frac{1}{N}\mathrm{Tr}\left[\Gamma^-\Gamma_j\right] \\
&= \left\|b^{0\perp}(k_2)\right\|\frac{1}{N}\mathrm{Tr}\left[\hat e_i^\perp\Gamma_i\Gamma_j\right] + \xi^+\frac{1}{N}\mathrm{Tr}\left[\frac{1}{2}\left(\hat e_i^r\Gamma_i + i\hat e_i^\nu\Gamma_i\right)\Gamma_j\right] + \xi^-\frac{1}{N}\mathrm{Tr}\left[\frac{1}{2}\left(\hat e_i^r\Gamma_i - i\hat e_i^\nu\Gamma_i\right)\Gamma_j\right] \\
&= \left\|b^{0\perp}(k_2)\right\|\hat e_i^\perp\underbrace{\frac{1}{N}\mathrm{Tr}\left[\Gamma_i\Gamma_j\right]}_{\delta_{ij}} + \frac{1}{2}\xi^+\left(\hat e_i^r\frac{1}{N}\mathrm{Tr}\left[\Gamma_i\Gamma_j\right] + i\hat e_i^\nu\frac{1}{N}\mathrm{Tr}\left[\Gamma_i\Gamma_j\right]\right) + \frac{1}{2}\xi^-\left(\hat e_i^r\frac{1}{N}\mathrm{Tr}\left[\Gamma_i\Gamma_j\right] - i\hat e_i^\nu\frac{1}{N}\mathrm{Tr}\left[\Gamma_i\Gamma_j\right]\right) \\
&= \left\|b^{0\perp}(k_2)\right\|\hat e_j^\perp + \xi^+\underbrace{\frac{1}{2}\left(\hat e_j^r + i\hat e_j^\nu\right)}_{\hat e^+} + \xi^-\underbrace{\frac{1}{2}\left(\hat e_j^r - i\hat e_j^\nu\right)}_{\hat e^-}
\end{aligned}$$

Now we would like to find out what is $\lambda \in \mathbb{C}$ corresponding to this pair (ξ^+, ξ^-) and so we have to solve the following equation for λ (k_2 is fixed an suppressed):

$$\xi_j \overset{!}{=} \eta_j \equiv b_j^0 + b_j\lambda^{-1} + \overline{b_j}\lambda$$

which implies

$$\overline{b_j}\lambda^2 + \left(b_j^0 - \xi_j\right)\lambda + b_j = 0$$

and now using Vieta's formula (which holds for quadratic equations over $\mathbb{C}$ as well) we have that

$$\lambda_1\lambda_2 = \frac{b_j}{\overline{(b_j)}}$$

Taking the absolute value of this equation we find that

$$|\lambda_1||\lambda_2| = 1$$

which implies that $|\lambda_1| = \frac{1}{|\lambda_2|}$. If $|\lambda_1| < 1$ that means that $|\lambda_2| > 1$ which contradicts the initial hypothesis and likewise for $|\lambda_2| < 1$ we have $|\lambda_1| > 1$, again, a contradiction. So it must be that $E = \pm\left\|b^{0\perp}(k_2)\right\|$, as desired. □

1.5.16. CLAIM. The edge system $H^\sharp(k_2)$ has a decaying solution at some k_2 if and only if the ellipse traced by $h^\parallel(k)$ (k_2 is fixed and k_1 is the parameter along the ellipse) encloses the origin of $\mathbb{R}^m$. If this condition is met, then the energy of that edge state is $E^\sharp(k_2) = \pm\left\|b^{0\perp}(k_2)\right\|$.

PROOF. From 1.4.2, as the first step, we are looking for a solution $\psi^\sharp \in l^2(\mathbb{Z}; \mathbb{C}^N)$ to the equations

$$b_j^0\Gamma_j\psi_n^\sharp + b_j\Gamma_j\psi_{n-1}^\sharp + \overline{b_j}\Gamma_j\psi_{n+1}^\sharp = E^\sharp\psi_n^\sharp \quad \forall n \in \mathbb{N}$$

together with the boundary condition that $\psi_0^\sharp \overset{!}{=} 0$. Make an Ansatz of the form $\psi_n^\sharp = \sum_j u_j\lambda_j^n$ (finite sum) to obtain

$$\begin{aligned} b_j^0\Gamma_j\left(\sum_l u_l\lambda_l^n\right) + b_j\Gamma_j\left(\sum_l u_l\lambda_l^{n-1}\right) + \overline{b_j}\Gamma_j\left(\sum_l u_l\lambda_l^{n+1}\right) &= E^\sharp\left(\sum_l u_l\lambda_l^n\right) \\ \sum_l\left(b_j^0\Gamma_j u_l\lambda_l^n + b_j\Gamma_j u_l\lambda_l^{n-1} + \overline{b_j}\Gamma_j u_l\lambda_l^{n+1}\right) &= \sum_l E^\sharp u_l\lambda_l^n \end{aligned}$$

so that (omitting l for brevity, but the following holds for each l):

$$b_j^0\Gamma_j u\lambda^n + b_j\Gamma_j u\lambda^{n-1} + \overline{b_j}\Gamma_j u\lambda^{n+1} = E^\sharp u\lambda^n \tag{14}$$

This Ansatz makes sense if $|\lambda| < 1$ as then our solution indeed decays into the bulk. This can be thought of as a generalized Bloch solution with $\lambda = \exp(ik_1)$ where now $\Im(k_1) > 0$. From Eq. (14) we have

$$\lambda\left\{\left[b^0 + b\lambda^{-1} + \overline{b}\lambda^1\right]\cdot\Gamma - E^\sharp\mathbb{1}\right\}u = 0 \tag{15}$$

Thus we have:

$$\lambda\left[\eta_j(\lambda)\Gamma_j - E^\sharp\mathbb{1}\right]u = 0 \tag{16}$$

and so using Eq. (8) we have

$$\lambda\left[\left\|b^{0\perp}(k_2)\right\|\Gamma^\perp + \eta^+(\lambda, k_2)\Gamma^+ + \eta^-(\lambda, k_2)\Gamma^- - E^\sharp\mathbb{1}\right]u = 0 \tag{17}$$

which implies (using the same procedure as in 1.5.14) the equation

$$\lambda^2\left[\eta^+(\lambda, k_2)\eta^-(\lambda, k_2) + \left\|b^{0\perp}(k_2)\right\|^2 - \left(E^\sharp\right)^2\right] = 0 \tag{18}$$

Note that contrary to how the eigenvalue equation is usually solved ($E^\sharp$ would be the unknown), we consider the unknown in Eq. (18) to be λ while k_2 and $E^\sharp$ are fixed.

1.5.17. CLAIM. $\overline{\eta_j(\lambda)} = \eta_j\left(\frac{1}{\overline{\lambda}}\right)$.

PROOF.

$$\begin{aligned}\overline{\eta_j(\lambda)} &\equiv \overline{\lambda^{-1}b_j+\lambda\overline{b_j}+b_j^0}\\ &= \overline{\lambda^{-1}}\,\overline{b_j}+\overline{\lambda}b_j+\overline{b_j^0}\\ &= \left(\frac{1}{\overline{\lambda}}\right)^{-1}b_j+\frac{1}{\overline{\lambda}}\overline{b_j}+\overline{b_j^0}\\ &\equiv \eta_j\left(\frac{1}{\overline{\lambda}}\right)\end{aligned}$$

□

1.5.18. CLAIM. If $\lambda\in\mathbb{C}\backslash\{0\}$ is a solution of Eq. (18) then so is $\frac{1}{(\overline{\lambda})}$.

PROOF. We assume Eq. (18) holds for some given $\lambda\in\mathbb{C}$. If this equation is true, then its complex conjugate should also be true:

$$\begin{aligned}\overline{\left\{\lambda^2\left\{\sum_j\left[\eta_j(\lambda)\right]^2\right\}\right\}} &= \overline{\left\{\lambda^2\left(E^\sharp\right)^2\right\}}\\ \left(\overline{\lambda}\right)^2\left\{\sum_j\left(\overline{\eta_j(\lambda)}\right)^2\right\} &= \left(\overline{\lambda}\right)^2\left(E^\sharp\right)^2\\ \left(\overline{\lambda}\right)^2\left\{\sum_j\left(\eta_j\left(\frac{1}{\overline{\lambda}}\right)\right)^2\right\} &= \left(\overline{\lambda}\right)^2\left(E^\sharp\right)^2\\ \left(\frac{1}{\overline{\lambda}}\right)^2\left\{\sum_j\left(\eta_j\left(\frac{1}{\overline{\lambda}}\right)\right)^2\right\} &= \left(\frac{1}{\overline{\lambda}}\right)^2\left(E^\sharp\right)^2\end{aligned}$$

which is just the original equation with λ replaced by $\frac{1}{\overline{\lambda}}$, so that the claim follows. □

Thus we conclude that for every solution of Eq. (18) within the unit circle, $\lambda = Re^{i\varphi}$ with $R<1$, there is a solution outside the unit circle $\frac{1}{\overline{\lambda}}=\frac{1}{Re^{-i\varphi}}=R^{-1}e^{i\varphi}$ $(R^{-1}>1)$. As a result, only half the solutions are decaying into the bulk and other other solutions correspond to a mirrored chain, defined on $-\mathbb{N}$.

1.5.19. CLAIM. Eq. (18) is an equation of order 4 in λ.

PROOF. We have

$$\begin{aligned}\lambda^2\eta^+\eta^- &= \lambda^2\frac{1}{2}\left(\eta^r-i\eta^\nu\right)\frac{1}{2}\left(\eta^r+i\eta^\nu\right)\\ &= \lambda^2\frac{1}{4}\left[\left(\eta^r\right)^2+\left(\eta^\nu\right)^2\right]\\ &= \lambda^2\frac{1}{4}\eta_j^{\parallel}\eta_j^{\parallel}\\ &= \left(b_j^{0\parallel}\lambda+b_j+\overline{b_j}\lambda^2\right)\left(b_j^{0\parallel}\lambda+b_j+\overline{b_j}\lambda^2\right)\end{aligned}$$

The other terms in the equation are all of order λ^2. □

Thus by the fundamental theorem of algebra Eq. (18) has 4 solutions in the complex plane. In light of 1.5.18, we have at most 2 solutions within the unit circle. Call these two solutions λ_1 and λ_2.

So the most general form of the edge wave function which is decaying is

$$\psi_n^\sharp=\sum_{i\in J_2}u_i\left(\lambda_i\right)^n$$

where u_i is a null-vector of the matrix $\lambda_i\left[\sum_j \eta_j(\lambda_i)\Gamma_j - E^\sharp \mathbb{1}\right]$.

Following the next step of 1.4.2, we need to employ the boundary condition and so we set $\psi_0^\sharp \overset{!}{=} 0$ which implies that $u_1 = -u_2$ and thus $\lambda_1\left[\sum_j \eta_j(\lambda_1)\Gamma_j - E^\sharp \mathbb{1}\right]$ and $\lambda_2\left[\sum_j \eta_j(\lambda_2)\Gamma_j - E^\sharp \mathbb{1}\right]$ share a null-vector. But that means that for a fixed $E^\sharp$ and k_2, the equation $\eta_j(\lambda)\Gamma_j u_1 = E^\sharp u_1$ has two solutions λ_1 and λ_2 within the unit circle, so that we may use 1.5.15 to conclude that if an edge state exists, then $E^\sharp(k_2) = \pm\left\|b^{0\perp}(k_2)\right\|$, showing the last part of our claim.

Furthermore, we have $\begin{cases}\left[\left\|b^{0\perp}\right\|\Gamma^\perp + \eta_1^+\Gamma^+ + \eta_1^-\Gamma^-\right]u_1 & = E^\sharp u_1 \\ \left[\left\|b^{0\perp}\right\|\Gamma^\perp + \eta_2^+\Gamma^+ + \eta_2^-\Gamma^-\right]u_1 & = E^\sharp u_1\end{cases}$ where we have abbreviated $\eta_i^\pm \equiv \eta^\pm(\lambda_i)$. We can now compute the anti-commutator:

$$\left\{\left\|b^{0\perp}\right\|\Gamma^\perp + \eta_1^+\Gamma^+ + \eta_1^-\Gamma^-, \left\|b^{0\perp}\right\|\Gamma^\perp + \eta_2^+\Gamma^+ + \eta_2^-\Gamma^-\right\} = \left[\left\|b^{0\perp}\right\|^2 + \eta_2^+\eta_1^- + \eta_2^-\eta_1^+\right]\mathbb{1}$$

yet we also have

$$\left\{\left\|b^{0\perp}\right\|\Gamma^\perp + \eta_1^+\Gamma^+ + \eta_1^-\Gamma^-, \left\|b^{0\perp}\right\|\Gamma^\perp + \eta_2^+\Gamma^+ + \eta_2^-\Gamma^-\right\}u = \left(E^\sharp\right)^2 u$$

so that we may conclude

$$\begin{cases}\eta^+(\lambda_1)\eta^-(\lambda_1) & = 0 \\ \eta^+(\lambda_2)\eta^-(\lambda_2) & = 0 \\ \eta^+(\lambda_2)\eta^-(\lambda_1) + \eta^-(\lambda_2)\eta^+(\lambda_1) & = 0\end{cases}$$

As a result, it appears that either $\eta^+(\lambda)$ has the two roots λ_1 and λ_2, or $\eta^-(\lambda)$ has two roots λ_1 and λ_2. But the third equation excludes the possibility that η^+ and η^- each have only one root λ_1 and λ_2 respectively.

We now proceed to show that the existence of the edge state at k_2 means the ellipse traced by $h^\parallel(k)\big|_{k_2}$ encloses the origin of $\mathbb{R}^m$:

(1) The number of zeros minus the number of poles of η^+ within the unit circle is given by $\frac{1}{2\pi i}\oint_{z\in S^1\subset\mathbb{C}}\frac{\eta^{+'}(z)}{\eta^+(z)}dz$.

(2) But η^+ has one pole (at $\lambda = 0$), and so, to have two zeros, we must have $\frac{1}{2\pi i}\oint\frac{\eta^{+'}(z)}{\eta^+(z)}dz \overset{!}{=} 1$.

(3) But $\frac{1}{2\pi i}\oint\frac{\eta^{+'}(z)}{\eta^+(z)}dz \overset{!}{=} 1$ iff $\eta^+(e^{ik})$ wraps around the origin counterclockwise once, for $k \in [0, 2\pi]$.

(4) If, however, $\eta^+(e^{ik})$ wraps around the origin clockwise, $\frac{1}{2\pi i}\oint\frac{\eta^{+'}(z)}{\eta^+(z)}dz = -1$ and so the number of zeros is 0 for η^+ (thus no edge states "from" η^+). But then, that means that $\eta^-(e^{ik})$ wraps around the origin counterclockwise (because η^- is the conjugate of η^+ when evaluated on the unit circle) and so $\frac{1}{2\pi i}\oint\frac{\eta^{-'}(z)}{\eta^-(z)}dz = 1$ and so η^- has two zeros, and thus, gives rise to an edge states.

(5) Observe that both $\eta^\pm(e^{ik_1})$ trace the same ellipse in $\mathbb{C}$ which $h^\parallel(k)\big|_{k_y}$ traces in some skewed plane of $\mathbb{R}^m$. So that if $h^\parallel(k)\big|_{k_y}$ wraps around the origin (for fixed k_2 and varying k_1) then either $\eta^+(\lambda)$ or $\eta^-(\lambda)$ has two zeros within the unit circle.

□

1.5.20. Claim. If $\eta^+(\lambda)$ has two roots λ_1 and λ_2 within the unit circle, then either $\eta^-(\lambda_1) \neq \eta^-(\lambda_2)$ or the ellipse lies on a straight line. The same holds when $+$ and $-$ are interchanged.

PROOF. Assume that $\eta^+(\lambda_1) = \eta^+(\lambda_2) = 0$. Recall that

$$\begin{aligned}\eta^+(\lambda) &= \eta^r(\lambda) - i\eta^\nu(\lambda)\\ &= \eta_j(\lambda)\left(e^r_j - ie^\nu_j\right)\\ &= \left(b^0 + b\lambda^{-1} + \overline{b}\lambda\right)\cdot\left(\hat{e}^r - i\hat{e}^\nu\right)\\ &= \left[b^0 + \left(\Re\{b\} + i\Im(b)\right)\lambda^{-1} + \left(\Re\{b\} - i\Im(b)\right)\lambda\right]\cdot\left(\hat{e}^r - i\hat{e}^\nu\right)\\ &= b^0\cdot\hat{e}^r - ib^0\cdot\hat{e}^\nu + \left(|\Re\{b\}| + i\Im(b)\cdot\hat{e}^r + \Im(b)\cdot\hat{e}^\nu\right)\lambda^{-1} + \left(|\Re\{b\}| - i\Im(b)\cdot\hat{e}^r - \Im(b)\cdot\hat{e}^\nu\right)\lambda\\ &= b^{0r} - ib^{0\nu} + \left(b^r + ib^{ir} + b^{i\nu}\right)\lambda^{-1} + \left(b^r - ib^{ir} - b^{i\nu}\right)\lambda\end{aligned}$$

and so if $\eta^+(\lambda)$ has two roots λ_1 and λ_2 it follows from Vieta's formula that

$$\lambda_1\lambda_2 = \frac{b^r + ib^{ir} + b^{i\nu}}{b^r - ib^{ir} - b^{i\nu}}$$

Now also compute

$$\begin{aligned}\eta^-(\lambda) &= \eta^r(\lambda) + i\eta^\nu(\lambda)\\ &= \eta_j(\lambda)\left(e^r_j + ie^\nu_j\right)\\ &= \left(b^0 + b\lambda^{-1} + \overline{b}\lambda\right)\cdot\left(\hat{e}^r + i\hat{e}^\nu\right)\\ &= \left[b^0 + \left(\Re\{b\} + i\Im(b)\right)\lambda^{-1} + \left(\Re\{b\} - i\Im(b)\right)\lambda\right]\cdot\left(\hat{e}^r + i\hat{e}^\nu\right)\\ &= b^0\cdot\hat{e}^r + ib^0\cdot\hat{e}^\nu + \left(|\Re\{b\}| + i\Im(b)\cdot\hat{e}^r - \Im(b)\cdot\hat{e}^\nu\right)\lambda^{-1} + \left(|\Re\{b\}| - i\Im(b)\cdot\hat{e}^r + \Im(b)\cdot\hat{e}^\nu\right)\lambda\\ &= b^{0r} + ib^{0\nu} + \left(b^r + ib^{ir} - b^{i\nu}\right)\lambda^{-1} + \left(b^r - ib^{ir} + b^{i\nu}\right)\lambda\end{aligned}$$

and assume that $\eta^-(\lambda_1) = \eta^-(\lambda_2)$, which implies that

$$\begin{aligned}\left(b^r + ib^{ir} - b^{i\nu}\right)\lambda_1^{-1} + \left(b^r - ib^{ir} + b^{i\nu}\right)\lambda_1 &= \left(b^r + ib^{ir} - b^{i\nu}\right)\lambda_2^{-1} + \left(b^r - ib^{ir} + b^{i\nu}\right)\lambda_2\\ \left(b^r - ib^{ir} + b^{i\nu}\right)\left(\lambda_1 - \lambda_2\right) &= \left(b^r + ib^{ir} - b^{i\nu}\right)\underbrace{\left(\lambda_2^{-1} - \lambda_1^{-1}\right)}_{\frac{\lambda_1-\lambda_2}{\lambda_1\lambda_2}}\\ \lambda_1\lambda_2 &= \frac{b^r + ib^{ir} - b^{i\nu}}{b^r - ib^{ir} + b^{i\nu}}\end{aligned}$$

Thus we obtain the constraint

$$\begin{aligned}\frac{b^r + ib^{ir} - b^{i\nu}}{b^r - ib^{ir} + b^{i\nu}} &= \frac{b^r + ib^{ir} + b^{i\nu}}{b^r - ib^{ir} - b^{i\nu}}\\ \left(b^r + ib^{ir} - b^{i\nu}\right)\left(b^r - ib^{ir} - b^{i\nu}\right) &= \left(b^r + ib^{ir} + b^{i\nu}\right)\left(b^r - ib^{ir} + b^{i\nu}\right)\\ \left(b^r - b^{i\nu}\right)^2 + \left(b^{ir}\right)^2 &= \left(b^r + b^{i\nu}\right)^2 + \left(b^{ir}\right)^2\\ b^r b^{i\nu} &= 0\end{aligned}$$

Which geometrically means that the ellipse reduces to a straight line (either along $\hat{e}^r$ or along $\hat{e}^\nu$).

The case with $+$ and $-$ interchanged gives the same constraint and thus leads to the same conclusion. □

1.5.21. CLAIM. When $N = 2$ then the sign of $E^\sharp(k_2)$ is given by

$$\boxed{E^\sharp(k_2) = \left[\left(\hat{e}^r \times \hat{e}^i\right)\cdot\hat{e}^\perp\right]\left\|b^{0\perp}(k_2)\right\|}$$

PROOF. Let $k_2 \in S^1$ be given. *Assume that for k_2, the ellipse does not lie on a straight line.*

First note that we may adiabatically (without closing the gap) apply a unitary transformation on $H^B(k)$, continuously in k, such that $\hat{e}^r = \hat{e}_1$, $\hat{e}^\nu = \hat{e}_2$ and $\hat{e}^\perp = \hat{e}_3$. Rotations will not change the magnitude of the vector $\|h(k)\|$ and so will not close the gap, and clearly rotations are continuous. This is exactly possible because $\hat{e}^\nu$ has an *unspecified* sign, and so we can make sure that $(\hat{e}^r, \hat{e}^\nu, \hat{e}^\perp)$ has right-handed orientation just as $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$. As a result, we will have $\hat{e}^i = \pm \hat{e}_2$ and so

$$\mathrm{sgn}\left(b^{i\nu}\right) = \mathrm{sgn}\left(\left\langle b^i, \hat{e}_2 \right\rangle\right) = \pm 1$$

The sign of $b^{i\nu}$ thus matches the sign of $\left[\left(\hat{e}^r \times \hat{e}^i\right) \cdot \hat{e}^\perp\right]$. So if $\left[\left(\hat{e}^r \times \hat{e}^i\right) \cdot \hat{e}^\perp\right] = +1$ then $\mathrm{sign}\left(b^{i\nu}\right) = +1$ and so $h^-(k)|_{k_y}$ goes counter-clockwise in $\mathbb{C}$ whereas if $\left[\left(\hat{e}^r \times \hat{e}^i\right) \cdot \hat{e}^\perp\right] = -1$ then $\mathrm{sign}\left(b^{i\nu}\right) = -1$ then it is $h^+(k)|_{k_y}$ that goes counter-clockwise in $\mathbb{C}$. This can be seen from

$$\begin{aligned} h^\pm(k)\big|_{k_2} &= h^r(k) \mp i h^\nu(k) \\ &= b^{0r} + 2b^r \cos(k_1) + 2b^{ir}\sin(k_1) \mp i\left[b^{0\nu} + 2b^{i\nu}\sin(k_1)\right] \\ &= \left(b^{0r} \mp i b^{0\nu}\right) + 2b^r\cos(k_1) + 2\left(b^{ir} \mp i b^{i\nu}\right)\sin(k_1) \end{aligned}$$

As we know from 1.5.16, the one of h^+ or h^- which goes counter-clockwise is the one of η^+ or η^- that has the two zeros within the unit circle (if it contains the origin). In conclusion:

- $\left[\left(\hat{e}^r \times \hat{e}^i\right) \cdot \hat{e}^\perp\right] = +1$ means η^- is the one that might have two zeros within the unit circle.
- $\left[\left(\hat{e}^r \times \hat{e}^i\right) \cdot \hat{e}^\perp\right] = -1$ means η^+ is the one that might have two zeros within the unit circle.

Assuming we have these relations, we may work with an explicit form of the three gamma matrices:

$$\Gamma^\perp = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\Gamma^\perp - \mathbb{1} = \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix}$$

$$\Gamma^\perp + \mathbb{1} = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\Gamma^r = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\Gamma^\nu = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\Gamma^\pm \equiv \frac{1}{2}\left(\Gamma^r \pm i\Gamma^\nu\right) = \frac{1}{2}\left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \pm \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}\right) = \begin{cases} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} & + \\ \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} & - \end{cases}$$

Next, divide the analysis into two cases:

(1) Assume that it is η^+ that has the two roots (rather than η^-) within the unit circle. So in this case $\left[\left(\hat{e}^r \times \hat{e}^i\right) \cdot \hat{e}^\perp\right] = -1$.

From Eq. (17) we have that

$$\begin{cases} \left[\left\|b^{0\perp}(k_2)\right\|\Gamma^\perp + \eta^-(\lambda_1, k_2)\Gamma^- - E^\sharp\mathbb{1}\right]u &= 0 \\ \left[\left\|b^{0\perp}(k_2)\right\|\Gamma^\perp + \eta^-(\lambda_2, k_2)\Gamma^- - E^\sharp\mathbb{1}\right]u &= 0 \end{cases}$$

Now we have two sub-cases:

(a) $E^\sharp = +\left\|b^{0\perp}(k_2)\right\|$:

In this case we have

$$\begin{cases} \left[\left\|b^{0\perp}(k_2)\right\|\left(\Gamma^\perp - \mathbb{1}\right) + \eta^-(\lambda_1, k_2)\Gamma^-\right]u &= 0 \\ \left[\left\|b^{0\perp}(k_2)\right\|\left(\Gamma^\perp - \mathbb{1}\right) + \eta^-(\lambda_2, k_2)\Gamma^-\right]u &= 0 \end{cases}$$

which translates into

$$\begin{cases} \left\{\left\|b^{0\perp}(k_2)\right\|\begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix} + \eta^-(\lambda_1, k_2)\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}\right\}u &= 0 \\ \left\{\left\|b^{0\perp}(k_2)\right\|\begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix} + \eta^-(\lambda_2, k_2)\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}\right\}u &= 0 \end{cases}$$

from which we learn that

$$\begin{cases}\eta^{-}(\lambda_1,k_2)u^{(1)}-2\|b^{0\perp}(k_2)\|u^{(2)}=0\\ \|b^{0\perp}(k_2)\|\eta^{-}(\lambda_2,k_2)u^{(1)}-2\|b^{0\perp}(k_2)\|u^{(2)}=0\end{cases}$$

or that

$$\begin{cases}u &= \begin{bmatrix}\left(\frac{2\|b^{0\perp}(k_2)\|}{\eta^{-}(\lambda_1,k_2)}\right)\\ 1\end{bmatrix}\\ u &= \begin{bmatrix}\left(\frac{2\|b^{0\perp}(k_2)\|}{\eta^{-}(\lambda_2,k_2)}\right)\\ 1\end{bmatrix}\end{cases}$$

But then it must be that $\eta^{-}(\lambda_1,k_2)=\eta^{-}(\lambda_2,k_2)$, which, as we learnt in 1.5.20 is not possible because *by hypothesis* the ellipse is not on a straight line, so we must conclude this case is not possible.

(b) $E^{\sharp}=-\|b^{0\perp}(k_2)\|$:
In this case we have

$$\begin{cases}\left[\|b^{0\perp}(k_2)\|\left(\Gamma^{\perp}+\mathbb{1}\right)+\eta^{-}(\lambda_1,k_2)\Gamma^{-}\right]u &=0\\ \left[\|b^{0\perp}(k_2)\|\left(\Gamma^{\perp}+\mathbb{1}\right)+\eta^{-}(\lambda_1,k_2)\Gamma^{-}\right]u &=0\end{cases}$$

which translates into

$$\begin{cases}\left\{\|b^{0\perp}(k_2)\|\begin{bmatrix}2&0\\0&0\end{bmatrix}+\eta^{-}(\lambda_1,k_2)\begin{bmatrix}0&0\\1&0\end{bmatrix}\right\}u &=0\\ \left\{\|b^{0\perp}(k_2)\|\begin{bmatrix}2&0\\0&0\end{bmatrix}+\eta^{-}(\lambda_2,k_2)\begin{bmatrix}0&0\\1&0\end{bmatrix}\right\}u &=0\end{cases}$$

from which we learn that

$$\begin{cases}\begin{cases}2\|b^{0\perp}(k_2)\|u^{(1)} &=0\\ \eta^{-}(\lambda_1,k_2)u^{(1)} &=0\end{cases}\\ \begin{cases}2\|b^{0\perp}(k_2)\|u^{(1)} &=0\\ \eta^{-}(\lambda_2,k_2)u^{(1)} &=0\end{cases}\end{cases}$$

or that

$$u=\begin{bmatrix}0\\1\end{bmatrix}$$

which leads to no contradictions.

We have thus shown that

$$\left[\left(\hat{e}^{r}\times\hat{e}^{i}\right)\cdot\hat{e}^{\perp}\right]=-1 \quad \boxed{\Longrightarrow} \quad E^{\sharp}=-\left\|b^{0\perp}(k_2)\right\|$$

(2) The other case leads to the complementary conclusion, namely, if $\eta^{-}(\lambda)$ has two roots within the unit circle then $\left[\left(\hat{e}^{r}\times\hat{e}^{i}\right)\cdot\hat{e}^{\perp}\right]=+1$, and we will find that to avoid contradictions it must be that $E^{\sharp}=+\|b^{0\perp}(k_2)\|$.

Thus when the ellipse does not lie on a straight line, we have proven the formula

$$E^{\sharp}(k_2)=\left[\left(\hat{e}^{r}\times\hat{e}^{i}\right)\cdot\hat{e}^{\perp}\right]\left\|b^{0\perp}(k_2)\right\|$$

Now, assuming that $E^{\sharp}(k_2)$ is continuous, we can take the limit $\hat{e}^{i}\to\pm\hat{e}^{r}$ (then the ellipse *is* on a straight line). In this limit, $E^{\sharp}(k_2)\to 0$. So it must be that when the ellipse lies on a straight line, $E^{\sharp}(k_2)=0$. □

1.5.22. CLAIM. If $N=4$ and there is an edge state at a given k_2 then there are in fact at least two edge states corresponding to both $E^{\sharp}(k_2)=+\|b^{0\perp}(k_2)\|$ and $E^{\sharp}(k_2)=-\|b^{0\perp}(k_2)\|$.

PROOF. Without loss of generality, assume that η^{+} has two zeros within the unit circle (the case for η^{-} proceeds analogously). Then the eigenvalue equation, depending on the sign of the energy, is either:

$$\begin{cases}\left[\|b^{0\perp}(k_2)\|\left(\Gamma^{\perp}-\mathbb{1}\right)+\eta^{-}(\lambda_1,k_2)\Gamma^{-}\right]u &=0\\ \left[\|b^{0\perp}(k_2)\|\left(\Gamma^{\perp}-\mathbb{1}\right)+\eta^{-}(\lambda_2,k_2)\Gamma^{-}\right]u &=0\end{cases} \quad \text{for} \quad E^{\sharp}(k_2)=+\left\|b^{0\perp}(k_2)\right\|$$

with the same u for both equations, or

$$\begin{cases} \left[\left\|b^{0\perp}(k_2)\right\|\left(\Gamma^\perp + \mathbb{1}\right) + \eta^-(\lambda_1, k_2)\Gamma^-\right] v &= 0 \\ \left[\left\|b^{0\perp}(k_2)\right\|\left(\Gamma^\perp + \mathbb{1}\right) + \eta^-(\lambda_2, k_2)\Gamma^-\right] v &= 0 \end{cases} \quad \text{for} \quad E^\sharp(k_2) = -\left\|b^{0\perp}(k_2)\right\|$$

with the same v for both equations. Our goal is to show that both duos of equations are possible simultaneously with u and v linearly independent (whereas in 1.5.21 only one was possible, which allowed us to determine the sign of the energy of the edge state).

For the case when $N = 4$, again we may work without loss of generality with a particular representation of the Gamma matrices so that:

$$\Gamma^\perp = \sigma_3 \otimes \sigma_0 = \mathrm{diag}(1, 1, -1, -1)$$

$$\Gamma^r = \sigma_1 \otimes \sigma_0 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

and

$$\Gamma^\nu = \sigma_2 \otimes \sigma_3 = \begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{bmatrix}$$

from which we then have

$$\Gamma^\perp - \mathbb{1} = \mathrm{diag}(0, 0, -2, -2)$$
$$\Gamma^\perp + \mathbb{1} = \mathrm{diag}(2, 2, 0, 0)$$

and

$$\Gamma^- = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

We find then the following two equations:

$$\begin{cases} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \eta^-(\lambda_1, k_2) \\ \eta^-(\lambda_1, k_2) & 0 & -2\left\|b^{0\perp}(k_2)\right\| & 0 \\ 0 & 0 & 0 & -2\left\|b^{0\perp}(k_2)\right\| \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = 0 \\ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \eta^-(\lambda_2, k_2) \\ \eta^-(\lambda_2, k_2) & 0 & -2\left\|b^{0\perp}(k_2)\right\| & 0 \\ 0 & 0 & 0 & -2\left\|b^{0\perp}(k_2)\right\| \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = 0 \end{cases} \quad \text{for} \quad E^\sharp(k_2) = +\left\|b^{0\perp}(k_2)\right\|$$

and

$$\begin{cases} \begin{bmatrix} 2\left\|b^{0\perp}(k_2)\right\| & 0 & 0 & 0 \\ 0 & 2\left\|b^{0\perp}(k_2)\right\| & 0 & \eta^-(\lambda_1, k_2) \\ \eta^-(\lambda_1, k_2) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = 0 \\ \begin{bmatrix} 2\left\|b^{0\perp}(k_2)\right\| & 0 & 0 & 0 \\ 0 & 2\left\|b^{0\perp}(k_2)\right\| & 0 & \eta^-(\lambda_2, k_2) \\ \eta^-(\lambda_2, k_2) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = 0 \end{cases} \quad \text{for} \quad E^\sharp(k_2) = -\left\|b^{0\perp}(k_2)\right\|$$

Then it's easy to verify that both duos of equations are possible to satisfy, the first with $u = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ and the second with $v = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, both of which are linearly independent and thus correspond to different solutions, each of which has an opposite sign of energy. What's more, neither of these solutions are obstructed by a requirement of the form $\eta^-(\lambda_1, k_2) = \eta^-(\lambda_2, k_2)$. □

1.6. The Edge Indices

Let $\{ E_i^\#(k_2) \}_{i \in I}$ denote the discrete spectrum of $H^\#(k_2)$. Assuming the following set is of finite order, we define:

$$\mathcal{CROSS} := \left\{ (k_2, i) \in [0, 2\pi) \times I \;\middle|\; E_i^\#(k_2) = E_F \wedge \left(E_i^\sharp\right)'(k_2) \neq 0 \right\}$$

and we assume further that $\nexists (k_2, i) \in [0, 2\pi) \times I$ such that $\left(E_i^\sharp\right)'(k_2) = 0$. Under these assumptions, $\mathcal{CROSS}$ contains all the points where the edge energy crosses the Fermi energy. We define two quantities:

1.6.1. DEFINITION. The edge-quantum-Hall-conductance-index:

$$\boxed{\mathcal{I}^\sharp_{QH}\left(H^\sharp\right) := -\sum_{(k_2,i)\in\mathcal{CROSS}} \frac{\left(E_i^\sharp\right)'(k_2)}{\left|\left(E_i^\sharp\right)'(k_2)\right|}} \tag{19}$$

1.6.2. DEFINITION. The edge-Kane-Mele-index:

$$\boxed{\mathcal{I}^\sharp_{KM}\left(H^\sharp\right) := \frac{1}{2}\left|\mathcal{CROSS}\right| \mod 2} \tag{20}$$

is defined only for time-reversal symmetric Hamiltonians due to the fact that for such Hamiltonians we have necessarily that $|\mathcal{CROSS}| \in 2\mathbb{N}$ due to 1.2.8.

1.6.3. REMARK. We may choose to take an arbitrary fiducial line $E_F(k_2)$ instead of a constant E_F, such that $E_F'(k_2) \neq 0$. Then, in general we need to replace in all the formulas above

$$\left(E_i^\sharp\right)'(k_2) \quad \mapsto \quad \frac{\left(E_i^\sharp\right)'(k_2) - E_F'(k_2)}{1 + \left(E_i^\sharp\right)'(k_2)\, E_F'(k_2)}$$

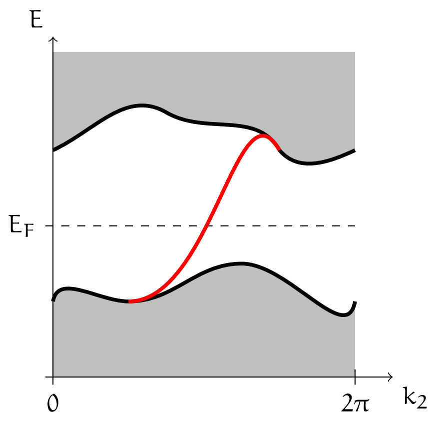

FIGURE 1.6.1. The bulk spectrum is in the shaded area, and the discrete edge spectrum is in red. In this configuration, $\mathcal{I}^\sharp_{QH}\left(H^\sharp\right) = -1$ because there is one crossing point with positive slope.

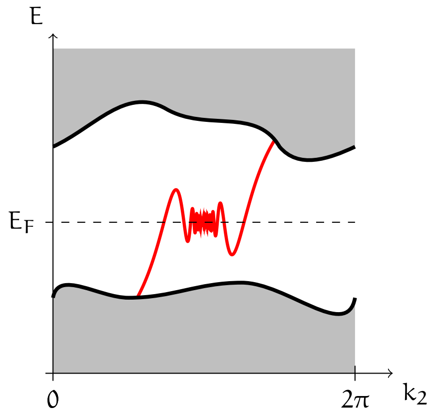

FIGURE 1.6.2. In this picture, the edge discrete spectrum has an infinite number of crossings. Such systems may be continuously deformed into systems where there would be only one simple crossing.

assuming $\left(E_i^\sharp\right)'(k_2)\,E_F'(k_2) \neq -1 \quad \forall k_2 \in S^1$. When $\left(E_i^\sharp\right)'(k_2)\,E_F'(k_2) = -1$ the sign is undefined, as $E_i^\sharp$ and E_F are perpendicular at that point. However, then, the curves may be slightly bent so that the sign is defined. This will not affect the overall count.

This definition is such that we are counting the "signed" number of times the edge energy crosses the Fermi energy, where the sign is determined by the relative slope.

1.6.4. REMARK. To complete the definition, we argue that any edge system may be brought to such a form as the one assumed in the beginning of this section, without affecting the overall count. This is justified in 1.6.5.

1.6.5. CLAIM. The edge Hamiltonian may be deformed continuously, without closing the gap, in a way that will not affect $\mathcal{I}_{QH}^\sharp(H^\sharp)$. If in addition, along the path of deformation, condition Eq. (3) is obeyed then $\mathcal{I}_{KM}^\sharp(H^\sharp)$ remains invariant as well.

PROOF. Due to the stability of the resolvent set under small perturbations, as well as the stability of the spectrum, we know that any such perturbation may either deform an existing gapless mode into another gapless mode, or establish new hills or bubbles, which in turn may grow to become two gapless modes, but there are no other possibilities. In either case we see the count for $\mathcal{I}_{QH}^\sharp(H^\sharp)$ will not change, as shifting a gapless mode leaves $\mathcal{CROSS}$ invariant, and when a hill suddenly crosses E_F, $|\mathcal{CROSS}| \mapsto |\mathcal{CROSS}|+2$, however, the two crossing points have opposite sign so that $\mathcal{I}_{QH}^\sharp(H^\sharp)$ again remains invariant. If a hill has a flat maximum, or if there is an infinite number of crossings from such a hill, we assume we may continuously deform away such problems such that the index becomes defined again. □

1.7. The Bulk Indices

Let $k \in \mathbb{T}^2$ be given. Let E_k be the eigenspace of $H^B(k)$ below E_F. This defines a complex vector bundle:

$$E = \left\{ (k,\psi) \in \mathbb{T}^2 \times \mathbb{C}^N \,\middle|\, \psi \in E_k \right\}$$

where we assume $H^B(k)$ acts on a fixed Hilbert space $\mathbb{C}^N$.

1.7.1. DEFINITION. The bulk-quantum-Hall-conductance-index is defined as:

$$\boxed{\mathcal{I}_{QH}(H) := Ch_1(E)} \tag{21}$$

where Ch_1 is the first Chern number of a vector bundle.

1.7.2. REMARK. In [Av83] it was shown that

$$\mathcal{I}_{QH}(H) = \sum_{j\in \text{Occupied}} \frac{i}{2\pi}\int_{\mathbb{T}^2} \mathrm{Tr}\left[dP_j \wedge P_j dP_j\right] \tag{22}$$

where P_j is the rank-one projector onto the jth occupied band, which is just what was originally found in [Th82]. Let X be a topological space. [Av83] argued that to specify maps $\mathbb{T}^2 \to X$, we need to specify two loops $S^1 \to X$ (the two

two basic circles of $\mathbb{T}^2$) and one map $S^2 \to X$ (the left-over sphere in $\mathbb{T}^2$). Thus the topological classification of $X^{\mathbb{T}^2}$ is given by two elements in $\pi_1(X)$ and one element in $\pi_2(X)$. Let $j \in J_{N-1}$ be fixed (it does not depend on k). Then, for us, X is the space of $N \times N$ Hermitian matrices where the jth and $(j+1)$th eigenvalue are never degenerate. It turns out that X is simply connected, so that we only need to specify an element $\pi_2(X)$, and [**Av83**] calculates this element to be given by the formula in Eq. (22).

In fact, in this perspective, the explicit definition of the Chern class of E is not used, because the argument is that Eq. (22) is the *only* topological invariant that can be associated with E, and as the Chern number is a topological invariant, the two are equal. The reason one starts with the Chern number and not directly with Eq. (22) is due to the fact it is simply the most *natural* context in which to discuss the topological classification of E.

1.7.3. REMARK. The gauge-invariant formula of [**Av83**] which we present in Eq. (22) reduces to the formulation from [**Th82**].

PROOF. Expanding the exterior derivative and using the shortcuts $\partial_{k_i} P_j = P_{j,i}$ and $A_{[i}B_{j]} = \frac{1}{2}[A_i, B_j]$ we get:

$$\begin{aligned}
\mathrm{Tr}\left[dP_j \wedge P_j dP_j\right] &= \mathrm{Tr}\left[\left(\sum_{i=1}^{2}\partial_{k_i}P_j dk_i\right)\wedge P_j\left(\sum_{l=1}^{2}\partial_{k_l}P_j dk_l\right)\right] \\
&= \mathrm{Tr}\left[\left(\partial_{k_1}P_j\right)P_j\left(\partial_{k_2}P_j\right)dk_1\wedge dk_2 + \left(\partial_{k_2}P_j\right)P_j\left(\partial_{k_1}P_j\right)dk_2\wedge dk_1\right] \\
&= \mathrm{Tr}\left[\left(\partial_{k_1}P_j\right)P_j\left(\partial_{k_2}P_j\right) - \left(\partial_{k_2}P_j\right)P_j\left(\partial_{k_1}P_j\right)\right]dk_1\wedge dk_2 \\
&= 2\mathrm{Tr}\left[\left(\partial_{k_{[1}}P_j\right)P_j\left(\partial_{k_{2]}}P_j\right)\right]dk_1\wedge dk_2 \\
&= 2\mathrm{Tr}\left[\left(\partial_{k_{[1}}|\psi_j\rangle\langle\psi_j|\right)|\psi_j\rangle\langle\psi_j|\left(\partial_{k_{2]}}|\psi_j\rangle\langle\psi_j|\right)\right]dk_1\wedge dk_2 \\
&= 2\mathrm{Tr}\left[\left(\left|\psi_{j,[1}\right\rangle\langle\psi_j| + |\psi_j\rangle\left\langle\psi_{j,[1}\right|\right)|\psi_j\rangle\langle\psi_j|\left(\left|\psi_{j,2]}\right\rangle\langle\psi_j| + |\psi_j\rangle\left\langle\psi_{j,2]}\right|\right)\right]dk_1\wedge dk_2 \\
&= 2\begin{pmatrix}\langle\psi_j|\left|\psi_{j,2]}\right\rangle\langle\psi_j|\left|\psi_{j,[1}\right\rangle + \\ \left\langle\psi_{j,2]}\right|\left|\psi_{j,[1}\right\rangle + \\ \left\langle\psi_{j,[1}\right||\psi_j\rangle\langle\psi_j|\left|\psi_{j,2]}\right\rangle + \\ \left\langle\psi_{j,[1}\right||\psi_j\rangle\left\langle\psi_{j,2]}\right||\psi_j\rangle\end{pmatrix}dk_1\wedge dk_2 \\
&\overset{*}{=} 2\left(\left\langle\psi_{j,2]}\,\middle|\,\psi_{j,[1}\right\rangle + \underbrace{\left\langle\psi_{j,[1}\,\middle|\,\psi_j\right\rangle\left\langle\psi_{j,2]}\,\middle|\,\psi_j\right\rangle}_{\text{Symmetric }1\leftrightarrow2}\right)dk_1\wedge dk_2 \\
&= -\left(\langle\psi_{j,1}\,|\,\psi_{j,2}\rangle - \langle\psi_{j,2}\,|\,\psi_{j,1}\rangle\right)dk_1\wedge dk_2 \\
&= \frac{1}{i}\langle\mathcal{F}_j,\hat{e}_3\rangle dk_1\wedge dk_2
\end{aligned}$$

where in $*$ we have used the fact that $\langle\psi_{j,i}\,|\,\psi_j\rangle = -\langle\psi_j\,|\,\psi_{j,i}\rangle$ because $\langle\psi_j\,|\,\psi_j\rangle = 1$, and $\mathcal{F}_j$ is the Berry curvature of the jth band. □

Despite the first introduction of the Kane-Mele index being in [**Ka05**], we follow instead the equivalent definition of [**Fu06**] (equation 3.25).[1]

Define a matrix

$$\boxed{w_{ij}(k) := \langle\psi_i(-k), \Theta\psi_j(k)\rangle} \tag{23}$$

where $\{\psi_i(k)\}_i$ is a set of eigenstates of $H^B(k)$ corresponding to the occupied states, each of which is chosen *continuously* throughout $\mathbb{T}^2$. Thus, $\{\psi_j\}_{j\in\text{Occupied}}$ is a continuous section in the occupied frame bundle over $\mathbb{T}^2$.

1.7.4. CLAIM. Such a global smooth choice of $\{\psi_i(k)\}_i$ is always possible for time-reversal-invariant systems, due to the fact that TRI forces $\mathcal{I}_{QH}(H) = 0$.

PROOF. A non-zero Chern number can be viewed as an obstruction to the choice of a smooth section of the occupied frame bundle over $\mathbb{T}^2$. Thus if we showed that $\mathcal{I}_{QH}(H) = 0$ necessarily for systems obeying Eq. (6) we would

[1]Note that [**Fu06**] provides a proof for the equivalence of the definition we use with the definition of [**Ka05**].

be finished. The first thing to note is that from Eq. (6) another equation is implied:

$$f\left(H^{B}\left(-k\right)\right)=\Theta f\left(H^{B}\left(k\right)\right)\Theta^{-1}\qquad\forall k\in\mathbb{T}^{2}$$

where f is any map from $\mathcal{B}\left(\mathbb{C}^{N}\right)\to\mathcal{B}\left(\mathbb{C}^{N}\right)$. In fact, the projectors are obtained by such a map $P_{j}\left(k\right)=f\left(H^{B}\left(k\right)\right)$ where f is zero outside of the subspace projected on by P_{j}. As a result we obtain

$$P_{j}\left(-k\right)=\Theta P_{j}\left(k\right)\Theta^{-1}\qquad\forall k\in\mathbb{T}^{2}\tag{24}$$

Furthermore, observe that for any operator A and anti-unitary operator T we have:

$$\begin{aligned}\overline{\mathrm{Tr}\left[A\right]} & = \mathrm{Tr}\left[A^{*}\right]\\ & = \sum_{j\in J}\left\langle \psi_{j},A^{*}\psi_{j}\right\rangle \\ & \overset{\psi_{j}\mapsto T^{-1}\psi_{j}}{=} \sum_{j\in J}\left\langle T^{-1}\psi_{j},A^{*}T^{-1}\psi_{j}\right\rangle \\ & = \sum_{j\in J}\left\langle AT^{-1}\psi_{j},T^{-1}\psi_{j}\right\rangle \\ & \overset{\left\langle a,b\right\rangle =\left\langle Tb,Ta\right\rangle }{=} \sum_{j\in J}\left\langle TT^{-1}\psi_{j},TAT^{-1}\psi_{j}\right\rangle \\ & = \sum_{j\in J}\left\langle \psi_{j},TAT^{-1}\psi_{j}\right\rangle \\ & = \mathrm{Tr}\left[TAT^{-1}\right]\end{aligned}$$

Next we show that $\mathcal{I}_{QH}\left(H\right)=0$ indeed for a system obeying Eq. (24). Observe that $\mathcal{I}_{QH}\left(H\right)\in\mathbb{Z}$ and in particular $\mathcal{I}_{QH}\left(H\right)=\overline{\mathcal{I}_{QH}\left(H\right)}$. As a result we have

$$\begin{aligned}\mathcal{I}_{QH}\left(H\right) & = \overline{\mathcal{I}_{QH}\left(H\right)}\\ & = \overline{\sum_{j\in Occupied}\frac{i}{2\pi}\int_{\mathbb{T}^{2}}\mathrm{Tr}\left[dP_{j}\left(k\right)\wedge P_{j}\left(k\right)dP_{j}\left(k\right)\right]}\\ & = \sum_{j\in Occupied}\frac{-i}{2\pi}\int_{\mathbb{T}^{2}}\overline{\mathrm{Tr}\left[dP_{j}\left(k\right)\wedge P_{j}\left(k\right)dP_{j}\left(k\right)\right]}\\ & = \sum_{j\in Occupied}\frac{-i}{2\pi}\int_{\mathbb{T}^{2}}\mathrm{Tr}\left[\Theta\left(dP_{j}\left(k\right)\wedge P_{j}\left(k\right)dP_{j}\left(k\right)\right)\Theta^{-1}\right]\\ & = \sum_{j\in Occupied}\frac{-i}{2\pi}\int_{\mathbb{T}^{2}}\mathrm{Tr}\left[\Theta dP_{j}\left(k\right)\Theta^{-1}\wedge\Theta P_{j}\left(k\right)\Theta^{-1}\Theta dP_{j}\left(k\right)\Theta^{-1}\right]\\ & \overset{\Theta\text{ is const.}}{=} \sum_{j\in Occupied}\frac{-i}{2\pi}\int_{\mathbb{T}^{2}}\mathrm{Tr}\left\{ d\left[\Theta P_{j}\left(k\right)\Theta^{-1}\right]\wedge\left[\Theta P_{j}\left(k\right)\Theta^{-1}\right]d\left[\Theta P_{j}\left(k\right)\Theta^{-1}\right]\right\} \\ & = \sum_{j\in Occupied}\frac{-i}{2\pi}\int_{\mathbb{T}^{2}}\mathrm{Tr}\left\{ d\left[P_{j}\left(-k\right)\right]\wedge\left[P_{j}\left(-k\right)\right]d\left[P_{j}\left(-k\right)\right]\right\} \\ & \overset{-k\mapsto k}{=} \sum_{j\in Occupied}\frac{-i}{2\pi}\int_{\mathbb{T}^{2}}\mathrm{Tr}\left\{ d\left[P_{j}\left(k\right)\right]\wedge\left[P_{j}\left(k\right)\right]d\left[P_{j}\left(k\right)\right]\right\} \\ & = -\mathcal{I}_{QH}\left(H\right)\end{aligned}$$

□

1.7.5. CLAIM. $w\left(k\right)=-\left[w\left(-k\right)\right]^{T}$

PROOF. Using the fact that Θ obeys $\langle\alpha,\beta\rangle = \langle\Theta\beta,\Theta\alpha\rangle$ we have

$$\begin{aligned} w_{ij}(k) &\equiv \left\langle \psi_i(-k), \Theta\psi_j(k)\right\rangle \\ &= \left\langle \Theta\Theta\psi_j(k), \Theta\psi_i(-k)\right\rangle \\ &= -\left\langle \psi_j(k), \Theta\psi_i(-k)\right\rangle \\ &= -w_{ji}(-k) \end{aligned}$$

□

1.7.6. REMARK. As a result, we see that $\mathrm{Pf}[w(k)]$ is defined $\forall k\in\mathrm{TRIM}$, as at such points $w(k)$ is anti-symmetric and, by hypothesis, there is always an even number of occupied bands.

1.7.7. DEFINITION. The bulk-Kane-Mele-index, defined only for time-reversal invariant Hamiltonians, is given by

$$\mathcal{I}_{KM}(H) := \frac{1}{i\pi}\log\left(\prod_{k\in\mathrm{TRIM}}\frac{\sqrt{\det[w(k)]}}{\mathrm{Pf}[w(k)]}\right) \tag{25}$$

1.7.8. REMARK. Naively, it would seem that $\mathcal{I}_{KM}(H)$ is always zero, due to $\det[A] = (\mathrm{Pf}[A])^2$. However, care must be taken with the branch of $\sqrt{\cdot}$ that is chosen, which has to be done globally on $\mathbb{T}^2$. As a result, even though the formula does not *explicitly* require one to compute $\det[w(k)]$ outside of $\mathrm{TRIM}\subset\mathbb{T}^2$, in order to make a continuous choice of $\sqrt{\det[w(k)]}$, knowledge of $\det[w(k)]$ along paths in $\mathbb{T}^2\setminus\mathrm{TRIM}$ connecting points in TRIM is necessary. It is in this part that the assumption of $\{\psi_j\}_j$ being a smooth section will be used.

It should also be noted that $\left(\prod_{k\in\mathrm{TRIM}}\frac{\sqrt{\det[w(k)]}}{\mathrm{Pf}[w(k)]}\right)\in\{1,-1\}$ and so $\mathcal{I}_{KM}(H)\in\mathbb{Z}_2$ indeed.

1.7.9. CLAIM. If $H^B:\mathbb{T}^2\to\mathcal{B}(\mathbb{C}^N)$ is deformed continuously without closing the gap then $\mathcal{I}_{QH}(H)$ remains invariant. If the deformation obeys the condition 1.3.1 along its path, then $\mathcal{I}_{KM}(H)$ remains invariant as well.

PROOF. The invariants we have defined are topological invariants, and as such, defined only up to continuous deformations. A continuous deformation of H^B induces on of E (the total space of the vector bundle) which is always defined as long as the gap remains open. The first Chern number is stable under such deformations. Furthermore, even though we have not defined it in such a way, it is possible to define $\mathcal{I}_{KM}(H)$ in terms of the frame bundle [**Gr13**] in such a way that it is also manifestly stable under continuous deformations. □

CHAPTER 2

The Simplest Quantum Hall System: The Two-Band Model

2.1. Setting

When $N = 2$, the most general Hermitian 2×2 matrix may be written as

$$H^B(k) = h_0(k)\,\mathbb{1}_{2\times 2} + \sum_{j=1}^{3} h_j(k)\,\sigma_j$$

where $h : \mathbb{T}^2 \to \mathbb{R}^4$. As the spectrum of this system is

$$E^B_{lower;upper}(k) = h_0(k) \pm \sqrt{\sum_{j=1}^{3}\left[h_j(k)\right]^2}$$

we see that continuously deforming the system from its initial specification into one where $h_0(k) = 0$ will never close the gap, as the gap condition 1.1.2 is given by

$$\sqrt{\sum_{j=1}^{3}\left[h_j(k)\right]^2} \neq 0$$

Then, as a result of 1.6.5 and 1.7.9, we may without loss of generality assume that $h_0(k) = 0$ so that $H^B(k)$ in fact conforms to 1.5.1.

Then 1.1.2 boils down to the assumption that

$$h(k) \neq 0 \forall k \in \mathbb{T}^2$$

where we refer to $h(k) \equiv \begin{bmatrix} h_1(k) \\ h_2(k) \\ h_3(k) \end{bmatrix} \in \mathbb{R}^3$ and so we may always define the unit vector

$$\hat{h}(k) := \frac{h(k)}{\|h(k)\|} \in S^2$$

2.1.1. Claim. Eq. (21) reduces to

$$\mathcal{I}_{QH}(H) = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{2\pi}\hat{h}(k)\cdot\left\{\left[\partial_{k_1}\hat{h}(k)\right]\times\left[\partial_{k_2}\hat{h}(k)\right]\right\}dk_1\,dk_2$$

which is just the degree of the mapping $\hat{h} : \mathbb{T}^2 \to S^2$:

$$\boxed{\mathcal{I}_{QH}(H) = \deg\left(\hat{h} : \mathbb{T}^2 \to S^2\right)}$$

Proof. We use the formula that

$$Ch_1(E) \equiv \frac{i}{2\pi}\int \mathrm{Tr}\left[dP_1 \wedge P_1\,dP_1\right]$$

where P_1 is the projector onto the occupied (lower) band. This projector is given by $P_1 = \frac{E^B_2\mathbb{1} - H^B}{E^B_2 - E^B_1}$. Indeed, if a general vector v is expanded as $v = \alpha_1 v_1 + \alpha_2 v_2$ where v_i are respective eigenvectors of H^B with eigenvalues E^B_i, then

$$\begin{aligned} P_1 v &= \frac{E_2^B \mathbb{1} - H^B}{E_2^B - E_1^B} (\alpha_1 v_1 + \alpha_2 v_2) \\ &= \frac{1}{E_2^B - E_1^B} \left(\alpha_1 \left(E_2^B - H^B \right) v_1 + \alpha_2 \left(E_2^B - H^B \right) v_2 \right) \\ &= \frac{1}{E_2^B - E_1^B} \left(\alpha_1 \left(E_2^B - E_1^B \right) v_1 + \alpha_2 \left(E_2^B - E_2^B \right) v_2 \right) \\ &= \alpha_1 v_1 \end{aligned}$$

as desired. Actually for our system there is an even more explicit expression for the projector given by

$$\begin{aligned} P_1 &= \frac{E_2 \mathbb{1} - H}{E_2 - E_1} \\ &= \frac{\|h\| \mathbb{1} - (h_j \sigma_j)}{2\|h\|} \\ &= \frac{1}{2}\mathbb{1} - \frac{1}{2}\hat{h}_j \sigma_j \end{aligned}$$

Then, a direct computation leads to the desired result

$$\begin{aligned} Ch_1(E) &= \frac{i}{2\pi} \int \mathrm{Tr}\left[dP_1 \wedge P_1 dP_1\right] \\ &= \frac{i}{2\pi} \int \mathrm{Tr}\left[(\partial_{k_1} P_1) P_1 \partial_{k_2} P_1 - (\partial_{k_2} P_1) P_1 \partial_{k_1} P_1 \right] dk_1 \wedge dk_2 \\ &= \frac{i}{2\pi} \int dk_1 \wedge dk_2 \\ & \quad \mathrm{Tr}\left[\left(\partial_{k_1} \left(\frac{1}{2}\mathbb{1} - \frac{1}{2}\hat{h}\cdot\sigma \right) \right) \left(\frac{1}{2}\mathbb{1} - \frac{1}{2}\hat{h}\cdot\sigma \right) \partial_{k_2} \left(\frac{1}{2}\mathbb{1} - \frac{1}{2}\hat{h}\cdot\sigma \right) \right] \\ & \quad \mathrm{Tr}\left[- \left(\partial_{k_2} \left(\frac{1}{2}\mathbb{1} - \frac{1}{2}\hat{h}\cdot\sigma \right) \right) \left(\frac{1}{2}\mathbb{1} - \frac{1}{2}\hat{h}\cdot\sigma \right) \partial_{k_1} \left(\frac{1}{2}\mathbb{1} - \frac{1}{2}\hat{h}\cdot\sigma \right) \right] \\ &= \frac{i}{2\pi} \int \frac{1}{8} \mathrm{Tr}\left[\left(\left(\partial_{k_1} \hat{h} \right)_i \sigma_i \right) (\mathbb{1} - e_j \sigma_j) \left((\partial_{k_2} e_k) \sigma_k \right) - \left((\partial_{k_2} e_i \sigma_i) \right) (\mathbb{1} - e_j \sigma_j) (\partial_{k_1} e_k \sigma_k) \right] dk_1 \wedge dk_2 \\ &= \frac{i}{2\pi} \int \frac{1}{8} dk_1 \wedge dk_2 \{ \\ & \quad \underbrace{\left[\left(\partial_{k_1} \hat{h}_i \right) \left(\partial_{k_2} \hat{h}_k \right) - \left(\partial_{k_2} \hat{h}_i \right) \left(\partial_{k_1} \hat{h}_k \right) \right] \underbrace{\mathrm{Tr}\left[\sigma_i \sigma_k\right]}_{2\delta_{ik}}}_{0} \\ & \quad - \left[\left(\partial_{k_1} \hat{h}_i \right) \hat{h}_j \left(\partial_{k_2} \hat{h}_k \right) - \left(\partial_{k_2} \hat{h}_i \right) \hat{h}_j \left(\partial_{k_1} \hat{h}_k \right) \right] \underbrace{\mathrm{Tr}\left[\sigma_i \sigma_j \sigma_k\right]}_{2i\varepsilon_{ijk}} \} \\ &= \frac{1}{2\pi} \int \frac{1}{4} \varepsilon_{ijk} \left\{ \left[\left(\partial_{k_1} \hat{h}_i \right) \hat{h}_j \left(\partial_{k_2} \hat{h}_k \right) - \left(\partial_{k_2} \hat{h}_i \right) \hat{h}_j \left(\partial_{k_1} \hat{h}_k \right) \right] \right\} dk_1 \wedge dk_2 \\ &= -\frac{1}{4\pi} \int \hat{h} \cdot \left[\left(\partial_{k_1} \hat{h} \right) \times \left(\partial_{k_2} \hat{h} \right) \right] dk_1 \wedge dk_2 \end{aligned}$$

□

2.2. Proof of the Bulk-Edge Correspondence for Singular Hopping Matrices

If the hopping matrix in Eq. (1) is of the form

$$A = \begin{bmatrix} a_{11} & 0 \\ a_{21} & 0 \end{bmatrix}$$

then

$$A\psi_0 = \begin{bmatrix} a_{11} & 0 \\ a_{21} & 0 \end{bmatrix} \begin{bmatrix} (\psi_0)_1 \\ (\psi_0)_2 \end{bmatrix} = \begin{bmatrix} a_{11} (\psi_0)_1 \\ a_{21} (\psi_0)_1 \end{bmatrix}$$

Thus it suffices to require merely $(\psi_0)_1 \stackrel{!}{=} 0$ as the boundary condition of the edge eigenvalue problem, and $(\psi_0)_2$ can in fact stay unconstrained. This possibility allows us to avoid having to find linear combinations of generalized

Bloch solutions as in 1.4.2 and we can look for non-zero edge solutions simply by imposing the boundary condition

$$\psi_0 \overset{!}{=} \begin{bmatrix} 0 \\ * \end{bmatrix} \tag{26}$$

We still don't know the edge spectrum, but we do know that at the points of incipience, it is equal to the bulk spectrum.

2.2.1. CLAIM. $\mathcal{I}_{QH}(H)$ is the signed number of points from $\mathbb{T}^2$ that reach the north pole of S^2 via the map $\hat{h} : \mathbb{T}^2 \to S^2$.

PROOF. It will be convenient later to understand what the formula in 2.1.1 means. To this end, we established the fact that

$$\frac{1}{4\pi}\int_0^{2\pi}\int_0^{2\pi} \hat{h}(k)\cdot\left\{\left[\partial_{k_1}\hat{h}(k)\right]\times\left[\partial_{k_2}\hat{h}(k)\right]\right\} dk_1 dk_2$$

is the formula for the degree of the map $\hat{h} : \mathbb{T}^2 \to S^2$, which is an integer counting the *signed* order of the set $\hat{h}^{-1}(\{p\})$ for any $p \in S^2$. To clarify, assume that for some choice of $p \in S^2$, $\hat{h}^{-1}(\{p\}) = \{k^1, \dots, k^m\}$ for some $m \in \mathbb{N}$. For each $j \in J_m$, the restricted map $\hat{h}$ in a neighborhood of k^j is a local diffeomorphism. Such diffeomorphisms can be either orientation preserving or reversing, depending on the sign of

$$\hat{h}(k)\cdot\left\{\left[\partial_{k_1}\hat{h}(k)\right]\times\left[\partial_{k_2}\hat{h}(k)\right]\right\}$$

Thus, if this local diffeomorphism in the neighborhood of k_j is orientation preserving, we count that point j as $+1$, whereas if the diffeomorphism is orientation reversing, we count it as -1. The total count of all m points in $\hat{h}^{-1}(\{p\})$ will give us the degree of the map, and this number will be independent of p (though for different p's, the unsigned count, m, might vary).

We could choose any point as $p \in S^2$ and the choice wouldn't matter for the computation the degree, and thus for $\mathcal{I}_{QH}(H)$, let us choose the north pole $N := \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \in S^2$. Thus, if at a point $k_j \in \hat{h}^{-1}(\{N\})$,

$$\partial_1\hat{h}_1(k_j)\,\partial_2\hat{h}_2(k_j) - \partial_1\hat{h}_2(k_j)\,\partial_2\hat{h}_1(k_j) > 0$$

we count j as $+1$ and if

$$\partial_1\hat{h}_1(k_j)\,\partial_2\hat{h}_2(k_j) - \partial_1\hat{h}_2(k_j)\,\partial_2\hat{h}_1(k_j) < 0$$

we count j as -1. □

2.2.2. DEFINITION. Define the supremum of the lower energy band as

$$E^B_{l,sup}(k_2) := \sup\left(\left\{ E^B_{lower}(k_1, k_2) \,\middle|\, k_1 \in S^1 \right\}\right)$$

2.2.3. DEFINITION. Denote the *discrete* edge spectrum as $E^\sharp(k_2)$ for all $k_2 \in S^1$. We know there is only one energy eigenvalue in the gap for the edge state, from 1.5.21.

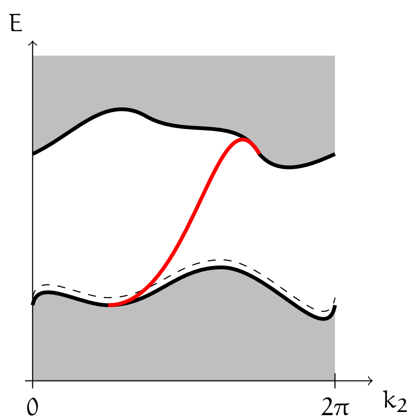

FIGURE 2.2.1. Another possibility to find the edge index is to set the fiducial line (in this picture the dashed line) infinitesimally close to $E^B_{l,sup}(k_2)$ (in this picture the thick lower line).

2.2.4. CLAIM. $\mathcal{I}^{\sharp}_{QH}(H^{\sharp})$ is given by the signed number of degeneracy points between $E^{\sharp}(k_2)$ and $E^{B}_{l,sup}(k_2)$, where the sign is obtained via the relative slope of the $E^{\sharp}(k_2)$ and $E^{B}_{l,sup}(k_2)$.

PROOF. We may take without loss of generality the Fermi energy to be infinitesimally close to $E^{B}_{l,sup}(k_2)$:

$$E_F(k_2) \overset{!}{=} E^{B}_{l,sup}(k_2)$$

and then 1.6.3 gives exactly the above definition. □

2.2.5. CLAIM. $\hat{h}^{-1}(\{N\})$ is the set of points in $\mathbb{T}^2$ such that $E^{B}_{l,sup}(k_2)$ is degenerate with $E^{\sharp}(k_2)$.

PROOF. In order to be able to compare the two descriptions, we first compute the eigenvectors of the bulk system *before* we allow for the possibility that k_1 is complex-valued (this generalization follows from 1.4.2). Consequently, $h \in \mathbb{R}^3$ for the purpose of this computation.

Let $k \in \mathbb{T}^2$ be given. The eigensystem equation is given by

$$\begin{bmatrix} +h_3 & h_1 - ih_2 \\ h_1 + ih_2 & -h_3 \end{bmatrix} \begin{bmatrix} v_1{}^{(n)} \\ v_2{}^{(n)} \end{bmatrix} = (-1)^n \|h\| \begin{bmatrix} v_1{}^{(n)} \\ v_2{}^{(n)} \end{bmatrix}$$

which gives an eigenvector $\begin{bmatrix} v_1{}^{(n)} \\ v_2{}^{(n)} \end{bmatrix}$ corresponding to the eigenvalue $E^{B}_{n} = (-1)^n \|h\|$ for $\begin{cases} n=1 & \text{lower} \\ n=2 & \text{upper} \end{cases}$.

From this equation two equations follow for v_1 and v_2:

$$\begin{cases} (h_3 - (-1)^n \|h\|)\, v_1{}^{(n)} + (h_1 - ih_2)\, v_2{}^{(n)} & = 0 \\ (h_1 + ih_2)\, v_1{}^{(n)} + \left(-h_3 - (-1)^n \|h\|\right) v_2{}^{(n)} & = 0 \end{cases}$$

dividing through $\|h\|$ (which is never zero by hypothesis) we get:

$$\begin{cases} \left(\hat{h}_3 - (-1)^n\right) v_1{}^{(n)} + \left(\hat{h}_1 - i\hat{h}_2\right) v_2{}^{(n)} & = 0 \\ \left(\hat{h}_1 + i\hat{h}_2\right) v_1{}^{(n)} + \left(-\hat{h}_3 - (-1)^n\right) v_2{}^{(n)} & = 0 \end{cases}$$

Note that, as before, even though we started with a general point $\begin{bmatrix} h_0 \\ h \end{bmatrix} \in \mathbb{R}^4$ such that $\|h\| \neq 0$, what matters for the eigenvectors is only the associated point $\hat{h} \in S^2$.

(1) Case 1: $\hat{h}_3 = 1$ (the north pole, where $\hat{h}_1 = \hat{h}_2 = 0$)

- Then we obtain
$$\begin{cases} \left(1 - (-1)^n\right) v_1{}^{(n)} & = 0 \\ \left(-1 - (-1)^n\right) v_2{}^{(n)} & = 0 \end{cases}$$
- Then for $n = 1$, $v_2{}^{(1)}$ is free and $v_1{}^{(1)}$ must be zero, so that we obtain that the general eigenvector corresponding to E^{B}_{1} is given by $\begin{bmatrix} 0 \\ \alpha \end{bmatrix}$ for some $\alpha \in \mathbb{C}\setminus\{0\}$.
- For $n = 2$, $v_1{}^{(2)}$ is free and $v_2{}^{(2)}$ must be zero, so that the general eigenvector corresponding to E^{B}_{2} is given by $\begin{bmatrix} \alpha \\ 0 \end{bmatrix}$ for some $\alpha \in \mathbb{C}\setminus\{0\}$.

(1) Case 2: $\hat{h}_3 = -1$ (the south pole, where $\hat{h}_1 = \hat{h}_2 = 0$)

- Then we obtain
$$\begin{cases} \left(-1 - (-1)^n\right) v_1{}^{(n)} & = 0 \\ \left(+1 - (-1)^n\right) v_2{}^{(n)} & = 0 \end{cases}$$
- For $n = 1$, $v_1{}^{(1)}$ is free and $v_2{}^{(1)}$ must be zero, so that we obtain that the general eigenvector corresponding to E^{B}_{1} is given by $\begin{bmatrix} \alpha \\ 0 \end{bmatrix}$ for some $\alpha \in \mathbb{C}\setminus\{0\}$.
- For $n = 2$, $v_2{}^{(2)}$ is free and $v_1{}^{(2)}$ must be zero, so that the general eigenvector corresponding to E^{B}_{2} is given by $\begin{bmatrix} 0 \\ \alpha \end{bmatrix}$ for some $\alpha \in \mathbb{C}\setminus\{0\}$.

(1) Case 3: $\hat{h}_3 \notin \{\pm 1\}$ (where either $\hat{h}_1 \neq 0$ or $\hat{h}_2 \neq 0$)

- Then we obtain

$$\begin{cases} {v_1}^{(n)} & = \frac{-\hat{h}_1+i\hat{h}_2}{\hat{h}_3-(-1)^n}{v_2}^{(n)} \\ {v_1}^{(n)} & = \frac{\hat{h}_3+(-1)^n}{\hat{h}_1+i\hat{h}_2}{v_2}^{(n)} \end{cases}$$

- The two equations are the same up to multiplication by a nonzero constant complex number and so the general eigenvector associated with E^B_n is given by $\begin{bmatrix} \frac{-\hat{h}_1+i\hat{h}_2}{\hat{h}_3-(-1)^n}\alpha \\ \alpha \end{bmatrix}$ for some $\alpha \in \mathbb{C}\backslash\{0\}$. Observe that the two components of this vector will never be zero, because we assume $\hat{h}_3 \notin \{\pm 1\}$.

The final conclusion from this analysis is that the non-normalized (but normalizable) eigenvectors for the bulk system are given, up to multiplication by non-zero complex factors by,

$$\begin{cases} \begin{cases} \psi_{lower} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ \psi_{upper} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{cases} & \hat{h}_3 = 1 \\ \begin{cases} \psi_{lower} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ \psi_{upper} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{cases} & \hat{h}_3 = -1 \\ \begin{cases} \psi_{lower} = \begin{bmatrix} \frac{-\hat{h}_1+i\hat{h}_2}{\hat{h}_3+1} \\ 1 \end{bmatrix} \\ \psi_{upper} = \begin{bmatrix} \frac{-\hat{h}_1+i\hat{h}_2}{\hat{h}_3-1} \\ 1 \end{bmatrix} \end{cases} & \hat{h}_3 \notin \{\pm 1\} \end{cases}$$

We can already see that the edge boundary condition Eq. (26) on the bulk eigenvectors are only fulfilled on special points on the sphere: on the north pole only for ψ_{lower} whereas on the south pole only for ψ_{upper}.

Hence we may conclude that for these points on the sphere, we exactly have degeneracy between edge energy eigenvalues and bulk energy eigenvalues, because these solutions *are* solutions of the bulk Hamiltonian H^B (with real values of k) yet they also obey the boundary conditions of the edge, and as we saw in 1.4.2, solutions of H^B which obey the edge boundary conditions are solutions of $H^\sharp$. □

2.2.6. REMARK. We were able to find these degeneracy points using the bulk Hamiltonian and the edge boundary conditions alone, with no analysis of the edge system nor its actual discrete spectrum. In fact, had the word "signed" not been used in the definition of (either of the bulk or the edge) quantum-Hall index, the correspondence proof would have been done at this point. Hence the missing fact from the correspondence proof is the matching of the signs, so that the counting would indeed be the same. All effort done from this point onward will be invested to that end.

Let $k^D \in h^{-1}(\{N\})$ be such a degeneracy point between $E^B_{l,sup}(k_2)$ and $E^\sharp(k_2)$. We will show that both signs of the edge and the bulk agree for k^D and thus complete the proof that

$$\boxed{\mathcal{I}_{QH}(H) = \mathcal{I}^\sharp_{QH}\left(H^\sharp\right)} \tag{27}$$

2.2.7. CLAIM. The equation $\boxed{h_1 = ih_2}$ determines the complex value of k_1 of the edge solution in terms of k_2.

PROOF. In general, to find $E^\sharp(k_2)$, we can solve the eigensystem of H^B, but assuming that k_1 can take on complex values in the upper plane (so that the edge wave-functions decay exponentially into the bulk, as we expect from edge states at the zeroth site), and impose the edge boundary $\psi_0 \stackrel{!}{=} 0$ and that $E^\sharp(k_2) \in \mathbb{R}$. However, those boundary conditions cannot be imposed on the same wave-functions (that is, eigenvectors) of $H^B(k_2)$ where we assumed $k_1 \in \mathbb{R}$. We need to "re-solve" the eigensystem allowing for $\Im(k_1) > 0$ and only then impose the boundary conditions. As a result, now we allow $h \in \mathbb{C}^3$. As such the matrix $\sum_{j=1}^3 h_j\sigma_j$ is no longer Hermitian and our eigenvalues are not *necessarily* real:

$$E^{\sharp}_{1,2} = \pm\sqrt{h_1 + h_2 + h_3}$$

The eigenvectors are given by the two equations which come from the eigenvalue equation $H^B(k)\begin{bmatrix} v_1{}^{(n)} \\ v_2{}^{(n)} \end{bmatrix} = \left(+(-1)^n\sqrt{h_1+h_2+h_3}\right)\begin{bmatrix} v_1{}^{(n)} \\ v_2{}^{(n)} \end{bmatrix}$:

$$\begin{cases} \left(h_3 - (-1)^n\sqrt{h_1+h_2+h_3}\right)v_1{}^{(n)} + (h_1 - ih_2)\, v_2{}^{(n)} & = 0 \\ (h_1 + ih_2)\, v_1{}^{(n)} + \left(-h_3 - (-1)^n\sqrt{h_1+h_2+h_3}\right)v_2{}^{(n)} & = 0 \end{cases}$$

We don't actually need to compute the eigenvectors, but rather, only check when they obey the boundary conditions, that is, when it would follow from the equations that $v_1{}^{(n)} = 0$ and $v_2{}^{(n)} \neq 0$, following Eq. (26). To that end, we get the equations:

$$\begin{cases} \left(h_3 - (-1)^n\sqrt{h_1+h_2+h_3}\right) & \neq 0 \\ (h_1 - ih_2) & = 0 \\ (h_1 + ih_2) & \neq 0 \\ \left(-h_3 - (-1)^n\sqrt{h_1+h_2+h_3}\right) & = 0 \end{cases}$$

These conditions are fulfilled when $h_1 = ih_2$: $(ih_2)^2 + (h_2)^2 = 0$, and when $E^e = -h_3$. Thus, the equation $h_1 = ih_2$ determines the complex value of k_1 in the edge in terms of k_2. □

If we had explicit expressions for h_1 and h_2 we could already look at the expression $E^{\sharp}(k_2)$ and compute its slope in the vicinity of k^D. Because we don't, we will make an approximation at $k^D + \delta$ with $\delta_2 \in \mathbb{R}$, $\delta_1 \in \mathbb{C}$ (in upper plane for decaying solution) and $|\delta_i| \ll 1 \forall i \in J_2$.

2.2.8. CLAIM. The edge spectrum near $E^B_{l,sup}(k_D)$ is obtained by taking $\Re\{\delta_1\} = 0$.

PROOF. To get the edge spectrum near k^D, we plug into E^B_{lower} complex values of k_1 such that the result is real, and that the corresponding eigenstates obey the boundary conditions and decay. Observe that k^D_1 is an extremal point of $E^B_{lower}(k)$ for fixed k_2, and as such, $\partial_1 E^B_{lower}(k^D) = 0$. Thus

$$E^B_{lower}\left(k^D_1 + \delta_1, k^D_2 + \delta_2\right) \approx E^B_{lower}\left(k^D\right) + \partial_2 E^B_{lower}\left(k^D\right)\delta_2 + \left[\partial_1^2 E^B_{lower}\left(k^D\right)\right]\delta_1^2$$

As a result we see that the only way for $E^B_{lower}(k^D_1 + \delta_1, k^D_2 + \delta_2)$ to be real (and thus, to represent the edge energy) is to have $\Re(\delta_1) = 0$ (and so δ_1 is *purely* imaginary in the upper complex plane). □

2.2.9. CLAIM. The signs of the edge index count and the bulk index count exactly match, proving Eq. (27).

PROOF. Now that we have all the ingredients, we may proceed as follows:

- The condition that $h_1 = ih_2$ translates to (in the vicinity of k^D):

$$\underbrace{h_1\left(k^D\right)}_{0} + i\left[\partial_1 h_1\left(k^D\right)\right]\Im\{\delta_1\} + \left[\partial_2 h_1\left(k^D\right)\right]\delta_2 \overset{!}{\approx} i\left\{\underbrace{h_2\left(k^D\right)}_{0} + i\left[\partial_1 h_2\left(k^D\right)\right]\Im\{\delta_1\} + \left[\partial_2 h_2\left(k^D\right)\right]\delta_2\right\}$$

  From which we obtain that

$$\begin{cases} \left[\partial_1 h_1\left(k^D\right)\right]\Im\{\delta_1\} & = \left[\partial_2 h_2\left(k^D\right)\right]\delta_2 \\ \left[\partial_2 h_1\left(k^D\right)\right]\delta_2 & = -\left[\partial_1 h_2\left(k^D\right)\right]\Im\{\delta_1\} \end{cases}$$

  or in shorthand notation

$$\begin{cases} h_{1,1}\Im\{\delta_1\} & = h_{2,2}\delta_2 \\ h_{2,1}\Im\{\delta_1\} & = -h_{1,2}\delta_2 \end{cases}$$

  These equation imply

$$\begin{cases} h_{1,1}{}^2\Im\{\delta_1\} & = h_{1,1}h_{2,2}\delta_2 \\ h_{2,1}{}^2\Im\{\delta_1\} & = -h_{2,1}h_{1,2}\delta_2 \end{cases}$$

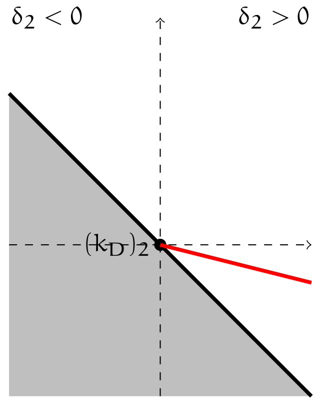

FIGURE 2.2.2. A linear zoom near $(k_D)_2$. Even though $E^\sharp((k_D)_2)$ (red line) has negative slope, relative to $E^B_{l,sup}((k_D)_2)$ (thick black line) it has positive slope. This has to be the case when $\delta_2 > 0$ because the the red line *must* always be above the thick black line.

which in turn implies

$$\boxed{\Im\{\delta_1\} = \frac{h_{1,1}h_{2,2} - h_{1,2}h_{2,1}}{{h_{1,1}}^2 + {h_{2,1}}^2}\delta_2}$$

- We know that $\Im\{\delta_1\} > 0$ (that's the condition for a decaying solution). Following 2.2.4, $sgn(\delta_2)$ gives us a way to determine the sign of the degeneracy point for the count of $\mathcal{I}^\sharp_{QH}(H^\sharp)$. Indeed, iff $\delta_2 > 0$ we get a plus sign for the count of the edge index because $E^\sharp(k_D)$ grows rightwards, which is happens iff the relative slope of $E^\sharp((k_D)_2)$ with $E^B_{l,sup}((k_D)_2)$ is positive, because $E^\sharp((k_D)_2 + \delta_2)$ must be above $E^B_{l,sup}((k_D)_2 + \delta_2)$ by definition; this is in agreement with 1.6.3. The analog argument holds if $\delta_2 < 0$. Observe $\delta_2 = 0$ is not possible by the stability of the edge spectrum.
- Use the fact that $\partial_i \hat{h}_j = \frac{1}{\|h\|}\left[\partial_i h_j - \left\langle \hat{h}, \partial_i h\right\rangle \hat{h}_j\right]$ to conclude that $\partial_i \hat{h}_j\left(k^D\right) = \frac{1}{h_3(k^D)}\partial_i h_j \forall j \in J_2$ where $h_3\left(k^D\right) > 0$. Thus, the signs are preserved and we can safely replace the condition

$$\partial_1\hat{h}_1\left(k^D\right)\partial_2\hat{h}_2\left(k^D\right) - \partial_1\hat{h}_2\left(k^D\right)\partial_2\hat{h}_1\left(k^D\right) > 0$$

by

$$\partial_1 h_1\left(k^D\right)\partial_2 h_2\left(k^D\right) - \partial_1 h_2\left(k^D\right)\partial_2 h_1\left(k^D\right) > 0$$

which is what we had in 2.2.1.
- Thus we see that the two signs *exactly match* because when $\delta_2 > 0$, $\hat{h}(k_D)$ is orientation preserving *and* the count of the edge index is $+1$, and the corresponding statement for $\delta_2 < 0$.

□

2.3. Bulk-Edge Correspondence for a General Two-Band Hamiltonian

We present our version of the proof in [**Mo11**], most of which is already contained in 1.5.16.

2.3.1. CLAIM. In a nearest-neighbor approximation, if for a fixed k_2, $\hat{h}(k)\big|_{k_2}$ is a loop on S^2 parametrized by k_1, then $Ch_1(E)$ is given by the signed number of times $\hat{h}(k)\big|_{k_2}$ crosses as a great circle on S^2, where the sign is:

- Positive if $\left(\hat{e}^r \times \hat{e}^i\right)\cdot\hat{e}^\perp$ went from -1 before crossing to $+1$ after crossing.
- Negative if $\left(\hat{e}^r \times \hat{e}^i\right)\cdot\hat{e}^\perp$ went from $+1$ before crossing to -1 after crossing.

PROOF. First note that in a nearest neighbor approximation we may follow the scheme of 1.5. However, even though the curve $h(k)|_{k_2}$ is planar, $\hat{h}(k)\big|_{k_2}$ is not necessarily a circle when projected on S^2, and so the area $\hat{h}(k)\big|_{k_2}$ encloses is not strictly speaking a cap on S^2, so we'll refer to it as a "cap".

We write the formula in 2.1.1 as:

$$\begin{aligned} \mathrm{Ch}_1(E) &= \frac{1}{4\pi}\int_0^{2\pi}\int_0^{2\pi} \hat{h}(k)\cdot\left\{\left[\partial_{k_1}\hat{h}(k)\right]\times\left[\partial_{k_2}\hat{h}(k)\right]\right\}dk_1\,dk_2 \\ &= \frac{1}{4\pi}\int_0^{2\pi}\underbrace{\left(\int_0^{2\pi}\hat{h}(k)\cdot\left\{\left[\partial_{k_1}\hat{h}(k)\right]\times\left[\partial_{k_2}\hat{h}(k)\right]\right\}dk_1\right)}_{f(k_2)}dk_2 \\ &= \frac{1}{4\pi}\int_0^{2\pi} f(k_2)\,dk_2 \end{aligned}$$

The integral in $\mathrm{Ch}_1(E)$ gives the total surface covered on the sphere covered by $\mathbb{T}^2$, so that the function f is the rate of change of area-covering, as we change k_2. That is, $\int_{k_2=k_2^{(1)}}^{k_2=k_2^{(2)}} f(k_2)\,dk_2$ gives the area on the sphere enclosed between the two curves $\hat{h}(k)\big|_{k_2^{(1)}}$ and $\hat{h}(k)\big|_{k_2^{(2)}}$. We may thus define the anti-derivative of $f(k_2)$ as $F(k_2)$ and so

$$\mathrm{Ch}_1(E) = \frac{1}{4\pi}\left[F(2\pi) - F(0)\right]$$

F is such that $F'(k_2) = f(k_2)$, but we have the freedom to define $F(k_2)$ with an arbitrary constant. Define the constant as follows: Let $k_2^{(0)} \in S^1$ be given such that $\hat{e}^{\perp}\left(k_2^{(0)}\right) \neq 0$. Define $F\left(k_2^{(0)}\right)$ as the area of the "cap" enclosed by the loop $\hat{h}(k)\big|_{k_2^{(0)}}$, where the "cap" is the one the vector $-\left(\hat{e}^r \times \hat{e}^i\right)$ points towards. If such a $k_2^{(0)} \in S^1$ does not exist then the claim is automatically satisfied as there are no crossings at all, and $\mathrm{Ch}_1(E) = 0$ indeed because if $\hat{h}(k)\big|_{k_2}$ covers any area, in order to obey the boundary conditions it will cover a negative area of the same amount, totaling in zero. $F(k_2)$ thus is the amount of area swept on S^2 going from $k_2^{(0)}$ to some k_2. As a side note, using the Guass-Bonnet theorem we could verify this directly:

$$\mathrm{Area}(k_2) = 2\pi\underbrace{\chi}_{1} - \int_{\hat{h}(k)|_{k_2}} k_g(s)\,ds$$

where $k_g(s)$ is the curvature along $\hat{h}(k)\big|_{k_2}$, s is the arc-length parametrization and χ is the Euler characteristic of a closed disc.

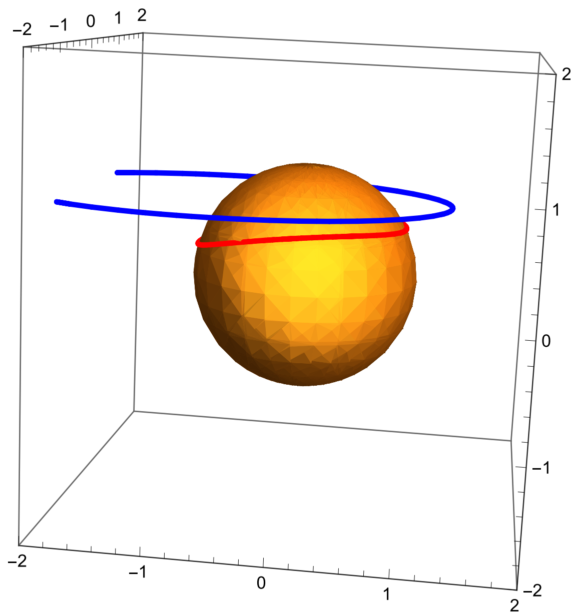

FIGURE 2.3.1. The ellipse projected onto S^2. The projection does not form a circle.

At any rate, now $\mathrm{Ch}_1(E)$ can be computed as the *signed* number of times F crosses the lines $2\pi\mathbb{Z}$, because $\hat{h}(k)\Big|_{k_2^{(0)}} = \hat{h}(k)\Big|_{k_2^{(0)}+2\pi}$ as $k_2 \in S^1$, so that $F\left(k_2^{(0)}+2\pi\right) = n \cdot F\left(k_2^{(0)}\right)$ for some $n \in \mathbb{Z}$:

$$\begin{aligned} \mathrm{Ch}_1(E) &= \frac{1}{4\pi}\left[F\left(k_2^{(0)}+2\pi\right) - F\left(k_2^{(0)}\right)\right] \\ &= n \end{aligned}$$

In order to have $n \neq 0$, the loop $\hat{h}(k)\Big|_{k_2}$ must cross as a great circle, and when this happens, F is a multiple of 2π, as that is the area of exactly half of S^2. Furthermore, at the crossings, $\hat{e}^\perp = 0$ because then the ellipse is not offset perpendicularly from the origin. So there, $(\hat{e}^r \times \hat{e}^i) \cdot \hat{e}^\perp = 0$.

The choice of "cap" we made for $F\left(k_2^{(0)}\right)$ ensures that the sign of the crossing must be counted as $+1$ if $(\hat{e}^r \times \hat{e}^i) \cdot \hat{e}^\perp$ went from being negative to positive and -1 if $(\hat{e}^r \times \hat{e}^i) \cdot \hat{e}^\perp$ went from being positive to negative:

- If it happens that $\left(\hat{e}^r\left(k_2^{(0)}\right) \times \hat{e}^i\left(k_2^{(0)}\right)\right) \cdot \hat{e}^\perp\left(k_2^{(0)}\right) > 0$, then $-\left(\hat{e}^r\left(k_2^{(0)}\right) \times \hat{e}^i\left(k_2^{(0)}\right)\right)$ points towards the larger "cap" defined by $\hat{h}(k)\Big|_{k_2^{(0)}}$.
- If it happens that $\left(\hat{e}^r\left(k_2^{(0)}\right) \times \hat{e}^i\left(k_2^{(0)}\right)\right) \cdot \hat{e}^\perp\left(k_2^{(0)}\right) < 0$, then $-\left(\hat{e}^r\left(k_2^{(0)}\right) \times \hat{e}^i\left(k_2^{(0)}\right)\right)$ points towards the smaller "cap" defined by $\hat{h}(k)\Big|_{k_2^{(0)}}$.

In either case we have that as F crosses the lines $2\pi\mathbb{Z}$ with positive slope, we necessarily have that $(\hat{e}^r(k_2) \times \hat{e}^i(k_2)) \cdot \hat{e}^\perp(k_2)$ goes from being -1 to $+1$. As F crosses the lines $2\pi\mathbb{Z}$ with negative slope, $(\hat{e}^r(k_2) \times \hat{e}^i(k_2)) \cdot \hat{e}^\perp(k_2)$ goes from $+1$ to -1. □

2.3.2. COROLLARY. *For nearest-neighbor two-band models we have*

$$\boxed{\mathcal{I}_{QH}(H) = \mathcal{I}^\sharp_{QH}\left(H^\sharp\right)}$$

PROOF. Without loss of generality, we set $E_F = 0$. Then, using 1.5.16 we know that there is a zero-energy edge state iff the ellipse $h(k)|_{k_2}$ contains the origin, and at these points $k_2 \in S^1$, $\hat{h}(k)\Big|_{k_2}$ is a great circle on S^2.

Furthermore, from 1.5.21 we know that the sign of the edge energy around zero is given by $(\hat{e}^r \times \hat{e}^i) \cdot \hat{e}^\perp$, so that following the definition Eq. (19):

- $-\frac{(E^\sharp)'(k_2)}{|(E^\sharp)'(k_2)|} = 1$ if $(\hat{e}^r \times \hat{e}^i) \cdot \hat{e}^\perp$ went from being -1 before the crossing to $+1$ after the crossing.
- $-\frac{(E^\sharp)'(k_2)}{|(E^\sharp)'(k_2)|} = -1$ if $(\hat{e}^r \times \hat{e}^i) \cdot \hat{e}^\perp$ went from being $+1$ before the crossing to -1 after the crossing.

□

CHAPTER 3

The Simplest Topological Insulator: The Four-Band Model

3.1. Gamma Matrices

3.1.1. DEFINITION. Define

$$\boxed{\Gamma_{i,j} := \sigma_i \otimes \sigma_j}$$

for any $(i, j) \in (\mathbb{Z}_4)^2$. In components we have

$$\left(\Gamma_{i,j}\right)_{\alpha,\beta} = \left(\sigma_i\right)_{\lfloor \frac{\alpha}{2} \rfloor, \lfloor \frac{\beta}{2} \rfloor} \left(\sigma_j\right)_{\alpha\%2,\, \beta\%2}$$

for any $(\alpha, \beta) \in (\mathbb{Z}_4)^2$, where % denotes modulo and $\lfloor x \rfloor$ denotes the floor of x. There are sixteen possible combinations, and thus sixteen $\Gamma_{i,j}$ matrices, of which fifteen are traceless (to be shown below).

3.1.2. CLAIM. $\left(\Gamma_{i,j}\right)^2 = \mathbb{1}_{4\times 4}$ and so $\left(\Gamma_{i,j}\right)^{-1} = \Gamma_{i,j}$ for any $(i, j) \in (\mathbb{Z}_4)^2$.

PROOF. Using the fact that $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$ we have:

$$\begin{aligned} \left(\Gamma_{i,j}\right)^2 &= \left(\sigma_i \otimes \sigma_j\right)\left(\sigma_i \otimes \sigma_j\right) \\ &= \left(\sigma_i \sigma_i\right) \otimes \left(\sigma_j \sigma_j\right) \\ &= \left(\mathbb{1}_{2\times 2}\right) \otimes \left(\mathbb{1}_{2\times 2}\right) \\ &= \mathbb{1}_{4\times 4} \end{aligned}$$

□

3.1.3. CLAIM. $\left(\Gamma_{i,j}\right)^* = \Gamma_{i,j}$ for any $(i, j) \in (\mathbb{Z}_4)^2$.

PROOF. Using the fact that $(A \otimes B)^* = (A^*) \otimes (B^*)$ we have and the Hermiticity of the Pauli matrices, we have:

$$\begin{aligned} \left(\Gamma_{i,j}\right)^* &= \left(\sigma_i \otimes \sigma_j\right)^* \\ &= \left(\sigma_i^*\right) \otimes \left(\sigma_j^*\right) \\ &= \sigma_i \otimes \sigma_j \\ &= \Gamma_{i,j} \end{aligned}$$

□

3.1.4. CLAIM. $\mathrm{Tr}\left[\Gamma_{i,j}\right] = 4\delta_{i,0}\delta_{j,0}$ for any $(i, j) \in (\mathbb{Z}_4)^2$.

PROOF. Using the fact that $\mathrm{Tr}[A \otimes B] = \mathrm{Tr}[A]\,\mathrm{Tr}[B]$ and the tracelessness of the Pauli matrices we have

$$\begin{aligned} \mathrm{Tr}\left[\Gamma_{i,j}\right] &= \mathrm{Tr}\left[\sigma_i \otimes \sigma_j\right] \\ &= \mathrm{Tr}\left[\sigma_i\right]\mathrm{Tr}\left[\sigma_j\right] \\ &= 2\delta_{i,0} 2\delta_{j,0} \\ &= 4\delta_{i,0}\delta_{j,0} \end{aligned}$$

□

3.1.5. CLAIM. $\left\{\Gamma_{i,j}, \Gamma_{l,m}\right\} = 0$ iff either (at least two indices are non-zero and non-equal, and another index is zero) or (all indices are non-zero, and two are non-equal and two are equal).

PROOF. In general we have

$$\begin{aligned}
\left\{\Gamma_{i,j},\,\Gamma_{l,m}\right\} &\equiv \Gamma_{i,j}\Gamma_{l,m}+\Gamma_{l,m}\Gamma_{i,j}\\
&= \left(\sigma_i\otimes\sigma_j\right)\left(\sigma_l\otimes\sigma_m\right)+\left(\sigma_l\otimes\sigma_m\right)\left(\sigma_i\otimes\sigma_j\right)\\
&= \left(\sigma_i\sigma_l\right)\otimes\left(\sigma_j\sigma_m\right)+\left(\sigma_l\sigma_i\right)\otimes\left(\sigma_m\sigma_j\right)\\
&= \begin{cases}
\sigma_i\otimes\left\{\sigma_j,\,\sigma_m\right\} & l=0\\
\begin{cases}
\sigma_l\otimes\left\{\sigma_j,\,\sigma_m\right\} & i=0\\
\begin{cases}
\left\{\sigma_l,\,\sigma_i\right\}\otimes\sigma_m & j=0\\
\begin{cases}
\left\{\sigma_l,\,\sigma_i\right\}\otimes\sigma_j & m=0\\
\left(\sigma_i\sigma_l\right)\otimes\left(\sigma_j\sigma_m\right)+\left(\sigma_l\sigma_i\right)\otimes\left(\sigma_m\sigma_j\right) & m\neq 0
\end{cases} & j\neq 0
\end{cases} & i\neq 0
\end{cases} & l\neq 0
\end{cases}\\
&= \begin{cases}
\begin{cases}
2\Gamma_{i,m} & j=0\\
\begin{cases}
2\Gamma_{i,j} & m=0\\
2\delta_{j,m}\Gamma_{i,0} & m\neq 0
\end{cases} & j\neq 0
\end{cases} & l=0\\
\begin{cases}
\begin{cases}
2\Gamma_{l,m} & j=0\\
\begin{cases}
2\Gamma_{l,j} & m=0\\
2\delta_{j,m}\Gamma_{l,0} & m\neq 0
\end{cases} & j\neq 0
\end{cases} & i=0\\
\begin{cases}
2\delta_{l,i}\Gamma_{0,m} & j=0\\
\begin{cases}
2\delta_{l,i}\Gamma_{0,j} & m=0\\
-\sum_{k=1}^{3}\sum_{r=1}^{3}\varepsilon_{jmr}\varepsilon_{ilk}\Gamma_{k,r}+\delta_{il}\delta_{jm}\Gamma_{0,0} & m\neq 0
\end{cases} & j\neq 0
\end{cases} & i\neq 0
\end{cases} & l\neq 0
\end{cases}
\end{aligned}$$

thus we see that there are basically six possibilities for the anti-commutator to be zero:

(1) $j\neq 0, m\neq 0, j\neq m, l=0$
(2) $j\neq 0, m\neq 0, j\neq m, i=0$
(3) $i\neq 0, l\neq 0, i\neq l, j=0$
(4) $i\neq 0, l\neq 0, i\neq l, m=0$
(5) $i\neq 0, l\neq 0, j\neq 0, m\neq 0, i=l, j\neq m$
(6) $i\neq 0, l\neq 0, j\neq 0, m\neq 0, i\neq l, j=m$

□

3.1.6. CLAIM. $\frac{1}{4}\mathrm{Tr}\left[\Gamma_{i,j}\Gamma_{i',j'}\right]=\delta_{i,i'}\delta_{j,j'}$ for any $(i,\,j,\,i',\,j')\in(\mathbb{Z}_4)^4$.

PROOF. Compute

$$\begin{aligned}
\frac{1}{4}\mathrm{Tr}\left[\Gamma_{i,j}\Gamma_{i',j'}\right] &= \frac{1}{4}\mathrm{Tr}\left[\Gamma_{i,j}\Gamma_{i',j'}\right]\\
&= \frac{1}{4}\mathrm{Tr}\left[\left(\sigma_i\otimes\sigma_j\right)\left(\sigma_{i'}\otimes\sigma_{j'}\right)\right]\\
&= \frac{1}{4}\mathrm{Tr}\left[\left(\sigma_i\sigma_{i'}\right)\otimes\left(\sigma_j\otimes\sigma_{j'}\right)\right]\\
&= \frac{1}{4}\mathrm{Tr}\left[\sigma_i\sigma_{i'}\right]\mathrm{Tr}\left[\sigma_j\otimes\sigma_{j'}\right]
\end{aligned}$$

- But $\mathrm{Tr}\left[\sigma_i\sigma_{i'}\right]=2\delta_{i,i'}$ using the tracelessness of the Pauli matrices:

$$\begin{aligned}
\mathrm{Tr}\left[\sigma_i\sigma_{i'}\right] &= \mathrm{Tr}\left[\delta_{i,0}\delta_{i',0}\mathbb{1}_{2\times 2}+\delta_{i,0}\left(1-\delta_{i',0}\right)\sigma_{i'}+\delta_{i',0}\left(1-\delta_{i,0}\right)\sigma_i+\left(1-\delta_{i,0}\right)\left(1-\delta_{i',0}\right)\left(i\sum_k\varepsilon_{ii'k}\sigma_k+\delta_{i,i'}\mathbb{1}_{2\times 2}\right)\right]\\
&= \delta_{i,0}\delta_{i',0}2+\left(1-\delta_{i,0}\right)\left(1-\delta_{i',0}\right)\left(\delta_{i,i'}2\right)\\
&= 2\delta_{i,i'}
\end{aligned}$$

□

3.1.7. CLAIM. $\left\{\,\Gamma_{i,j}\,\right\}$ is a linearly independent subset of the vector space $\mathrm{Mat}_{4\times 4}(\mathbb{C})$.

PROOF. The Pauli matrices form a linearly independent set in $\mathrm{Mat}_{2\times 2}(\mathbb{C})$, and a tensor product of the bases gives rise to a basis of the tensor product vector space: $\mathrm{Mat}_{4\times 4}(\mathbb{C})=\mathrm{Mat}_{2\times 2}(\mathbb{C})\otimes\mathrm{Mat}_{2\times 2}(\mathbb{C})$. □

3.1.8. COROLLARY. $\mathrm{span}\left(\left\{ \Gamma_{i,j} \,\middle|\, (i,j) \in (\mathbb{Z}_4)^2 \right\}\right) = \mathrm{Herm}(4)$ *due to the fact that all the* $\Gamma_{i,j}$ *matrices are Hermitian and* $\dim(\mathrm{Herm}(4)) = 16$.

3.1.9. CLAIM. Any given matrix $A \in \mathrm{Mat}_{4\times 4}(\mathbb{C})$ may be expanded (with coefficients not necessarily real) in the $\{\Gamma_{i,j}\}$ basis of Hermitian matrices as:

$$A = \sum_{(i,j)\in(\mathbb{Z}_4)^2} \frac{1}{4}\mathrm{Tr}\left[A\Gamma_{i,j}\right]\Gamma_{i,j}$$

PROOF. Write a general $A \in \mathrm{Mat}_{4\times 4}(\mathbb{C})$ as $A = \frac{1}{2}\underbrace{(A + A^*)}_{B_1} - \frac{1}{2}i\underbrace{[i(A - A^*)]}_{B_2}$.

- Observe that $(B_1, B_2) \in [\mathrm{Herm}(4)]^2$ by construction.
- Write $B_l = \sum_{(i,j)\in(\mathbb{Z}_4)^2} c^l_{i,j}\Gamma_{i,j} \forall l \in J_2$, which is always possible because of the preceding claim, where the coefficients are real.
- Multiply B_l by $\Gamma_{i',j'}$ and take the trace to get:

$$\begin{aligned}
\mathrm{Tr}\left[B_l\Gamma_{i',j'}\right] &= \mathrm{Tr}\left[\sum_{(i,j)\in(\mathbb{Z}_4)^2} c^l_{i,j}\Gamma_{i,j}\Gamma_{i',j'}\right] \\
&= \sum_{(i,j)\in(\mathbb{Z}_4)^2} c^l_{i,j}\mathrm{Tr}\left[\Gamma_{i,j}\Gamma_{i',j'}\right] \\
&= \sum_{(i,j)\in(\mathbb{Z}_4)^2} \delta_{ii'}\delta_{jj'}4c^l_{i,j} \\
&= 4c^l_{i',j'}
\end{aligned}$$

- Thus we have

$$\begin{aligned}
A &= \frac{1}{2}B_1 - \frac{1}{2}iB_2 \\
&= \frac{1}{2}\sum_{(i,j)\in(\mathbb{Z}_4)^2} c^1_{i,j}\Gamma_{i,j} - \frac{1}{2}i\sum_{(i,j)\in(\mathbb{Z}_4)^2} c^2_{i,j}\Gamma_{i,j} \\
&= \frac{1}{2}\sum_{(i,j)\in(\mathbb{Z}_4)^2} c^1_{i,j}\Gamma_{i,j} - \frac{1}{2}i\sum_{(i,j)\in(\mathbb{Z}_4)^2} c^2_{i,j}\Gamma_{i,j}4 \\
&= \frac{1}{2}\sum_{(i,j)\in(\mathbb{Z}_4)^2} \frac{1}{4}\mathrm{Tr}\left[B_1\Gamma_{i,j}\right]\Gamma_{i,j} - \frac{1}{2}i\sum_{(i,j)\in(\mathbb{Z}_4)^2} \frac{1}{4}\mathrm{Tr}\left[B_2\Gamma_{i,j}\right]\Gamma_{i,j}4 \\
&= \frac{1}{2}\sum_{(i,j)\in(\mathbb{Z}_4)^2} \frac{1}{4}\left\{\mathrm{Tr}\left[B_1\Gamma_{i,j}\right] - i\mathrm{Tr}\left[B_2\Gamma_{i,j}\right]\right\}\Gamma_{i,j} \\
&= \sum_{(i,j)\in(\mathbb{Z}_4)^2} \frac{1}{4}\mathrm{Tr}\left[\left(\frac{1}{2}B_1 - \frac{1}{2}iB_2\right)\Gamma_{i,j}\right]\Gamma_{i,j} \\
&= \sum_{(i,j)\in(\mathbb{Z}_4)^2} \frac{1}{4}\mathrm{Tr}\left[A\Gamma_{i,j}\right]\Gamma_{i,j}
\end{aligned}$$

□

3.1.10. DEFINITION. Define an inner product $\langle A, B\rangle := \frac{1}{4}\mathrm{Tr}[A^*B]$ on $\mathrm{Mat}_{4\times 4}(\mathbb{C})$.

3.1.11. CLAIM. This is indeed an inner product.

PROOF. Firstly, $\langle A, B\rangle = \frac{1}{4}\mathrm{Tr}[A^*B] = \overline{\frac{1}{4}\mathrm{Tr}\left[(A^*B)^*\right]} = \overline{\frac{1}{4}\mathrm{Tr}[B^*A]} \equiv \overline{\langle B, A\rangle}$.

- Let $A \in \mathrm{Mat}_{4\times 4}(\mathbb{C})$ be given. Then

$$\begin{aligned}\langle A,\, A\rangle &= \frac{1}{4}\mathrm{Tr}\left[A^* A\right]\\ &= \frac{1}{4}\mathrm{Tr}\left[\left(\sum_{i,j} c_{i,j}\Gamma_{i,j}\right)^*\left(\sum_{i',j'} c_{i',j'}\Gamma_{i',j'}\right)\right]\\ &= \frac{1}{4}\mathrm{Tr}\left[\left(\sum_{i,j} \overline{c_{i,j}}\Gamma_{i,j}\right)\left(\sum_{i',j'} c_{i',j'}\Gamma_{i',j'}\right)\right]\\ &= \frac{1}{4}\sum_{i,j}\sum_{i',j'}\overline{c_{i,j}}c_{i',j'}\mathrm{Tr}\left[\Gamma_{i,j}\Gamma_{i',j'}\right]\\ &= \sum_{i,j}\left|c_{i,j}\right|^2\\ &\geqslant 0\end{aligned}$$

from this computation we also see that $\langle A,\, A\rangle = 0$ iff $A = 0$.
- Next, to verify conjugate-linearity in the first slot,

$$\begin{aligned}\langle \alpha A + \beta B,\, C\rangle &= \frac{1}{4}\mathrm{Tr}\left[(\alpha A + \beta B)^* C\right]\\ &= \overline{\alpha}\frac{1}{4}\mathrm{Tr}\left[A^* C\right] + \overline{\beta}\frac{1}{4}\mathrm{Tr}\left[B^* C\right]\\ &= \overline{\alpha}\langle A,\, C\rangle + \overline{\beta}\langle A,\, C\rangle\end{aligned}$$

- Thus $\langle , \rangle$ is indeed an inner product, and in fact we have also shown that $\{\Gamma_{i,j}\}$ is an orthonormal basis in this inner product.

□

3.1.12. CLAIM. Six of the $\{\Gamma_{i,j}\}$ matrices are time-reversal invariant and the remaining ten are odd under time-reversal. In particular, the even ones are given by

$$\boxed{\mathrm{TREI} := \{(2,\,1),\,(2,\,2),\,(2,\,3),\,(0,\,0),\,(1,\,0),\,(3,\,0)\}} \tag{28}$$

where TREI stands for "Time-reversal Even Indices".

PROOF. Using the definition given in 1.2.3, we have that

$$\varepsilon = -i\Gamma_{0,2}$$

- Let $(i,\, j) \in (\mathbb{Z}_4)^2$ be given.
- Then using the above preceding claims:

$$\begin{aligned}\Theta\Gamma_{i,j}\Theta^{-1} &= -i\Gamma_{0,2}C\Gamma_{i,j}\left(-i\Gamma_{0,2}C\right)^{-1}\\ &= -i\Gamma_{0,2}C\Gamma_{i,j}C\left(+i\Gamma_{0,2}\right)\\ &= -i\Gamma_{0,2}\overline{\Gamma_{i,j}}\underbrace{CC}_{1}\left(+i\Gamma_{0,2}\right)\\ &= \Gamma_{0,2}\overline{\Gamma_{i,j}}\Gamma_{0,2}\end{aligned}$$

- Compute $\Gamma_{i,j}\Gamma_{0,2}$:

$$\begin{aligned}\Gamma_{i,j}\Gamma_{0,2} &= \left(\sigma_i\otimes\sigma_j\right)\left(\sigma_0\otimes\sigma_2\right)\\ &= \left(\sigma_i\sigma_0\right)\otimes\left(\sigma_j\sigma_2\right)\\ &= \sigma_i\otimes\left(\delta_{j,0}\sigma_2 + \left(1-\delta_{j,0}\right)\left[i\sum_{l=1}^{3}\varepsilon_{lj2}\sigma_l + \delta_{j,2}\sigma_0\right]\right)\\ &= \delta_{j,0}\Gamma_{i,2} + \left(1-\delta_{j,0}\right)\left(i\sum_{l=1}^{3}\varepsilon_{lj2}\Gamma_{i,l} + \delta_{j,2}\Gamma_{i,0}\right)\end{aligned}$$

and $\Gamma_{0,2}\Gamma_{i,j}$:

$$\begin{aligned}\Gamma_{0,2}\Gamma_{i,j} &= (\sigma_0\otimes\sigma_2)(\sigma_i\otimes\sigma_j)\\ &= (\sigma_0\sigma_i)\otimes(\sigma_2\sigma_j)\\ &= \sigma_i\otimes\left(\delta_{j,0}\sigma_2+(1-\delta_{j,0})\left[i\sum_{l=1}^{3}\varepsilon_{l2j}\sigma_l+\delta_{j,2}\sigma_0\right]\right)\\ &= \delta_{j,0}\Gamma_{i,2}+(1-\delta_{j,0})\left(i\sum_{l=1}^{3}\varepsilon_{l2j}\Gamma_{i,l}+\delta_{j,2}\Gamma_{i,0}\right)\end{aligned}$$

- Now use the fact that $\overline{\sigma_i}=\sigma_i(-1)^{\delta_{i,2}}$ and so

$$\begin{aligned}\overline{\Gamma_{i,j}} &= \overline{\sigma_i\otimes\sigma_j}\\ &= \overline{\sigma_i}\otimes\overline{\sigma_j}\\ &= (-1)^{\delta_{i,2}+\delta_{j,2}}\Gamma_{i,j}\end{aligned}$$

to get:

$$\begin{aligned}T\Gamma_{i,j}T^{-1} &= (-1)^{\delta_{i,2}+\delta_{j,2}}\Gamma_{0,2}\Gamma_{i,j}\Gamma_{0,2}\\ &= (-1)^{\delta_{i,2}+\delta_{j,2}}\Gamma_{0,2}\left[\delta_{j,0}\Gamma_{i,2}+(1-\delta_{j,0})\left(i\sum_{l=1}^{3}\varepsilon_{lj2}\Gamma_{i,l}+\delta_{j,2}\Gamma_{i,0}\right)\right]\\ &= (-1)^{\delta_{i,2}+\delta_{j,2}}\left[\delta_{j,0}\underbrace{\Gamma_{0,2}\Gamma_{i,2}}_{\Gamma_{i,0}}+(1-\delta_{j,0})\left(i\sum_{l=1}^{3}\varepsilon_{lj2}\underbrace{\Gamma_{0,2}\Gamma_{i,l}}_{\left(i\sum_{k=1}^{3}\varepsilon_{k2l}\Gamma_{i,k}+\delta_{l,2}\Gamma_{i,0}\right)}+\delta_{j,2}\underbrace{\Gamma_{0,2}\Gamma_{i,0}}_{\Gamma_{i,2}}\right)\right]\\ &= (-1)^{\delta_{i,2}+\delta_{j,2}}\left[\delta_{j,0}\Gamma_{i,j}+(1-\delta_{j,0})\left(-\sum_{k=1}^{3}\underbrace{\sum_{l=1}^{3}\varepsilon_{lj2}\varepsilon_{lk2}}_{\delta_{j,k}\delta_{2,2}-\delta_{j,2}\delta_{k,2}}\Gamma_{i,k}+\delta_{j,2}\Gamma_{i,j}\right)\right]\\ &= (-1)^{\delta_{i,2}+\delta_{j,2}}\left[\delta_{j,0}\Gamma_{i,j}+(1-\delta_{j,0})\left(-\Gamma_{i,j}+2\delta_{j,2}\Gamma_{i,j}\right)\right]\\ &= (-1)^{\delta_{i,2}+\delta_{j,2}}\left[\delta_{j,0}\Gamma_{i,j}+(1-\delta_{j,0})\left(-(1-\delta_{j,2}+\delta_{j,2})\Gamma_{i,j}+2\delta_{j,2}\Gamma_{i,j}\right)\right]\\ &= \delta_{j,0}(-1)^{\delta_{i,2}+\delta_{j,2}}\Gamma_{i,j}+(1-\delta_{j,0})(1-\delta_{j,2})(-1)^{\delta_{i,2}+\delta_{j,2}+1}\Gamma_{i,j}+(1-\delta_{j,0})\delta_{j,2}(-1)^{\delta_{i,2}+\delta_{j,2}}\Gamma_{i,j}\\ &= \delta_{j,0}(-1)^{\delta_{i,2}}\Gamma_{i,j}+\delta_{j,2}(-1)^{\delta_{i,2}+1}\Gamma_{i,j}+(1-\delta_{j,0})(1-\delta_{j,2})(-1)^{\delta_{i,2}+1}\Gamma_{i,j}\\ &= \delta_{j,0}(-1)^{\delta_{i,2}}\Gamma_{i,j}+(1-\delta_{j,0})(-1)^{\delta_{i,2}+1}\Gamma_{i,j}\end{aligned}$$

- As a result we see that there are exactly 6 combination of indices for which $\Theta\Gamma_{i,j}\Theta^{-1}=\Gamma_{i,j}$: $j=0$, $i\neq 2$ (3 indices) and $j\neq 0$ and $i=2$ (3 indices). This matches the definition of Eq. (28). For the other 10 indices, $\Theta\Gamma_{i,j}\Theta^{-1}=-\Gamma_{i,j}$.

□

3.1.13. Claim. Six of the $\{\Gamma_{i,j}\}$ matrices are spacetime-inversion invariant and the remaining ten are odd under this composite transformation. In particular, the even ones are given by

$$\boxed{STREI := \{(0,0),(1,0),(2,0),(3,1),(3,2),(3,3)\}} \quad (29)$$

where STREI stands for "Space-Time-Reversal Even Indices".

Proof. Following [Fu07], we define the parity (space reversal) operator Π as

$$\Pi := \Gamma_{1,0}$$

An even index pair (i,j) is such that

$$(\Pi\Theta)\Gamma_{i,j}(\Pi\Theta)^{-1}=\Gamma_{i,j}$$

- Let $(i,j)\in(\mathbb{Z}_4)^2$ be given.

- Then using the above we have:

$$\begin{aligned}\Pi\Theta\Gamma_{i,j}(\Pi\Theta)^{-1} &= \Gamma_{1,0}(-i)\Gamma_{0,2}C\Gamma_{i,j}\left(\Gamma_{1,0}(-i)\Gamma_{0,2}C\right)^{-1}\\ &= \Gamma_{1,0}(-i)\Gamma_{0,2}C\Gamma_{i,j}C\Gamma_{0,2}(+i)\Gamma_{1,0}\\ &= \Gamma_{1,0}\Gamma_{0,2}\overline{\Gamma_{i,j}}\Gamma_{0,2}\Gamma_{1,0}\\ &= \Gamma_{1,0}T\Gamma_{i,j}T^{-1}\Gamma_{1,0}\\ &= \Gamma_{1,0}\left[\delta_{j,0}(-1)^{\delta_{i,2}}\Gamma_{i,j}+\left(1-\delta_{j,0}\right)(-1)^{\delta_{i,2}+1}\Gamma_{i,j}\right]\Gamma_{1,0}\\ &= \delta_{j,0}(-1)^{\delta_{i,2}}\Gamma_{1,0}\Gamma_{i,j}\Gamma_{1,0}+\left(1-\delta_{j,0}\right)(-1)^{\delta_{i,2}+1}\Gamma_{1,0}\Gamma_{i,j}\Gamma_{1,0}\end{aligned}$$

- Compute $\Gamma_{i,j}\Gamma_{1,0}$:

$$\begin{aligned}\Gamma_{i,j}\Gamma_{1,0} &= \left(\sigma_i\otimes\sigma_j\right)\left(\sigma_1\otimes\sigma_0\right)\\ &= \left(\sigma_i\sigma_1\right)\otimes\left(\sigma_j\sigma_0\right)\\ &= \left(\delta_{i,0}\sigma_1+\left(1-\delta_{i,0}\right)\left(i\sum_{l=1}^{3}\varepsilon_{i1l}\sigma_l+\delta_{i1}\sigma_0\right)\right)\sigma_j\\ &= \delta_{i,0}\Gamma_{1,j}+\left(1-\delta_{i,0}\right)\left(i\sum_{l=1}^{3}\varepsilon_{i1l}\Gamma_{l,j}+\delta_{i1}\Gamma_{0,j}\right)\end{aligned}$$

and $\Gamma_{1,0}\Gamma_{i,j}$:

$$\begin{aligned}\Gamma_{1,0}\Gamma_{i,j} &= \left(\sigma_1\otimes\sigma_0\right)\left(\sigma_i\otimes\sigma_j\right)\\ &= \left(\sigma_1\sigma_i\right)\otimes\left(\sigma_0\sigma_j\right)\\ &= \left(\delta_{i,0}\sigma_1+\left(1-\delta_{i,0}\right)\left(i\sum_{l=1}^{3}\varepsilon_{1il}\sigma_l+\delta_{i1}\sigma_0\right)\right)\sigma_j\\ &= \delta_{i,0}\Gamma_{1,j}+\left(1-\delta_{i,0}\right)\left(i\sum_{l=1}^{3}\varepsilon_{1il}\Gamma_{l,j}+\delta_{i1}\Gamma_{0,j}\right)\end{aligned}$$

- As a result we have that

$$\begin{aligned}\Gamma_{1,0}\Gamma_{i,j}\Gamma_{1,0} &= \Gamma_{1,0}\left\{\delta_{i,0}\Gamma_{1,j}+\left(1-\delta_{i,0}\right)\left(i\sum_{l=1}^{3}\varepsilon_{i1l}\Gamma_{l,j}+\delta_{i,1}\Gamma_{0,j}\right)\right\}\\ &= \delta_{i,0}\underbrace{\Gamma_{1,0}\Gamma_{1,j}}_{\Gamma_{0,j}}+\left(1-\delta_{i,0}\right)\left(i\sum_{l=2}^{3}\varepsilon_{i1l}\underbrace{\Gamma_{1,0}\Gamma_{l,j}}_{i\sum_{l'=2}^{3}\varepsilon_{1ll'}\Gamma_{l',j}}+\delta_{i,1}\underbrace{\Gamma_{1,0}\Gamma_{0,j}}_{\Gamma_{1,j}}\right)\\ &= \delta_{i,0}\Gamma_{i,j}+\left(1-\delta_{i,0}\right)\left(\sum_{l'=2}^{3}\underbrace{\sum_{l=2}^{3}\varepsilon_{i1l}\varepsilon_{1l'l}}_{\delta_{i,1}\delta_{1,l'}-\delta_{i,l'}\delta_{1,1}}\Gamma_{l',j}+\delta_{i,1}\Gamma_{i,j}\right)\\ &= \delta_{i,0}\Gamma_{i,j}+\left(1-\delta_{i,0}\right)\left(-\left(1-\delta_{i,1}\right)\Gamma_{i,j}+\delta_{i,1}\Gamma_{i,j}\right)\\ &= -\left(1-\delta_{i,0}\right)\left(1-\delta_{i,1}\right)\Gamma_{i,j}+\left(\delta_{i,0}+\delta_{i,1}\right)\Gamma_{i,j}\\ &= (-1)^{\delta_{i,2}+\delta_{i,3}}\Gamma_{i,j}\end{aligned}$$

so that

$$\begin{aligned}\Pi\Theta\Gamma_{i,j}(\Pi\Theta)^{-1} &= \delta_{j,0}(-1)^{\delta_{i,2}}(-1)^{\delta_{i,2}+\delta_{i,3}}\Gamma_{i,j}+\left(1-\delta_{j,0}\right)(-1)^{\delta_{i,2}+1}(-1)^{\delta_{i,2}+\delta_{i,3}}\Gamma_{i,j}\\ &= \delta_{j,0}(-1)^{\delta_{i,3}}\Gamma_{i,j}+\left(1-\delta_{j,0}\right)(-1)^{1+\delta_{i,3}}\Gamma_{i,j}\end{aligned}$$

- Thus we see that those indices that are $\Pi\Theta$ invariant are $j=0$ and $i\neq 3$ or alternatively $j\neq 0$ and $i=3$: $(0,0)$, $(1,0)$, $(2,0)$, $(3,1)$, $(3,2)$, $(3,3)$, as in Eq. (29).

□

3.2. Setting

As a consequence of 3.1.9, when $N = 4$, the most general Bloch decomposed Hamiltonian may be written as

$$H^B(k) = \sum_{(i,j)\in(\mathbb{Z}_4)^2} d_{i,j}(k)\,\Gamma_{i,j}$$

with real coefficients

$$d_{i,j}(k) = \frac{1}{4}\mathrm{Tr}\left[H^B(k)\,\Gamma_{i,j}\right]$$

but we don't use the particular form of the $d_{i,j}$ coefficients.

Using 1.6.5 and 1.7.9 we may without loss of generality assume that $d_{0,0}(k) = 0$, using the fact that it would merely shift the bulk spectrum by a constant amount at each point k, but cannot close the gap. Furthermore, we assume that $H^B(k)$ is time-reversal invariant, as in Eq. (3), which now after Bloch decomposition on the k_1 axis is given by 1.3.1:

$$H^B(-k) = \Theta H^B(k)\,\Theta^{-1} \tag{30}$$

and finally we assume that there is always ($\forall k \in \mathbb{T}^2$) a gap between the two lower bands and the two upper bands. Note that we do allow for the two lower bands intersect, and similarly for the two upper bands.

3.2.1. CLAIM. Due to Eq. (30) it follows that

$$d_{i,j}(-k) = d_{i,j}(k) \quad \forall (i,j) \in TREI$$

and

$$d_{i,j}(-k) = -d_{i,j}(k) \quad \forall (i,j) \notin TREI$$

PROOF.

- Assume Eq. (30).
- Then

$$\begin{aligned}
\Theta\left(\sum_{(i,j)\in(\mathbb{Z}_4)^2} d_{i,j}(k)\,\Gamma_{i,j}\right)\Theta^{-1} &= \sum_{(i,j)\in(\mathbb{Z}_4)^2} d_{i,j}(-k)\,\Gamma_{i,j}\\
\left[\left(\sum_{(i,j)\in TREI} d_{i,j}(k)\,\underbrace{\Theta\Gamma_{i,j}\Theta^{-1}}_{\Gamma_{i,j}}\right) + \left(\sum_{(i,j)\in TREI^c} d_{i,j}(k)\,\underbrace{\Theta\Gamma_{i,j}\Theta^{-1}}_{-\Gamma_{i,j}}\right)\right] &= \sum_{(i,j)\in(\mathbb{Z}_4)^2} d_{i,j}(-k)\,\Gamma_{i,j}\\
\sum_{(i,j)\in TREI} d_{i,j}(k)\,\Gamma_{i,j} - \sum_{(i,j)\in TREI^c} d_{i,j}(k)\,\Gamma_{i,j} &= \sum_{(i,j)\in(\mathbb{Z}_4)^2} d_{i,j}(-k)\,\Gamma_{i,j}
\end{aligned}$$

- Now we can use the inner product and the fact that the $\Gamma_{i,j}$ matrices are orthogonal with respect to it deduce the claim.

□

The following claim is not strictly necessary for the succession of the correspondence proof.

3.2.2. CLAIM. The most general Hamiltonian can be described by a total of 10 real functions on $\mathbb{T}^2$ (instead of the original 15).

PROOF. As a result of the above symmetries there are a few simplifications we can make to the Hamiltonian (written here over two lines to fit on the page)

$$
\begin{aligned}
d_{i,j}(k)\Gamma_{i,j} &= \begin{bmatrix} d_{03}(k)+d_{30}(k)+d_{3,3}(k) & d_{01}(k)+d_{31}(k)+i\left[-d_{02}(k)-d_{32}(k)\right] & \downarrow & \downarrow \\ \cdots & -d_{03}(k)+d_{30}(k)-d_{33}(k) & \downarrow & \downarrow \\ \cdots & \cdots & \downarrow & \downarrow \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \\
&= \begin{bmatrix} \uparrow & \uparrow & d_{10}(k)+d_{13}(k)+i\left[-d_{23}(k)-d_{20}(k)\right] & d_{11}(k)-d_{22}(k)+i\left[-d_{12}(k)-d_{21}(k)\right] \\ \cdots & \uparrow & d_{11}(k)+d_{22}(k)+i\left[d_{12}(k)-d_{21}(k)\right] & d_{10}(k)-d_{13}(k)+i\left[d_{23}(k)-d_{20}(k)\right] \\ \cdots & \cdots & d_{03}(k)-d_{30}(k)-d_{33}(k) & d_{01}(k)-d_{31}(k)+i\left[d_{32}(k)-d_{02}(k)\right] \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \\
&= \begin{bmatrix} d_{03}(k)+d_{30}(k)+d_{3,3}(k) & d_{01}(k)+d_{31}(k)+i\left[-d_{02}(k)-d_{32}(k)\right] & \downarrow & \downarrow \\ \cdots & d_{03}(-k)+d_{30}(-k)+d_{33}(-k) & \downarrow & \downarrow \\ \cdots & \cdots & \downarrow & \downarrow \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \\
&= \begin{bmatrix} \uparrow & \uparrow & d_{10}(k)+d_{13}(k)-i\left[d_{23}(k)+d_{20}(k)\right] & d_{11}(k)-d_{22}(k)+i\left[-d_{12}(k)-d_{21}(k)\right] \\ \cdots & \uparrow & -d_{11}(-k)+d_{22}(-k)+i\left[-d_{12}(-k)-d_{21}(-k)\right] & d_{10}(-k)+d_{13}(-k)+i\left[d_{23}(-k)+d_{20}(-k)\right] \\ \cdots & \cdots & d_{03}(k)-d_{30}(k)-d_{33}(k) & d_{01}(k)-d_{31}(k)+i\left[d_{32}(k)-d_{02}(k)\right] \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \\
&= \begin{bmatrix} d_{03}(k)+d_{30+33}(k) & d_{01}(k)+d_{31}(k)-i\left[d_{32}(k)+d_{02}(k)\right] & \downarrow & \downarrow \\ \cdots & d_{03}(-k)+d_{30+33}(-k) & \downarrow & \downarrow \\ \cdots & \cdots & \downarrow & \downarrow \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \\
&= \begin{bmatrix} \uparrow & \uparrow & d_{10+13}(k)-id_{23+20}(k) & d_{11-22}(k)-id_{12+21}(k) \\ \cdots & \uparrow & -d_{11-22}(-k)-id_{12+21}(-k) & d_{10+13}(-k)+id_{23+20}(-k) \\ \cdots & \cdots & d_{03}(k)-d_{30+33}(k) & d_{01}(k)-d_{31}(k)+i\left[d_{32}(k)-d_{02}(k)\right] \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \\
&= \begin{bmatrix} d_1(k) & z_3(k) & \overline{z_5(k)} & \overline{z_6(k)} \\ \cdots & d_1(-k) & -\overline{z_6(-k)} & \overline{z_5(-k)} \\ \cdots & \cdots & d_2(k) & z_4(k) \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix}
\end{aligned}
$$

where we use the shorthand notation of $d_{ij\pm lm}(k)$ to denote $d_{ij}(k) \pm d_{lm}(k)$, and have defined the two real functions

$$
\begin{aligned}
d_1(k) &:= d_{03}(k) + d_{30+33}(k) \\
d_2(k) &:= d_{03}(k) - d_{30+33}(k)
\end{aligned}
$$

and four complex functions

$$
\begin{aligned}
z_3(k) &:= d_{01}(k) + d_{31}(k) - i\left[d_{32}(k) + d_{02}(k)\right] \\
z_4(k) &:= d_{01}(k) - d_{31}(k) + i\left[d_{32}(k) - d_{02}(k)\right] \\
z_5(k) &:= d_{10+13}(k) - id_{23+20}(k) \\
z_6(k) &:= d_{11-22}(k) - id_{12+21}(k)
\end{aligned}
$$

The fact we merge the $d_{ij\pm lm}(k)$ coefficients is because their constituents do not appear independently. So we have reduced the problem from 15 real functions,

$$\left\{ d_{(i,j)} \right\}_{(i,j)\in(\mathbb{Z}_4)^2\setminus\{(0,0)\}} \subset \mathbb{R}^{\mathbb{T}^2}$$

to 10 real functions on $\mathbb{T}^2$:

$$\{d_1, d_2\} \cup \{\Re\{z_i\}, \Im\{z_i\}\}_{i\in\{3,4,5,6\}} \subset \mathbb{R}^{\mathbb{T}^2}$$

For the new functions, we have the following symmetries:

- $\Re\{z_3(k)\} \equiv d_{01}(k) + d_{31}(k) = -d_{01}(-k) - d_{31}(-k) \equiv -\Re\{z_3(-k)\}$
- $\Im\{z_3(k)\} \equiv -d_{32}(k) - d_{02}(k) = d_{32}(-k) + d_{02}(-k) \equiv -\Im\{z_3(-k)\}$
- Thus, $z_3(k) = -z_3(-k)$.
- Similarly, $z_4(k) = -z_4(-k)$.

- $(d_1 + d_2)(k) = -(d_1 + d_2)(-k)$.

There are no other symmetries. □

3.2.3. CLAIM. Let $A \subset (\mathbb{Z}_4)^2 \setminus \{(0,0)\}$ be given such that $\{\Gamma_i, \Gamma_j\} = 2\delta_{i,j} \forall (i,j) \in A^2$. If

$$d_j(k) = \frac{1}{4}\mathrm{Tr}\left[H^B(k)\Gamma_j\right] = 0 \quad \forall j \in A^c$$

then 1.7.7 reduces to

$$\boxed{\mathcal{I}_{KM}(H) = \begin{cases} 0 & |A \cap TREI| > 1 \\ \frac{1}{i\pi}\log\left(\prod_{k\in TRIM}\mathrm{sgn}(d_e(k))\right) & A \cap TREI = \{e\} \end{cases}} \tag{31}$$

PROOF. We divide into two cases according to Eq. (31):

(1) Case 1: $A \cap TREI = \{e\}$.

The following proof is a generalization of one given in [Fu07] for the case of spacetime-inversion symmetric systems, where here Γ_e takes the role of space-inversion.

3.2.4. CLAIM. $\left[H^B(k), \Gamma_e\Theta\right] = 0$.

PROOF. We calculate

$$\begin{aligned}\left[H^B(k), \Gamma_e\Theta\right] &= \left[\sum_{i\in A} d_i(k)\Gamma_i, \Gamma_e\Theta\right] \\ &= \sum_{i\in A} d_i(k)[\Gamma_i, \Gamma_e\Theta] \\ &= \sum_{i\in A\setminus\{e\}} d_i(k)[\Gamma_i, \Gamma_e\Theta] + d_e(k)[\Gamma_e, \Gamma_e\Theta]\end{aligned}$$

But

$$\begin{aligned}[\Gamma_e, \Gamma_e\Theta] &= \Gamma_e\Gamma_e\Theta - \Gamma_e\Theta\Gamma_e \\ &\overset{e\in TREI}{=} \Gamma_e\Gamma_e\Theta - \Gamma_e\Gamma_e\Theta \\ &= 0\end{aligned}$$

and

$$\begin{aligned}[\Gamma_i, \Gamma_e\Theta] &= \Gamma_i\Gamma_e\Theta - \Gamma_e\Theta\Gamma_i \\ &\overset{i\notin TREI}{=} \Gamma_i\Gamma_e\Theta + \Gamma_e\Gamma_i\Theta \\ &= \underbrace{\{\Gamma_i, \Gamma_e\}}_{0}\Theta \\ &= 0\end{aligned}$$

□

3.2.5. CLAIM. $H^B(-k) = \Gamma_e H^B(k)(\Gamma_e)^{-1}$

PROOF. From 3.2.4 it follows that

$$\begin{aligned} H^B(k) &= \Gamma_e \Theta H^B(k) (\Gamma_e \Theta)^{-1} \\ &= \Gamma_e \Theta H^B(k) \Theta^{-1} (\Gamma_e)^{-1} \end{aligned}$$

and using Eq. (30) we then have that

$$\begin{aligned} H^B(-k) &= \Theta H^B(k) \Theta^{-1} \\ &= \Theta \left[\Gamma_e \Theta H^B(k) \Theta^{-1} (\Gamma_e)^{-1} \right] \Theta^{-1} \\ &= \Theta \Theta \Gamma_e H^B(k) (\Gamma_e)^{-1} \Theta^{-1} \Theta^{-1} \\ &= (-1) \Gamma_e H^B(k) (\Gamma_e)^{-1} (-1) \\ &= \Gamma_e H^B(k) (\Gamma_e)^{-1} \end{aligned}$$

where we have used that if $[A, B] \Longrightarrow [A^{-1}, B^{-1}]$ as well as $A^2 = -1 \Longrightarrow (A^{-1})^2 = -1$. □

3.2.6. DEFINITION. Define a 2×2 matrix by its components

$$\nu_{m,n}(k) = \langle \psi_m(k), \Gamma_e \Theta \psi_n(k) \rangle \quad \forall (m, n) \in (J_2)^2$$

where $\psi_n(k) \in \mathbb{C}^4$ is the nth eigenstate of $H^B(k)$ and we are assuming that the 1 and 2 bands are the occupied ones.

3.2.7. CLAIM. $\nu(k)$ is an anti-symmetric matrix.

PROOF. Note that due to Θ being anti-linear, we have that $\langle \Theta\phi, \Theta\chi \rangle = \overline{\langle \phi, \chi \rangle} = \langle \chi, \phi \rangle$ so that

$$\begin{aligned} \nu_{mn}(k) &\equiv \langle \psi_m(k), \Gamma_e \Theta \psi_n(k) \rangle \\ &= \langle \Theta \Gamma_e \Theta \psi_n(k), \Theta \psi_m(k) \rangle \\ &\overset{e \in TREI}{=} \langle \Gamma_e \Theta \Theta \psi_n(k), \Theta \psi_m(k) \rangle \\ &= -\langle \Gamma_e \psi_n(k), \Theta \psi_m(k) \rangle \\ &= -\left\langle \psi_n(k), (\Gamma_e)^* \Theta \psi_m(k) \right\rangle \\ &\overset{(\Gamma_l)^* = \Gamma_l}{=} -\langle \psi_n(k), \Gamma_e \Theta \psi_m(k) \rangle \\ &\equiv -\nu_{nm}(k) \end{aligned}$$

□

3.2.8. COROLLARY. *The Pfaffian of* $\nu(k)$ *is defined and it is given by*

$$\mathrm{Pf}[\nu(k)] = \nu_{12}(k)$$

3.2.9. CLAIM. $|\mathrm{Pf}[\nu(k)]| = 1$.

PROOF. Using 3.2.4 we have that $\psi_m(k)$ and $\Gamma_e\Theta\psi_m(k)$ are both eigenstates of the same energy.

CLAIM. $\Gamma_e\Theta\psi_m(k)$ is linearly independent of $\psi_m(k)$.

PROOF. Assume otherwise. Then

$$\Gamma_e\Theta\psi_m(k) = \alpha\psi_m(k) \tag{32}$$

for some $\alpha \in \mathbb{C}$. Apply $\Gamma_e\Theta$ on both sides of Eq. (32) to obtain on the one hand:

$$\Gamma_e\Theta\Gamma_e\Theta\psi_m(k) = -\psi_m(k)$$

and on the other hand

$$\begin{aligned}\Gamma_e\Theta\Gamma_e\Theta\psi_m(k) &= \Gamma_e\Theta\alpha\psi_m(k)\\ &= \overline{\alpha}\Gamma_e\Theta\psi_m(k)\\ &= |\alpha|^2\psi_m(k)\end{aligned}$$

so that we have $|\alpha|^2 = -1$ which is not possible. □

As a result, because there are only two states, we conclude that $\psi_1(k) = e^{i\theta(k)}\Gamma_e\Theta\psi_2(k)$ for some $\theta : \mathbb{T}^2 \to \mathbb{R}$.

We then have that

$$\begin{aligned}|\mathrm{Pf}[v(k)]| &= |v_{12}(k)|\\ &= |\langle\psi_1(k), \Gamma_e\Theta\psi_2(k)\rangle|\\ &= \left|\left\langle\psi_1(k), e^{-i\theta(k)}\psi_1(k)\right\rangle\right|\\ &= \left|e^{-i\theta(k)}\langle\psi_1(k), \psi_1(k)\rangle\right|\\ &= 1\end{aligned}$$

□

3.2.10. CLAIM. Without loss of generality, we may assume that we are in such a gauge such that $\mathrm{Pf}[v(k)] = 1$.

PROOF. Under the action of a gauge transformation of the form

$$\psi_n(k) \overset{G}{\mapsto} e^{i\alpha(k)\delta_{n,1}}\psi_n(k)$$

$\mathrm{Pf}[v(k)]$ transforms as

$$\begin{aligned}\mathrm{Pf}[v(k)] &\overset{G}{\mapsto} \left\langle e^{i\alpha(k)}\psi_1(k), \Gamma_e\Theta\psi_2(k)\right\rangle\\ &= e^{-i\alpha(k)}\langle\psi_1(k), \Gamma_e\Theta\psi_2(k)\rangle\\ &= e^{-i\alpha(k)}\mathrm{Pf}[v(k)]\end{aligned}$$

Thus, according to 3.2.9, $\mathrm{Pf}[v(k)] = e^{-i\theta(k)}$ and so if we pick $\alpha = -\theta$ then we can make sure that $\mathrm{Pf}[v(k)] = 1$ for all $k \in \mathbb{T}^2$. □

3.2.11. CLAIM. Using 3.2.10 we then have that

$$\det[w(k)] = 1$$

where w was defined in Eq. (23).

PROOF. Observe that

$$\mathrm{span}\left(\{\Theta\psi_m(k)\}_{m=1}^2\right)=\mathrm{span}\left(\{\psi_m(-k)\}_{m=1}^2\right)$$

so that

$$\begin{aligned}
v_{mn}(-k) &= \langle\psi_m(-k),\Gamma_e\Theta\psi_n(-k)\rangle\\
&= \sum_{l\in J_2}\langle\psi_m(-k),\Theta\psi_l(k)\rangle\langle\Theta\psi_l(k),\Gamma_e\Theta\psi_n(-k)\rangle\\
&= \sum_{l\in J_2} w_{ml}(k)\langle\Theta\psi_l(k),\Gamma_e\Theta\psi_n(-k)\rangle\\
&= \sum_{l\in J_2} w_{ml}(k)\left\langle(\Gamma_e)^*\Theta\psi_l(k),\Theta\psi_n(-k)\right\rangle\\
&= \sum_{l\in J_2} w_{ml}(k)\langle\Gamma_e\Theta\psi_l(k),\Theta\psi_n(-k)\rangle\\
&= \sum_{(l,r)\in(J_2)^2} w_{ml}(k)\langle\Gamma_e\Theta\psi_l(k),\psi_r(k)\rangle\langle\psi_r(k),\Theta\psi_n(-k)\rangle\\
&= \sum_{(l,r)\in(J_2)^2} w_{ml}(k)\overline{\langle\psi_r(k),\Gamma_e\Theta\psi_l(k)\rangle}\left\langle\Theta^2\psi_n(-k),\Theta\psi_r(k)\right\rangle\\
&= \sum_{(l,r)\in(J_2)^2} w_{ml}(k)\overline{v_{rl}(k)}(-1)w_{nr}(k)\\
&\overset{v=-v^T}{=} \sum_{(l,r)\in(J_2)^2} w_{ml}(k)\overline{v_{lr}(k)}w_{nr}(k)
\end{aligned}$$

so that we find the matrix equation

$$v(-k)=w(k)\overline{v(k)}[w(k)]^T$$

Taking the Pfaffian of this equation we have then that

$$\mathrm{Pf}[v(-k)]=\mathrm{Pf}\left[w(k)\overline{v(k)}[w(k)]^T\right]$$

and using the identity $\mathrm{Pf}\left[XAX^T\right]=\mathrm{Pf}[A]\det[X]$ we then have

$$\mathrm{Pf}[v(-k)]=\mathrm{Pf}\left[\overline{v(k)}\right]\det[w(k)]$$

and the result follows. □

Note that because $H^B(k)$ is comprised of anti-commuting gamma matrices, we may employ 1.5 to obtain that the two lower bands are always-degenerate with energy

$$E^B_{lower}(k)=-\|d(k)\|$$

Next, due to the fact that $\det[w(k)]=1$ for all $k\in\mathbb{T}^2$, we don't need to worry about picking the right branch of $\sqrt{\det[w(k)]}$ continuously over $\mathbb{T}^2$ and thus Eq. (25) reduces to

$$\mathcal{I}_{KM}(H):=\frac{1}{i\pi}\log\left(\prod_{k\in TRIM}\frac{1}{\mathrm{Pf}[w(k)]}\right)$$

and our only concern is to compute $\mathrm{Pf}[w(k)]$ at $k\in TRIM$. But At $k\in TRIM$, $H^B(k)=d_e(k)\Gamma_e$ because of $d_i(-k)=-d_i(k)\,\forall i\notin TREI$. Thus we have

$$\begin{aligned}
d_e(k)\Gamma_e\psi_n(k) &= -|d_e(k)|\psi_n(k)\\
\Gamma_e\psi_n(k) &= -\mathrm{sgn}(d_e(k))\psi_n(k)
\end{aligned}$$

Then we calculate $w(k)$ at $k \in \text{TRIM}$:

$$\begin{aligned} w_{mn}(k) &\equiv \langle \psi_m(-k), \Theta\psi_n(k)\rangle \\ &= \langle \psi_m(k), \Theta\psi_n(k)\rangle \\ &= \langle \psi_m(k), \Gamma_e\Gamma_e\Theta\psi_n(k)\rangle \\ &= \langle \Gamma_e\psi_m(k), \Gamma_e\Theta\psi_n(k)\rangle \\ &= -\text{sgn}(d_e(k))\langle \psi_m(k), \Gamma_e\Theta\psi_n(k)\rangle \\ &= -\text{sgn}(d_e(k))\, v_{mn}(k) \end{aligned}$$

so that

$$\begin{aligned} \text{Pf}[w(k)] &= w_{12}(k) \\ &= -\text{sgn}(d_e(k))\, v_{12}(k) \\ &= -\text{sgn}(d_e(k))\,\text{Pf}[v(k)] \\ &= -\text{sgn}(d_e(k)) \end{aligned}$$

And the result follows using the fact that $|\text{TRIM}| \in 2\mathbb{N}$.

Note that in particular, $d_e(k) \neq 0 \forall k \in \text{TRIM}$ because otherwise $d = 0$ at such a point, and then the gap closes, which by hypothesis is not possible.

(2) Case 2: $|A \cap \text{TREI}| > 1$.

(a) Case 2.1: $A \subseteq \text{TREI}$.

In this case we have that all $d_j(k)$ coefficients are symmetric, and as a result, the TRI condition $H^B(-k) = \Theta H^B(k)\Theta^{-1}$ becomes $\left[H^B(k), \Theta\right] = 0$ by virtue of $H^B(-k) = H^B(k)$.

3.2.12. DEFINITION. Define a matrix u by its components

$$u_{mn}(k) := \langle \psi_m(k), \Theta\psi_n(k)\rangle \,\forall (m, n) \in (J_2)^2$$

It is easy to verify just as above that u is anti-symmetric (unlike w, but like v) on the whole of $\mathbb{T}^2$.

3.2.13. CLAIM. $|\text{Pf}[u(k)]| = 1$.

PROOF. Using $\left[H^B(k), \Theta\right] = 0$ we have that $\psi_n(k)$ and $\Theta\psi_n(k)$ are eigenstates of the same energy, but as above, they cannot be linearly dependent so that $\psi_1(k) = e^{i\theta(k)}\Theta\psi_2(k)$ for some $\theta : \mathbb{T}^2 \to \mathbb{R}$. □

Again, we pick a gauge in which $\text{Pf}[u(k)] = 1$ and similarly we have again that $u(-k) = w(k)\overline{u(k)}[w(k)]^T$ so that $\det[w(k)] = 1$ here as well. On $k \in \text{TRIM}$, $w = u$ and so $\text{Pf}[w(k)] = 1$ for all $k \in \text{TRIM}$. As a result, in this case we find that

$$\mathcal{I}_{KM}(H) = 0$$

(b) Case 2.2: $H^B(k) = H^B_0 \forall k \in \mathbb{T}^2$.

Here we actually still have $H^B(k) = H^B(-k)$ trivially and so the preceding case covers this one.

(c) Case 2.3: None of the above.

3.2.14. CLAIM. If $|A \cap \text{TREI}| > 1$ then $H^B(k)$ is nullhomotopic (to be justified in 3.2.15).

As a result, we may adiabatically transform $H^B(k)$ to a constant and so $\mathcal{I}_{KM}(H) = 0$ again.

□

3.2.15. REMARK. The formula in 3.2.3 can also be justified using a geometric argument.

PROOF. First note that without loss of generality we may assume that $\left|E^B(k)\right| = 1$, as such a smooth change to H^B would not close the gap. As a result, $\|d(k)\| = 1$ at all points $k \in \mathbb{T}^2$. Also note that due to the Clifford algebra, the maximal value of $|A|$ is 5 so that in the general case we therefore have $d(k) \in S^4$ and this defines a map $\mathbb{T}^2 \ni k \mapsto d(k) \in S^4$ which we seek to classify, up to homotopies which preserve TRI. Note that in this setting, preserving TRI means preserving the evenness or oddness of the componenets of d.

Our way to make this classification follows the beginning of [**Mo07**] closely: we work with the EBZ ("effective brillouin zone"), where due to Eq. (30), $H^B(k)$ can be fully specified on merely *half* of $\mathbb{T}^2$, with special boundary

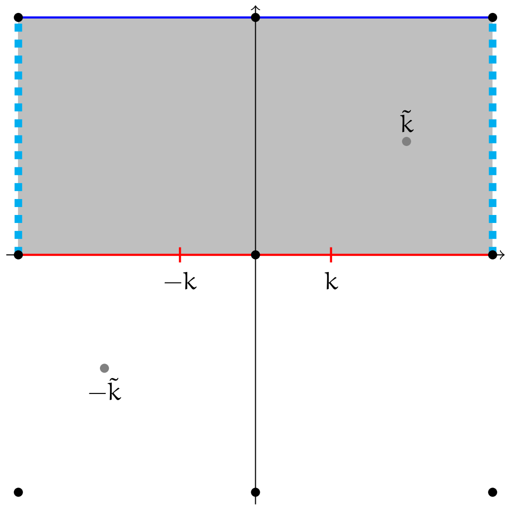

FIGURE 3.2.1. Instead of specifying Hamiltonians on the whole of $\mathbb{T}^2$, we only need to specify Hamiltonians in the shaded area. Within that area, TRI does not need to be enforced. The dashed cyan lines are stiched together as before to form a cylinder, and the red and blue circles must still obey TRI, because their k and $-k$ partners are both included in the effective brillouin zone.

conditions. In the interior of the half-torus there is no need to employ Eq. (30) because there is no partner $-k$ included in the EBZ for each given $k \in \text{EBZ}$. That is, except at the boundary circles.

Concretely, we pick the EBZ half torus to work on as $k_1 \in [-\pi, \pi]$ and $k_2 \in [0, \pi]$. Then, the upper-right quadrant $k \in [0, \pi] \times [0, \pi]$ specifies what happens on the lower-left quadrant $k \in [-\pi, 0] \times [-\pi, 0]$ and similarly the upper-left quadrant specifies what happens on the lower-right quadrant, all thanks to Eq. (30). We still need to stich together the two boundaries at the lines $k_1 = \pi$ and $k_1 = -\pi$ so that we are left with a cylinder: $(k_1, k_2) \in S^1 \times [0, \pi]$ where k_1 can be thought of as the angle parameter of the cylinder and k_2 is the "height" parameter of the cylinder. Notice that the two circles at the top and the bottom of $S^1 \times [0, \pi]$ *are* included in the EBZ.

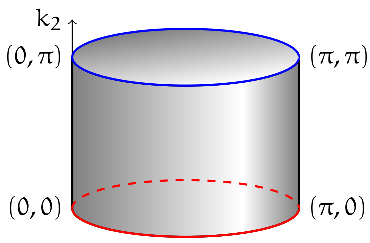

FIGURE 3.2.2. The resulting cylinder from the effective Brillouin zone. The upper and lower discs are not included, but their boundary circles (red and blue) are, and only on them do we enforce TRI.

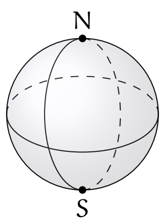

FIGURE 3.2.3. A path on S^4 (here depicted as S^2 for simplicity) which has to start at N and end at S cannot be deformed into one that starts and ends at N.

We now turn to the boundary conditions: Even though $H^B(k)$ has no further conditions on $S^1 \times (0, \pi)$, on the boundary circles, $S^1 \times \{0\}$ and $S^1 \times \{\pi\}$, however, we must obey Eq. (30), because the partners k and $-k$ do both belong to the EBZ for these circles.

To classify the maps from the cylinder $S^1 \times [0, \pi] \to S^4$ with special boundary conditions, we start by classifying maps from the boundary circles $S^1 \to S^4$ with special boundary conditions. For definiteness pick the lower boundary circle $S^1 \times \{0\}$. Then we write for breviy $d(k_1, 0)$ as $d_1(k_1)$. If there were no boundary conditions, this classification would be given by $\pi_1(S^4)$ which is just $\{1\}$ and so there is just one trivial class in this case. Otherwise, the special conditions force that $d_i(0) = d_i(\pi) = 0$ for all $i \in A \backslash TREI$ and otherwise they force that the loop $S^1 \to S^4$ is symmetric:

$$d_i(-k_1) = \begin{cases} d_i(k_1) & i \in TREI \\ -d_i(k_1) & i \notin TREI \end{cases}$$

so that it suffices to specify what happens just from $k_1 = 0$ until $k_1 = \pi$. Thus, the class of loops $S^1 \to S^4$ obeying the special boundary conditions is the class of *paths* $[0, \pi] \to S^4$ which end and start on

$$\left\{ d \in S^4 \;\middle|\; d_i = 0 \forall i \in A \backslash TREI \right\} =: \hat{S}$$

In general the possible classes of these maps are all nullhomotopic if $\hat{S}$ is a path connected subset of S^4: given a mapping $d : S^1 \to S^4$ that is not constant, we may find a path $\gamma : [0, 1] \to \hat{S}$ connecting $\gamma(0) = d(0)$ and $\gamma(1) = d(\pi)$ and then define a homotopy between a path $d : [0, \pi] \to S^4$ and a loop $\tilde{d} : [0, \pi] \to S^4$ which follows γ, and so $\tilde{d}(\pi) = \tilde{d}(0)$. We may then concatenate this homotopy with a homotopy that shrinks the loop $\tilde{d} : [0, \pi] \to S^4$ to a point, and thus $d : S^1 \to S^4$ is nullhomotopic. If, however, $\hat{S}$ is not path-connected, then we see that the classes of paths $d : [0, \pi] \to S^4$ are organized by the path-connected components of $\hat{S}$.

3.2.16. CLAIM. $\hat{S}$ is path-connected if $|A \backslash TREI| \leqslant 1$. $\hat{S}$ has two path-connected components if $|A \backslash TRIE| \in \{2, 3, 4\}$. There are no other possibilities.

PROOF. As the largest value of $|A|$ is five we see that the possibilities are $|A \backslash TREI| \in \{0, 1, 2, 3, 4, 5\}$. First note that if $|A \backslash TREI| = 5$ then $d_i(0) = 0$ for all $i \in A$ and so, in particular, $d(0) \notin S^4$. As a result, it is not possible that $|A \backslash TREI| = 5$.

If $|A \backslash TREI| = 0$, then $\hat{S} \equiv \left\{ d \in S^4 \;\middle|\; d_i = 0 \forall i \in \underbrace{A \backslash TREI}_{\varnothing} \right\} = S^4$ which is path-connected.

If $|A \backslash TREI| = 1$, then $\hat{S}$ is a sphere of lower dimension $\hat{S} \equiv \left\{ d \in S^4 \;\middle|\; d_i = 0 \forall i \in A \backslash TREI \right\} \cong S^3$ which is path-connected.

If $|A \backslash TREI| = 4$, then since on $\hat{S}$, $d_i = 0 \forall i \in A \backslash TREI$, there is only one index left which is not zero, call it e: $\{e\} = A \cap TREI$, and since all other indices are zero, that one index must be ± 1, as we must have at all times $\|d\| = 1$. As a result, we have only two points $\hat{S} = \{d_N, d_S\}$ where $(d_N)_e = 1$, $(d_S)_e = -1$. The two-point-set has two path-connected components.

If $|A \backslash TREI| \in \{2, 3\}$, then it *turns out* (by using 3.1.5) that if we make the additional requirement that the set $\{\Gamma_i\}_{i \in A}$ anti-commutes, then we can find either two or three odd gamma-matrices which anti-commute, and additionally only *one* even gamma matrix which also anti-commutes with the other odd ones. To reiterate, in this case, it turns out that $A \cap TREI = \{e\}$ just as in the case $|A \backslash TREI| = 4$ and so we again have only two points $\hat{S} = \{d_N, d_S\}$ where $(d_N)_e = 1$, $(d_S)_e = -1$.

In particular, our analysis is valid even when $|A| < 5$. □

As a result of the above claim, we only need to consider the case where $\hat{S}$ has two path-connected components, which we call $\hat{S}_N$ and $\hat{S}_S$. Then $A \cap TREI = \{e\}$.

3.2.17. CLAIM. $\prod_{k \in TRIM} \operatorname{sgn}(d_e(k)) = -1$ iff $d : S^1 \times [0, \pi] \to S^4$ is not nullhomotopic, and $\prod_{k \in TRIM} \operatorname{sgn}(d_e(k)) = +1$ iff d is nullhomotopic.

PROOF. For $d : S^1 \times \{0\} \to S^4$ (the lower boundary circle) there are in general four possibilities:

- NN: $d(0,0) \in \hat{S}_N$ and $d(\pi,0) \in \hat{S}_N$.
- SS: $d(0,0) \in \hat{S}_S$ and $d(\pi,0) \in \hat{S}_S$.
- NS: $d(0,0) \in \hat{S}_N$ and $d(\pi,0) \in \hat{S}_S$.
- SN: $d(0,0) \in \hat{S}_S$ and $d(\pi,0) \in \hat{S}_N$.

and $d : S^1 \times \{\pi\} \to S^4$ (the upper circle) is classified exactly the same. To classify the full maps $d : S^1 \times [0,\pi] \to S^4$, observe that what happens in the interior of the cylinder ($S^1 \times (0,\pi)$) is completely unconstrained and so it is only the two loops on the boundaries ($d : S^1 \times \{0\} \to S^4$ and $d : S^1 \times \{\pi\} \to S^4$) which determine the class of the full map $d : S^1 \times [0,\pi] \to S^4$.

Next, observe that we may adiabatically rotate S^4 so as to exchange $\hat{S}_N \leftrightarrow \hat{S}_S$. This can be done independently $\forall k_2 \in S^1$. As a result we really only have four classes for the whole cylinder map:

- NN at $k_2 = 0$, NN at $k_2 = \pi$.
- NN at $k_2 = 0$, NS at $k_2 = \pi$.
- NS at $k_2 = 0$, NN at $k_2 = \pi$.
- NS at $k_2 = 0$, NS at $k_2 = \pi$.

We can write this in a more suggestive form, which codifies the geometry of $\mathbb{T}^2$ by $\begin{bmatrix} k_2=\pi, k_1=0 & k_2=\pi, k_1=\pi \\ k_2=0, k_1=0 & k_2=0, k_1=\pi \end{bmatrix}$:

- $\begin{bmatrix} N & N \\ N & N \end{bmatrix}$
- $\begin{bmatrix} N & S \\ N & N \end{bmatrix}$
- $\begin{bmatrix} N & N \\ N & S \end{bmatrix}$
- $\begin{bmatrix} N & S \\ N & S \end{bmatrix}$

The next freedom we can exploit is to exchange $k_1 \leftrightarrow k_2$ so that a map like $\begin{bmatrix} N & S \\ N & S \end{bmatrix}$ becomes $\begin{bmatrix} S & S \\ N & N \end{bmatrix}$, after which we may compose another switch on S^4 of $\hat{S}_N \leftrightarrow \hat{S}_S$ to obtain in total:

$$\begin{bmatrix} N & S \\ N & S \end{bmatrix} \mapsto \begin{bmatrix} S & S \\ N & N \end{bmatrix} \mapsto \begin{bmatrix} N & N \\ N & N \end{bmatrix}$$

As a result, we see that there really are only two classes of maps, indexed by the number of S appearing on $k \in TRIM$: One S means the map is not null homotopic, and no S means the map is null homotopic. This statement may be encoded in the following expression:

$$\begin{cases} \prod_{k \in TRIM} \operatorname{sgn}(d_e(k)) = -1 & \text{non-nullhomotopic} \\ \prod_{k \in TRIM} \operatorname{sgn}(d_e(k)) = +1 & \text{null-homotopic} \end{cases}$$

□

We thus have a new meaning for the Kane-Mele index, inspired by [Mo07]. □

3.3. Bulk-Edge Correspondence Proof for the Case of a Dirac Hamiltonian

We assume the same assumptions of 3.2.3. In particular, we may use 1.5. We deal with the case where $A \cap TREI = \{e\}$. Otherwise, $H^B(k)$ is nullhomotopic, in which case its edge index is easily zero because the ellipse-point on S^4 would never contain the origin and so for constant $H^B(k)$ there are never zero energy edge modes.

Following 3.2.3 we have that Eq. (25) reduces to

$$\begin{aligned}(-1)^{\mathcal{I}_{KM}(H)} &= \prod_{k\in TRIM} \operatorname{sgn}(d_e(k)) \\ &= \operatorname{sgn}\left(d_e\left(\begin{bmatrix}0\\0\end{bmatrix}\right)\right)\operatorname{sgn}\left(d_e\left(\begin{bmatrix}0\\\pi\end{bmatrix}\right)\right)\operatorname{sgn}\left(d_e\left(\begin{bmatrix}\pi\\0\end{bmatrix}\right)\right)\operatorname{sgn}\left(d_e\left(\begin{bmatrix}\pi\\\pi\end{bmatrix}\right)\right) \\ &= \operatorname{sgn}\left(\underbrace{d_e\left(\begin{bmatrix}0\\0\end{bmatrix}\right)d_e\left(\begin{bmatrix}\pi\\0\end{bmatrix}\right)}_{M(k_2)|_{k_2=0}}\right)\operatorname{sgn}\left(\underbrace{d_e\left(\begin{bmatrix}0\\\pi\end{bmatrix}\right)d_e\left(\begin{bmatrix}\pi\\\pi\end{bmatrix}\right)}_{M(k_2)|_{k_2=\pi}}\right)\end{aligned}$$

where we have defined

$$M(k_2) := d_e\left(\begin{bmatrix}0\\k_2\end{bmatrix}\right)d_e\left(\begin{bmatrix}\pi\\k_2\end{bmatrix}\right)$$

So as we go with k_2 from 0 to π, $\mathcal{I}_{KM}(H) = 0$ if $M(k_2)$ changes sign an *even* number of times, whereas $\mathcal{I}_{KM}(H) = 1$ if $M(k_2)$ changes sign an *odd* number of times. $M(k_2)$ changes sign when it is zero, and thus, we are looking for the parity of the number of zeros of the function M on the domain $k_2 \in [0, \pi]$.

3.3.1. CLAIM. We may assume that $H^B(k)$ has been adiabatically changed (without closing the gap) that b^r lies along the $\hat{e}_e$ (recall $e = A \cap TREI$) direction, $b^r \perp b^i$, and that $b^0 \cdot b^i = 0$ for all k.

PROOF. We assume that $\hat{e}^r$ lies along the $\hat{e}_e$ direction in gamma-space. This should always be possible to achieve via adiabatic continuous rotations in gamma-space, which is isomorphic to $\mathbb{R}^5$ at each k_2. Observe that these rotations are continuous in k_2 (because $b(k_2)$ is continuous in k_2), and further more, this is possible to achieve for each k_2 adiabatically because the band gap never closes during these rotations, as $E^B = \pm\|d(k)\|$ shows ($SO(5)$ rotations should not affect the energy bands). The change to make $b^r \perp b^i$ should also be possible without closing the gap. It amounts to shrinking the $\hat{e}^r$ component of b^i to zero. There should be no obstruction to shrink the $\hat{e}^i$ component of b^0 to zero, even when $b^0 \cdot \hat{e}^r = 0$, because we may always keep a non-zero $b^{0\perp}$ to keep the gap open. Notice that we do all these changes while keeping each component d_j even or odd respectively in k.

First, to make sure that $b^r \perp b^i$, examine $d_e(k)$ (b^r is already along $\hat{e}_e$):

$$d_e(k) \equiv b_e^0(k_2) + 2b_e^r(k_2)\cos(k_1) + 2b_e^i(k_2)\sin(k_1)$$

so that making sure that $b^r \perp b^i$ means shrinking $b_e^i(k_2) \to 0$. As we do this, $d_e(k)$ stays even in k. Next, we want to make sure that $b^0 \cdot b^i = 0$. We have

$$d_i(k) = b_i^0(k_2) + 2b_i^i(k_2)\sin(k_1)$$

where the subscript i denotes the $\hat{e}_i$ component. Again, we may shrink $b_i^0(k_2) \to 0$ while keeping $d_i(k)$ odd in k.

In conclusion, along the homotopy to our desired $H^B(k)$, we keep time-reversal invariance *and* the gap. □

3.3.2. CLAIM. $M(k_2)$ changes sign exactly at those points $k_2 \in [0, \pi)$ where there is an edge state incipient out of or into the bulk. Thus

$$\mathcal{I}_{KM}(H) = \mathcal{I}^\sharp_{KM}\left(H^\sharp\right)$$

PROOF.

- Our model for $d_{i,j}(k)$ is, as given by 1.5.1:
$$d_{i,j}(k) = b_{i,j}^0(k_2) + 2b_{i,j}^r(k_2)\cos(k_1) + 2b_{i,j}^i(k_2)\sin(k_1)$$
- Then the ellipse lives on the plane defined by $\hat{e}^i$ and $\hat{e}^r$.
- We know that there are exactly two edge states in the gap via 1.5.22, and that they are at the energies $\pm\|b^{0\perp}\|$. Thus, if an edge state is incipient at the lower band for some k_2, there is another state simultaneously incipient at the upper band. It is therefore not important to make sure we deal only with incipience at the lower band or upper band, as those points give exactly the same count.
- We know that there is an edge state at a particular k_2 when the ellipse defined by
$$b^{0\|}(k_2) + 2b^r(k_2)\cos(k_1) + 2b^i(k_2)\sin(k_1)$$

includes the origin inside of it. Thus, an edge state is exactly incipient when $b^{0\|}(k_2)$ lies on the ellipse defined by $2b^r(k_2)\cos(k_1)+2b^i(k_2)\sin(k_1)$, that is, $b^{0\|}(k_2)=2b^r(k_2)\cos(k_1)+2b^i(k_2)\sin(k_1)$ for k_1 defined by the orientation of $b^{0\|}(k_2)$: $\cos(k_1):=\underbrace{\frac{b^{0\|}}{\|b^{0\|}\|}\hat{e}^r}_{1}$ and $\sin(k_1):=\underbrace{\frac{b^{0\|}}{\|b^{0\|}\|}\hat{e}^i}_{0}$.

- Thus by components we have:

$$\begin{cases}\underbrace{b^{0\|}(k_2)\cdot\hat{e}^i}_{0} & =\underbrace{2b^r(k_2)\cdot\hat{e}^i}_{0}\cos(k_1)+2b^i(k_2)\cdot\hat{e}^i\underbrace{\sin(k_1)}_{0}\\ \underbrace{b^{0\|}(k_2)\cdot\hat{e}^r}_{\left(b^{0\|}(k_2)\right)_e} & =\underbrace{2b^r(k_2)\cdot\hat{e}^r}_{(2b^r(k_2))_e}\underbrace{\cos(k_1)}_{1}+2\underbrace{b^i(k_2)\cdot\hat{e}^r}_{0}\sin(k_1)\end{cases}$$

- From the second equation we have $b^{0\|}(k_2)\cdot\hat{e}^r=2b^r(k_2)\cdot\hat{e}^r\cos(k_1)$, but $\hat{e}^r$ extracts exactly the $\hat{e}_e$ component of the vectors by hypothesis, so that we get: $\left(b^{0\|}(k_2)\right)_e=2(b^r(k_2))_e\cos(k_1)$ which means $\left(b^0(k_2)\right)_e=2(b^r(k_2))_e\cos(k_1)$ as $b^{0\perp}$ doesn't have any $\hat{e}_e$ component by its definition.
- So we have $\left(b^0(k_2)\right)_e-2(b^r(k_2))_e=0$ and so

$$\begin{aligned}M(k_2) &\equiv \left[\left(b^0(k_2)\right)_e-2(b^r(k_2))_e\right]\left[\left(b^0(k_2)\right)_e+2(b^r(k_2))_e\right]\\ &= 0\end{aligned}$$

at this point. The other possibility is that $b^{0\|}(k_2)\cdot\hat{e}^r=-\left(b^{0\|}(k_2)\right)_e$ which makes the other term zero.
- Either way, $M(k_2)$ changes sign at that point.

□

3.4. Proof for the General Case

So far we have shown the correspondence for a subclass of Hamiltonians which we call "Dirac". It turns out that for these simple systems, we are still able to find a non-zero $\mathbb{Z}_2$ invariant and so in this sense, we have already achieved the goal of examining the simplest non-trivial system.

In case H^B is not of "Dirac" form, we have no simple formula which characterizes the existence of edge states as in 1.5. However, it may be possible to generalize Eq. (31) in the following sense. A "Dirac" Hamiltonian has four bands, which come in two pairs. The lower pair and upper pair are always degenerate along k_2. In contrast, the generic Hamiltonian has four bands which intersect only on TRIM. However, it is always possible to make a time-reversal invariant homotopy which would squeeze together the lower pair and the upper pair, so as to ultimately bring it to the "Dirac" form. Once this has been made, Eq. (31) may be applied. Thus, future work might examine the prescription of how to make this time-reversal invariant homotopy, which would prescribe which indices of the fifteen indices end up being in A, and thus providing a generalization of Eq. (31).

Part 2

Physical Background

In this part we present a bridge between the results of the previous part and their relevance to physical systems.

CHAPTER 4

Lattice Models from Continuum Models

Our goal in this section is to convince the reader that starting from the usual description of non-interacting electrons in a crystal of atoms (with no magnetic field) it is legitimate to describe the system as a lattice.

4.0.1. CLAIM. The bulk continuum problem of an independent electron in a crystal reduces to an infinite discrete matrix eigenvalue problem.

PROOF. We start by a summary of notation and basic facts to give some context:

- Let a differential operator H be given by $H = -\frac{1}{2}\Delta + V$ where $V \in \mathbb{R}^{\mathbb{R}^3}$ acts by multiplication and is such that $H \in \mathcal{B}\left(L^2\left(\mathbb{R}^3; \mathbb{C}\right)\right)$.
- Let $\left\{a_j\right\}_{j\in J_3} \in \mathbb{R}^3$ be a triplet of three linearly independent vectors.
- Define "the lattice" as the set

$$\mathtt{Lat}\left(\left\{a_j\right\}_{j\in J_3}\right) := \left\{ \sum_{j\in J_3} n_j a_j \in \mathbb{R}^3 \,\middle|\, n_j \in \mathbb{Z} \forall j \in J_3 \right\}$$

and we denote an general element of $\mathtt{Lat}\left(\left\{a_j\right\}_{j\in J_3}\right)$ by R. The "primitive cell" is defined as

$$\mathtt{PrimCell}\left(\left\{a_j\right\}_{j\in J_3}\right) := \left\{ \sum_{j\in J_3} t_j a_j \in \mathbb{R}^3 \,\middle|\, t_j \in [0, 1]\, \forall j \in J_3 \right\}$$

4.0.2. DEFINITION. For all $R \in \mathtt{Lat}\left(\left\{a_j\right\}_{j\in J_3}\right)$, define a map $T_R \in \mathcal{B}\left(L^2\left(\mathbb{R}^3; \mathbb{C}\right)\right)$ by the action

$$T_R \psi \mapsto \left(r \mapsto \psi\left(r + R\right) \qquad \forall r \in \mathbb{R}^3\right)$$

for all $\psi \in L^2\left(\mathbb{R}^3; \mathbb{C}\right)$.

- Assume that V is such that $[V, T_R] = 0$ for any $R \in \mathtt{Lat}\left(\left\{a_j\right\}_{j\in J_3}\right)$. Then $[H, T_R] = 0$ for any $R \in \mathtt{Lat}\left(\left\{a_j\right\}_{j\in J_3}\right)$ because $[\Delta, T_R] = 0$.
- Note also that $[T_R, T_{R'}] = 0$.
- As a result we may pick eigenvectors of H which are simultaneous eigenvectors of all the T_R's. Index the eigenvalues of T_R with k where k ranges in $\mathbb{R}^3$ and the eigenvalues of H with $\alpha \in A$ for some discrete indexing set A. Then we may index the eigenfunctions of H and T_R as $\left\{\psi_{\alpha, k}\right\}_{(\alpha, k)\in A\times\mathbb{R}^3}$.
- Bloch's theorem ([As76] equation 8.3) states that

$$\psi_{\alpha, k}\left(r\right) = \exp\left(i\left\langle k, r\right\rangle\right) u_{k, \alpha}\left(r\right)$$

for all $r \in \mathbb{R}^3$ where $u_{k, \alpha}$ are some functions which are invariant under the action of T_R.
- Define

$$\begin{cases} b_1 & := 2\pi\frac{a_2\times a_3}{\langle a_1, (a_2\times a_3)\rangle} \\ b_2 & := 2\pi\frac{a_3\times a_1}{\langle a_1, (a_2\times a_3)\rangle} \\ b_3 & := 2\pi\frac{a_1\times a_2}{\langle a_1, (a_2\times a_3)\rangle} \end{cases}$$

Then "the reciprocal lattice" is $\mathtt{Lat}\left(\left\{b_j\right\}_{j\in J_3}\right)$. A typical element from $\mathtt{Lat}\left(\left\{b_j\right\}_{j\in J_3}\right)$ will be denoted by K. Then the primitive cell spanned by $\left\{b_j\right\}_{j\in J_3}$ is called BZ1:

$$\mathtt{BZ1}\left(\left\{a_j\right\}_{j\in J_3}\right) \equiv \mathtt{PrimCell}\left(\left\{b_j\right\}_{j\in J_3}\right)$$

- It turns out that $\psi_{\alpha,k} = \psi_{\alpha,k+K}$ for all $K \in \mathrm{Lat}\left(\{b_j\}_{j\in J_3}\right)$ (and so we need not consider general $k \in \mathbb{R}^3$ but only $k \in BZ1\left(\{a_j\}_{j\in J_3}\right)$).
- Thus $\{\psi_{\alpha,k}\}_{(\alpha,k)\in A\times BZ1\left(\{a_j\}_{j\in J_3}\right)}$ form a basis for the one-particle Hilbert space $L^2\left(\mathbb{R}^3,\mathbb{C}\right)$, which we denote by $\{|\alpha,k\rangle\}_{(\alpha,k)\in A\times BZ1\left(\{a_j\}_{j\in J_3}\right)}$.
- Because $\psi_{\alpha,k}$ are periodic in the k parameter, we may view them as functions of k and thus write a Fourier expansion as

$$\psi_{\alpha,k}(r) = \sum_{R\in \mathrm{Lat}\left(\{a_j\}_{j\in J_3}\right)} \tilde{\psi}_{\alpha,R}(r)\exp\left(i\langle k, R\rangle\right)$$

- $\tilde{\psi}_{\alpha,R}(r)$ are called “Wannier functions” and are given by the inversion

$$\tilde{\psi}_{\alpha,R}(r) = \frac{1}{v_0}\int_{BZ1\left(\{a_j\}_{j\in J_3}\right)} \psi_{\alpha,k}(r)\exp\left(-i\langle k, R\rangle\right)dk$$

  where $v_0 := \langle a_1, (a_2\times a_3)\rangle$.

4.0.3. CLAIM. $\tilde{\psi}_{\alpha,R}(r)$ is not a function of two independent variables r and R but rather depends only on the difference $r-R$.

PROOF. For some $R' \in \mathrm{Lat}\left(\{a_j\}_{j\in J_3}\right)$,

$$\begin{aligned}
\tilde{\psi}_{\alpha,R+R'}\left(r+R'\right) &= \frac{1}{v_0}\int_{BZ1\left(\{a_j\}_{j\in J_3}\right)} \psi_{\alpha,k}\left(r+R'\right)\exp\left(-i\left\langle k, R+R'\right\rangle\right)dk \\
&= \frac{1}{v_0}\int_{BZ1\left(\{a_j\}_{j\in J_3}\right)} \psi_{\alpha,k}(r)\exp\left(i\left\langle k, R'\right\rangle\right)\exp\left(-i\left\langle k, R+R'\right\rangle\right)dk \\
&= \frac{1}{v_0}\int_{BZ1\left(\{a_j\}_{j\in J_3}\right)} \psi_{\alpha,k}(r)\exp\left(-i\langle k, R\rangle\right)dk \\
&= \tilde{\psi}_{\alpha,R}(r)
\end{aligned}$$

□

4.0.4. CLAIM. $\tilde{\psi}_{\alpha,R}(r)$ and $\tilde{\psi}_{\alpha',R'}(r)$ are orthogonal if $R\neq R'$ or if $\alpha\neq\alpha'$.

PROOF. Assuming the Bloch functions are orthonormal:

$$\begin{aligned}\langle \alpha,\, k \,|\, \alpha',\, k' \rangle &\equiv \int_{\mathrm{PrimCell}\left(\{a_j\}_{j\in J_3}\right)} \overline{\psi_{\alpha,\,k}\,(r)}\psi_{\alpha',\,k'}\,(r)\,dr \\ &= \delta_{\alpha,\,\alpha'}\delta^3\,(k-k')\end{aligned}$$

we have

$$\begin{aligned}\int_{\mathrm{PrimCell}\left(\{a_j\}_{j\in J_3}\right)} \overline{\tilde\psi_{\alpha,\,R}\,(r)}\tilde\psi_{\alpha',\,R'}\,(r)\,dr &= \int_{\mathrm{PrimCell}\left(\{a_j\}_{j\in J_3}\right)} \overline{\frac{1}{v_0}\int_{\mathrm{BZ1}\left(\{a_j\}_{j\in J_3}\right)} \psi_{\alpha,\,k}\,(r)\exp\left(-i\,\langle k,\,R\rangle\right)dk}\,\times \\ &\quad \times\frac{1}{v_0}\int_{\mathrm{BZ1}\left(\{a_j\}_{j\in J_3}\right)} \psi_{\alpha',\,k'}\,(r)\exp\left(-i\,\langle k',\,R'\rangle\right)dk'dr \\ &= \frac{1}{v_0^2}\int_{\mathrm{PrimCell}\left(\{a_j\}_{j\in J_3}\right)}\int_{\mathrm{BZ1}\left(\{a_j\}_{j\in J_3}\right)}\int_{\mathrm{BZ1}\left(\{a_j\}_{j\in J_3}\right)} \overline{\psi_{\alpha,\,k}\,(r)}\exp\left(i\,\langle k,\,R\rangle\right)\times \\ &\quad \times\psi_{\alpha',\,k'}\,(r)\exp\left(-i\,\langle k',\,R'\rangle\right)dkdk'dr \\ &= \frac{\delta_{\alpha,\,\alpha'}}{v_0^2}\int\int_{\left[\mathrm{BZ1}\left(\{a_j\}_{j\in J_3}\right)\right]^2} \delta^3\,(k-k')\exp\left(i\,\langle k,\,R\rangle - i\,\langle k',\,R'\rangle\right)dkdk' \\ &= \frac{1}{v_0^2}\delta_{\alpha,\,\alpha'}\int_{\mathrm{BZ1}\left(\{a_j\}_{j\in J_3}\right)} \exp\left(i\,\langle k,\,R-R'\rangle\right)dk \\ &= \frac{1}{v_0^2}\delta_{\alpha,\,\alpha'}\,(2\pi)^3\,\delta^3\,(R-R')\end{aligned}$$

□

- As a result, $\tilde\psi_{\alpha,\,R}\,(r)$ also form a basis for the one particle Hilbert space $L^2\,(\mathbb{R}^3;\,\mathbb{C})$, which we denote by $\{|\alpha,\,R\rangle\}_{(\alpha,\,R)\in A\times \mathrm{Lat}\left(\{a_j\}_{j\in J_3}\right)}$.
- A general vector in $L^2\,(\mathbb{R}^3,\,\mathbb{C})$, $|v\rangle$, can then be expanded as
$$|v\rangle = \sum_{(\alpha,\,R)\in A\times\mathrm{Lat}\left(\{a_j\}_{j\in J_3}\right)} \langle\alpha,\,R\,|\,v\rangle\,|\alpha,\,R\rangle$$
- Thus instead of encoding $|v\rangle$ as a sequence $\{\langle\alpha,\,k\,|\,v\rangle\}_{(\alpha,\,k)\in A\times\mathrm{BZ1}\left(\{a_j\}_{j\in J_3}\right)}$ which is in general indexed by a continuum (because $\left|\mathrm{BZ1}\left(\{a_j\}_{j\in J_3}\right)\right| = \mathfrak{c}$) we are able to encode $|v\rangle$ as $\{\langle\alpha,\,R\,|\,v\rangle\}_{(\alpha,\,R)\in\mathbb{R}\times\mathrm{Lat}\left(\{a_j\}_{j\in J_3}\right)}$ which is in general indexed by a countable set (because $\mathrm{Lat}\left(\{a_j\}_{j\in J_3}\right)\simeq\mathbb{Z}^3$ and so $\left|\mathrm{Lat}\left(\{a_j\}_{j\in J_3}\right)\right| = \aleph_0$).
- As a result, our Hilbert space is made isomorphic to $l^2\left(\mathbb{Z}^3;\,\mathbb{C}^{|A|}\right)$.
- We are looking for eigenvalues and eigenvectors of the matrix $\langle\lambda,\,R\,|\,H\,|\,\lambda',\,R'\rangle$:
$$\boxed{\sum_{(\alpha',\,R')\in\in A\times\mathrm{Lat}\left(\{a_j\}_{j\in J_3}\right)} \langle\alpha,\,R\,|\,H\,|\,\alpha',\,R'\rangle\,\langle\alpha',\,R'\,|\,\psi\rangle = E\,\langle\alpha,\,R\,|\,\psi\rangle}$$

□

Now we can follow a very similar procedure to 1.3:
- Due to 4.0.3 we have:
$$\begin{aligned}\langle\alpha,\,R\,|\,H\,|\,\alpha',\,R'\rangle &\equiv \int_{\mathbb{R}^3}\left[\tilde\psi_{\alpha,\,R}\,(r)\right]^* H\tilde\psi_{\alpha',\,R'}\,(r)\,d^3r \\ &\overset{r\mapsto r+R}{=} \int_{\mathbb{R}^3}\left[\tilde\psi_{\alpha,\,R}\,(r+R)\right]^* H\tilde\psi_{\alpha',\,R'}\,(r+R)\,d^3r \\ &= \int_{\mathbb{R}^3}\left[\tilde\psi_{\alpha,\,0}\,(r)\right]^* H\tilde\psi_{\alpha',\,R'-R}\,(r)\,d^3r \\ &= \langle\alpha,\,0\,|\,H\,|\,\alpha',\,R'-R\rangle\end{aligned}$$

- ◦ As a result we need only carry one index of R on the $\langle\alpha,\,R|H|\alpha',\,R'\rangle$ matrix: $\langle\alpha,\,0|H|\alpha',\,R\rangle$.
- Because $\langle\alpha,\,R|H|\alpha',\,R'\rangle$ is periodic in R (that is, $\langle\alpha,\,R|H|\alpha',\,R'\rangle = \langle\alpha,\,R+R''|H|\alpha',\,R'+R''\rangle$) we may employ Bloch's theorem *again* to conclude that its eigenvectors should be of the form
$$\langle\alpha,\,R|\psi\rangle = \exp\left(i\langle k,\,R\rangle\right)u^{(d)}{}_{\alpha,k}(R)$$
where $k\in BZ1\left(a_j\right)$ and again $u^{(d)}{}_{\alpha,k}(R)$ have the same periodicity of the potential $R\mapsto R+R''$ and so we might as well drop the R index from $u^{(d)}{}_{\alpha,k}(R)$ and simply write $u^{(d)}{}_{\alpha,k}$.
- Plug this into the Schroedinger equation to obtain:
$$\begin{aligned}\sum_{(\alpha',R')}\left\langle\alpha,\,R\,\middle|\,H\,\middle|\,\alpha',\,R'\right\rangle\exp\left(i\left\langle k,\,R'\right\rangle\right)u^{(d)}{}_{\alpha',k} &= E_k\exp\left(i\langle k,\,R\rangle\right)u^{(d)}{}_{\alpha,k}\\ \sum_{(\alpha',R')}\left\langle\alpha,\,0\,\middle|\,H\,\middle|\,\alpha',\,R'-R\right\rangle\exp\left(i\left\langle k,\,R'\right\rangle\right)u^{(d)}{}_{\alpha',k} &= E_k\exp\left(i\langle k,\,R\rangle\right)u^{(d)}{}_{\alpha,k}\\ \sum_{(\alpha',R')}\left\langle\alpha,\,0\,\middle|\,H\,\middle|\,\alpha',\,R'-R\right\rangle\exp\left(i\left\langle k,\,R'-R\right\rangle\right)u^{(d)}{}_{\alpha',k} &= E_k u^{(d)}{}_{\alpha,k}\\ \sum_{\alpha}\sum_{R'}\left\langle\alpha,\,0\,\middle|\,H\,\middle|\,\alpha',\,R'\right\rangle\exp\left(i\left\langle k,\,R'\right\rangle\right)u^{(d)}{}_{\alpha',k} &= E_k u^{(d)}{}_{\alpha,k}\end{aligned}$$
- Define $H^{(d)}(k)\in\mathrm{Herm}(|A|)$ by its components $\left(H^{(d)}(k)\right)_{(\alpha,\alpha')} := \sum_{R'}\langle\alpha,\,0|H|\alpha',\,R'\rangle\exp\left(i\langle k,\,R'\rangle\right)$.
- Then the last equation becomes
$$\boxed{H^{(d)}(k)\,u^{(d)}{}_k = E_k u^{(d)}{}_k}$$
where $u^{(d)}{}_k\in\mathbb{C}^{|A|}$ is a vector with components $u^{(d)}{}_{\alpha,k}$.

As a result we have separated the problem into infinitely many problems (indexed by $k\in BZ1\left(a_j\right)$), namely, for each $k\in BZ1\left(a_j\right)$ we are looking to find the eigensystem of the $|A|\times|A|$ Hermitian matrix $H^{(d)}(k)$.

CHAPTER 5

Magnetic Translation Operators

We follow the presentation of [Ko85] for the magnetic translation operators. These can then be used to perform a Wannier decomposition in the presence of a magnetic field, as is done in [Wi00].

- The Hamiltonian for a 2D non-interacting electron system in a uniform magnetic field perpendicular to the plane is
$$H = \frac{1}{2m}(p+eA)^2 + U(x_1, x_2)$$
where
$$p = -i\hbar\nabla$$
and
$$U(x_1+a_1, x_2) = U(x_1, x_2+a_2) = U(x_1, x_2)$$
- Define $R_n = n_1 a_1 \hat{e}_1 + n_2 a_2 \hat{e}_2$ where $n \in \mathbb{Z}^2$, and $\hat{e}_i$ is the unit vector in the direction i for all $i \in J_2$.
- The most general vector potential such that the magnetic field is a constant (given by B) is given by $A(r) = \frac{1}{2}B\times r + \nabla\Lambda(r)$, where $\Lambda(r)$ is some function.
- As such, H has an explicit r dependence.

5.0.5. CLAIM. Under translation by R_n, the Hamiltonian is not invariant.

PROOF.

- Plug in $r+R_n$ into the Hamiltonian instead of r. The momentum stays the same, of course, as does the potential U:
$$\begin{aligned} H(r+R_n) &= \frac{1}{2m}(p+eA(r+R_n))^2 + U(r) \\ &= \frac{1}{2m}\left(p+e\left(\frac{1}{2}B\times(r+R_n)+\nabla\Lambda(r+R_n)\right)\right)^2 + U(r) \\ &= \frac{1}{2m}\left(p+eA(r)+e\left(\frac{1}{2}B\times R_n+\nabla\Lambda(r+R_n)-\nabla\Lambda(r)\right)\right)^2 + U(r) \\ &= H(r)+\frac{1}{2m}\left[\left(p+eA(r)+e\left(\frac{1}{2}B\times R_n+\nabla\Lambda(r+R_n)-\nabla\Lambda(r)\right)\right)^2-(p+eA(r))^2\right] \end{aligned}$$
- In general, there is no reason why $\frac{1}{2m}\left[\left(p+eA(r)+e\left(\frac{1}{2}B\times R_n+\nabla\Lambda(r+R_n)-\nabla\Lambda(r)\right)\right)^2-(p+eA(r))^2\right]$ should be zero (for instance, in $\Lambda=0$ gauge, we have
$$\frac{1}{2m}\left[(p+eA(r))\,e\left(\frac{1}{2}B\times R_n\right)+e\left(\frac{1}{2}B\times R_n\right)(p+eA(r))+e^2\left(\frac{1}{2}B\times R_n\right)^2\right]$$

□

- 4.0.2 is represented as $T_{R_n} = \exp\left(\frac{i}{\hbar}R_n\cdot p\right) = \exp(R_n\cdot\nabla)$.
- As we have just seen, $[T_{R_n}, H] \neq 0$.
- The difference between $A(r)$ and $A(r+R_n)$ is given by:
$$\begin{aligned} A(r)-A(r-R_n) &= \left[\frac{1}{2}B\times r+\nabla\Lambda(r)\right]-\left[\frac{1}{2}B\times(r+R_n)+\nabla\Lambda(r+R_n)\right] \\ &= \nabla\Lambda(r)-\frac{1}{2}B\times R_n-\nabla\Lambda(r+R_n) \\ &= \nabla\left[\Lambda(r)-\Lambda(r+R_n)-\frac{1}{6}(B\times R_n)\cdot r\right] \end{aligned}$$

5.0.6. DEFINITION. Define the magnetic translation operators

$$\boxed{\hat{T}_{R_n} \equiv \exp\left(\frac{i}{\hbar} R_n \cdot \left(p + \frac{1}{2} e\,(r \times B)\right)\right)}$$

5.0.7. CLAIM. $\hat{T}_{R_n} = T_{R_n} \exp\left(\frac{i}{\hbar}\frac{1}{2} e\,(B \times R_n) \cdot r\right)$.

PROOF.

- Observe that

$$\begin{aligned}\frac{i}{\hbar} R_n \cdot \frac{1}{2} e\,(r \times B) &= \frac{i}{\hbar}\frac{1}{2} e \sum_j (R_n)_j\,(r \times B)_j \\ &= \frac{i}{\hbar}\frac{1}{2} e \sum_{j,l,m} (R_n)_j\,\varepsilon_{jlm} r_l B_m \\ &= \frac{i}{\hbar}\frac{1}{2} e \sum_{j,l,m} \varepsilon_{jlm}\,(R_n)_j\,r_l B_m\end{aligned}$$

whereas

$$\begin{aligned}\frac{i}{\hbar}\frac{1}{2} e\,(B \times R_n) \cdot r &= \frac{i}{\hbar}\frac{1}{2} e \sum_j (B \times R_n)_j\,r_j \\ &= \frac{i}{\hbar}\frac{1}{2} e \sum_{j,l,m} \varepsilon_{jlm} B_l\,(R_n)_m\,r_j \\ &= \frac{i}{\hbar}\frac{1}{2} e \sum_{l,m,j} \varepsilon_{lmj}\,(R_n)_j\,r_l B_m \\ &= \frac{i}{\hbar}\frac{1}{2} e \sum_{l,m,j} \varepsilon_{jlm}\,(R_n)_j\,r_l B_m\end{aligned}$$

so the two exponents are the same. The only question is why may we factor out the momentum exponent.
- To see this we use the Baker-Campbell-Hausdorff formula, and in order to use it we need to compute the commutator and hope that it vanishes:

$$\begin{aligned}\left[\frac{i}{\hbar} R_n \cdot p,\ \frac{i}{\hbar}\frac{1}{2} e R_n \cdot (r \times B)\right] &= -\frac{1}{\hbar^2}\frac{1}{2} e \left[\sum_i (R_n)_i\,p_i,\ \sum_j (R_n)_j\,(r \times B)_j\right] \\ &= -\frac{1}{\hbar^2}\frac{1}{2} e \sum_i \sum_j (R_n)_i\,(R_n)_j \sum_{l,m} \varepsilon_{jlm} B_m\,[p_i,\ r_l] \\ &= \frac{i}{\hbar}\frac{1}{2} e \sum_i \sum_j \sum_m (R_n)_i\,(R_n)_j\,\varepsilon_{jim} B_m\end{aligned}$$

which vanishes due to the anti-symmetry of ε_{jim}.

□

5.0.8. CLAIM. If $\Lambda = 0$ then $\left[\hat{T}_{R_n},\ H\right] = 0$.

PROOF.

- Observe that when $\Lambda = 0$, $A\,(r + R_n) = \frac{1}{2} B \times (r + R_n) = A\,(r) + \frac{1}{2} B \times R_n$.
- Using the above computations we have $\hat{T}_{R_n} H\,(r,\ p) = T_{R_n} \exp\left(\frac{i}{\hbar}\frac{1}{2} e\,(B \times R_n) \cdot r\right) H\,(r,\ p)$.
- $\exp\left(\frac{i}{\hbar}\frac{1}{2} e\,(B \times R_n) \cdot r\right)$ can be seen as translation of p by $-\frac{1}{2} e\,(B \times R_n)$ and so we have

$$\exp\left(\frac{i}{\hbar}\frac{1}{2} e\,(B \times R_n) \cdot r\right) H\,(r,\ p) = \frac{1}{2m}\left(\left(p - \frac{1}{2} e\,(B \times R_n)\right) + eA\right)^2 + U\,(r)$$

- But then, applying T_{R_n} on this we obtain:

$$\begin{aligned}\hat{T}_{R_n} H(r,p) &= T_{R_n}\left[\frac{1}{2m}\left(\left(p-\frac{1}{2}e(B\times R_n)\right)+eA(r)\right)^2+U(r)\right]\\ &= \frac{1}{2m}\left(\left(p-\frac{1}{2}e(B\times R_n)\right)+eA(r)+e\frac{1}{2}B\times R_n\right)^2+U(r)\\ &= H(r,p)\end{aligned}$$

□

5.0.9. CLAIM. The commutator is given by:

$$\left[\hat{T}_{R_n},\hat{T}_{R_m}\right]=2iT_{R_n}T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)\sin\left(\frac{1}{2}\frac{1}{\hbar}eB\cdot(R_m\times R_n)\right)$$

PROOF.

- Compute

$$\begin{aligned}\left[\hat{T}_{R_n},\hat{T}_{R_m}\right] &= \left[T_{R_n}\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)\right]\\ &= \left[T_{R_n}\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),T_{R_m}\right]\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)+\\ &\quad +T_{R_m}\left[T_{R_n}\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)\right]\\ &= T_{R_n}\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),T_{R_m}\right]\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)+\\ &\quad +[T_{R_n},T_{R_m}]\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)+\\ &\quad +T_{R_m}T_{R_n}\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)\right]+\\ &\quad +T_{R_m}\left[T_{R_n},\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)\right]\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right)\end{aligned}$$

- But of course $[T_{R_n},T_{R_m}]=0$ and also $\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)\right]=0$ and so we have

$$\begin{aligned}\left[\hat{T}_{R_n},\hat{T}_{R_m}\right] &= T_{R_n}\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),T_{R_m}\right]\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)+\\ &= +T_{R_m}\left[T_{R_n},\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_m)\cdot r\right)\right]\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right)\end{aligned}$$

and so our main task reduces to evaluate $\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),T_{R_m}\right]$:

$$\begin{aligned}\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),T_{R_m}\right] &= \left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right),\exp\left(\frac{i}{\hbar}R_m\cdot p\right)\right]\\ &= \exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right)\exp\left(\frac{i}{\hbar}R_m\cdot p\right)-\exp\left(\frac{i}{\hbar}R_m\cdot p\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r\right)\end{aligned}$$

- To use the Baker Hausdorff Campbell formula we need the commutators

$$\begin{aligned}\left[\frac{i}{\hbar}\frac{1}{2}e(B\times R_n)\cdot r,\frac{i}{\hbar}R_m\cdot p\right] &= -\frac{1}{\hbar^2}\frac{1}{2}e\left[\sum_j(B\times R_n)_j r_j,\sum_i(R_m)_i p_i\right]\\ &= -\frac{1}{\hbar^2}\frac{1}{2}e\sum_j\sum_i\sum_l\sum_k\varepsilon_{jlk}B_l(R_n)_k(R_m)_i\, i\hbar\delta_{ji}\\ &= \frac{i}{\hbar}\frac{1}{2}e\sum_j\sum_l\sum_k B_l\varepsilon_{ljk}(R_n)_k(R_m)_j\\ &= \frac{1}{2}\frac{i}{\hbar}eB\cdot(R_m\times R_n)\end{aligned}$$

and thus

$$\left[\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r,\ \left[\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r,\ \frac{i}{\hbar}R_m\cdot p\right]\right]=0$$

and

$$\left[\frac{i}{\hbar}R_m\cdot p,\ \left[\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r,\ \frac{i}{\hbar}R_m\cdot p\right]\right]=0$$

and so

$$\begin{aligned}
\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\exp\left(\frac{i}{\hbar}R_m\cdot p\right) &= \exp\left(\frac{i}{\hbar}R_m\cdot p\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\times\\
&\quad\times\exp\left(\left[\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r,\ \frac{i}{\hbar}R_m\cdot p\right]\right)\\
&= \exp\left(\frac{i}{\hbar}R_m\cdot p\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)\\
&= T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)
\end{aligned}$$

- As a result we find the commutator

$$\begin{aligned}
\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right),T_{R_m}\right] &= \exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)T_{R_m}-T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\\
&= T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)\\
&\quad -T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\\
&= T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\left(\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)-1\right)
\end{aligned}$$

and

$$\begin{aligned}
\left[T_{R_n},\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\right] &= -\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right),T_{R_n}\right]\\
&= -T_{R_n}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\left(\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_n\times R_m\right)\right)-1\right)\\
&= T_{R_n}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\left(1-\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_n\times R_m\right)\right)\right)
\end{aligned}$$

- Finally we have

$$\begin{aligned}
\left[\hat{T}_{R_n},\hat{T}_{R_m}\right] &= T_{R_n}\left[\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right),T_{R_m}\right]\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)+\\
&\quad +T_{R_m}\left[T_{R_n},\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\right]\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\\
&= T_{R_n}T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\left(\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)-1\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)+\\
&\quad +T_{R_m}T_{R_n}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\left(1-\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_n\times R_m\right)\right)\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\\
&= T_{R_n}T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\left(\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)-1\right)+\\
&\quad -T_{R_n}T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\left(\exp\left(-\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)-1\right)\\
&= T_{R_n}T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\times\\
&\quad\times\left(\exp\left(\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)-\exp\left(-\frac{1}{2}\frac{i}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)\right)\\
&= 2iT_{R_n}T_{R_m}\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_n\right)\cdot r\right)\exp\left(\frac{i}{\hbar}\frac{1}{2}e\left(B\times R_m\right)\cdot r\right)\sin\left(\frac{1}{2}\frac{1}{\hbar}eB\cdot\left(R_m\times R_n\right)\right)
\end{aligned}$$

□

- So we see that the magnetic translation operators of different translation parameter R_m do not commute in general, unless $\sin\left(\frac{1}{2}\frac{1}{\hbar}eB\cdot(R_m\times R_n)\right)=0$ which implies $\frac{1}{2}\frac{1}{\hbar}eB\cdot(R_m\times R_n)=\pi\alpha$ for some $\alpha\in\mathbb{Z}$, or $\frac{e}{\hbar}B\cdot(R_m\times R_n)=\alpha$ for some $\alpha\in\mathbb{Z}$.
  - Because B is along the z-axis we can already write $\frac{e}{\hbar}B\cdot(R_m\times R_n)=\frac{e}{\hbar}|B||R_m\times R_n|$.
  - In general,

$$|R_m\times R_n|=|(m_1a_1\hat{e}_1+m_2a_2\hat{e}_2)\times(n_1a_1\hat{e}_1+n_2a_2\hat{e}_2)|=m_1a_1n_2a_2-m_2a_2n_1a_1=a_1a_2(m_1n_2-m_2n_1)$$

  - Thus we have
$$\frac{e}{\hbar}B\cdot(R_m\times R_n)=\frac{e}{\hbar}|B|a_1a_2(m_1n_2-m_2n_1)$$
  - Assume that $\frac{e}{\hbar}|B|a_1a_2\in\mathbb{Q}$. Then we could write
$$\frac{e}{\hbar}|B|a_1a_2=\frac{p}{q}$$
where $p\in\mathbb{Z}$ and $q\in\mathbb{N}\backslash\{0\}$ and $\gcd(p,q)=1$.
  - Then
$$\frac{e}{\hbar}B\cdot(R_m\times R_n)=\frac{p}{q}(m_1n_2-m_2n_1)\overset{!}{=}\alpha$$
where $\alpha\in\mathbb{Z}$.
  - There is a "trick" to make sure $\frac{p}{q}(m_1n_2-m_2n_1)\in\mathbb{Z}$: always work with multiples of q in one (or both) of the basis vectors, so that n_1 and m_1 will always contain a multiple of q. We can also do this for n_2 or m_2 alternatively. This is effectively making the replacement $a_1\to qa_1$ (this choice is not canonical, it's just one simple alternative).
- Define
$$R'_n=n_1qa_1\hat{e}_1+n_2a_2\hat{e}_2$$
where $n\in\mathbb{Z}^2$, and $\hat{e}_i$ is the unit vector in the direction i for all $i\in\{1,2\}$.
- Then we have $\left[\hat{T}_{R'_n},\hat{T}_{R'_m}\right]=0$.
- As a result, we may diagonalize H and all of $\left\{\hat{T}_{R'_n}\,\middle|\,n\in\mathbb{Z}^2\right\}$ simultaneously.
- To find the eigenvalues of $\hat{T}_{R'_n}$:
  - They must have absolute value 1 because $\hat{T}_{R'_n}$ should be unitary, so write the eigenvalues as $\exp(i\varphi_n)$.
  - Now that $\left[\hat{T}_{R'_n},\hat{T}_{R'_m}\right]=0$, we have $\hat{T}_{R'_n}\hat{T}_{R'_m}=\hat{T}_{R'_n+R'_m}$. The only continuous choice of φ_n which satisfies this is $\varphi_n=R'_n\cdot k+\alpha$ for some $k\in\mathbb{R}^3$ and $\alpha\in\mathbb{R}$.
  - α would merely introduce a global phase and so we may choose $\alpha=0$ [TODO].
  - But $\exp(iR'_n\cdot k)=\exp(iR'_n\cdot k)\,1=\exp(iR'_n\cdot k)\exp(iR'_n\cdot\mathbf{K}')=\exp(iR'_n\cdot(k+\mathbf{K}'))$ where $\mathbf{K}'$ is a reciprocal lattice vector to $\{qa_1\hat{e}_1,a_2\hat{e}_2\}$. So our eigenvalues are only those inside the $BZ1'$.
- So label the eigenfunctions of H and all of $\left\{\hat{T}_{R'_n}\,\middle|\,n\in\mathbb{Z}^2\right\}$ by $\psi_{\lambda,k}(r)$ where λ labels eigenvalues of H and $k\in BZ1'$.
- Define $u_{\lambda,k}(r):=\exp(-ir\cdot k)\psi_{\lambda,k}(r)$.

5.0.10. CLAIM. The action of translation on $u_{\lambda,k}$ is given by:

$$T_{R'_n}u_{\lambda,k}(r)\equiv u_{\lambda,k}(r+R'_n)=\exp\left(i\pi p\left(\frac{n_2}{qa_1}\hat{x}-\frac{n_1}{a_2}\hat{y}\right)\cdot r\right)u_{\lambda,k}(r)$$

for all $n\in\mathbb{Z}^2$.
Note: This is called the generalized Bloch conditions.

PROOF.

- So

$$\begin{aligned}
u_{\lambda,k}\left(r+R'_n\right) &= \exp\left(-i\left(r+R'_n\right)\cdot k\right)\psi_{\lambda,k}\left(r+R'_n\right)\\
&= \exp\left(-i\left(r+R'_n\right)\cdot k\right)T_{R'_n}\psi_{\lambda,k}(r)\\
&= \exp\left(-i\left(r+R'_n\right)\cdot k\right)\exp\left(-\frac{i}{\hbar}\frac{1}{2}e\left(B\times R'_n\right)\cdot r\right)\hat{T}_{R'_n}\psi_{\lambda,k}(r)\\
&= \exp\left(-i\left(r+R'_n\right)\cdot k\right)\exp\left(-\frac{i}{\hbar}\frac{1}{2}e\left(B\times R'_n\right)\cdot r\right)\exp\left(iR'_n\cdot k\right)\psi_{\lambda,k}(r)\\
&= \exp\left(-ir\cdot k\right)\exp\left(-\frac{i}{\hbar}\frac{1}{2}e\left(B\times R'_n\right)\cdot r\right)\psi_{\lambda,k}(r)\\
&= \exp\left(-ir\cdot k\right)\exp\left(-\frac{i}{\hbar}\frac{1}{2}e\left(B\times R'_n\right)\cdot r\right)\exp\left(ir\cdot k\right)u_{\lambda,k}(r)\\
&= \exp\left(-\frac{i}{\hbar}\frac{1}{2}e\left(B\times R'_n\right)\cdot r\right)u_{\lambda,k}(r)\\
&= \exp\left(-i\pi\frac{p}{q}\left(\hat{z}\times\left(n_1q\frac{1}{a_2}\hat{x}+n_2\frac{1}{a_1}\hat{y}\right)\right)\cdot r\right)u_{\lambda,k}(r)\\
&= \exp\left(-i\pi\frac{p}{q}\left(n_1q\frac{1}{a_2}\hat{y}-n_2\frac{1}{a_1}\hat{x}\right)\cdot\left(r_x\hat{x}+r_y\hat{y}\right)\right)u_{\lambda,k}(r)\\
&= \exp\left(i\pi p\left(\frac{n_2}{qa_1}\hat{x}-\frac{n_1}{a_2}\hat{y}\right)\cdot r\right)u_{\lambda,k}(r)
\end{aligned}$$

□

- Note that a gauge transformation of $A\mapsto A+\nabla f$ changes the phase of the wave function $\psi\mapsto\exp\left(-\frac{ie}{\hbar}f\right)\psi$.

5.0.11. CLAIM. The phase change around the boundary of the magnetic unit cell is gauge-invariant.

PROOF.

- The phase change around one magnetic unit cell should be given by:

$$T_{-a_2\hat{e}_2}T_{-qa_1\hat{e}_1}T_{a_2\hat{e}_2}T_{qa_1\hat{e}_1}\psi(r)$$

- Using the one before the above claim, we have:

$$\begin{aligned}
T_{qa_1\hat{e}_1}\psi(r) &= T_{qa_1\hat{e}_1}\exp\left(ir\cdot k\right)u_{\lambda,k}(r)\\
&= \exp\left(i\left(r+qa_1\hat{e}_1\right)\cdot k\right)T_{qa_1\hat{e}_1}u_{\lambda,k}(r)\\
&= \exp\left(i\left(r+qa_1\hat{e}_1\right)\cdot k\right)\exp\left(i\pi p\left(-\frac{1}{a_2}\hat{y}\right)\cdot r\right)u_{\lambda,k}(r)
\end{aligned}$$

- Then

$$\begin{aligned}
T_{a_2\hat{e}_2}T_{qa_1\hat{e}_1}\psi(r) &= T_{a_2\hat{e}_2}\exp\left(i\left(r+qa_1\hat{e}_1\right)\cdot k\right)\exp\left(i\pi p\left(-\frac{1}{a_2}\hat{y}\right)\cdot r\right)u_{\lambda,k}(r)\\
&= \exp\left(i\left(r+qa_1\hat{e}_1+a_2\hat{e}_2\right)\cdot k\right)\exp\left(i\pi p\left(-\frac{1}{a_2}\hat{y}\right)\cdot\left(r+a_2\hat{e}_2\right)\right)T_{a_2\hat{e}_2}u_{\lambda,k}(r)\\
&= \exp\left(i\left(r+qa_1\hat{e}_1+a_2\hat{e}_2\right)\cdot k\right)\exp\left(i\pi p\left(-\frac{1}{a_2}\hat{y}\right)\cdot\left(r+a_2\hat{e}_2\right)\right)\exp\left(i\pi p\left(\frac{1}{qa_1}\hat{x}\right)\cdot r\right)u_{\lambda,k}(r)
\end{aligned}$$

- The third leg is then:

$$\begin{aligned}
T_{-qa_1\hat{e}_1}T_{a_2\hat{e}_2}T_{qa_1\hat{e}_1}\psi(r) &= T_{-qa_1\hat{e}_1}\exp\left(i\left(r+qa_1\hat{e}_1+a_2\hat{e}_2\right)\cdot k\right)\times\\
&\quad\times\exp\left(i\pi p\left(-\frac{1}{a_2}\hat{y}\right)\cdot\left(r+a_2\hat{e}_2\right)\right)\exp\left(i\pi p\left(\frac{1}{qa_1}\hat{x}\right)\cdot r\right)u_{\lambda,k}(r)\\
&= \exp\left(i\left(r+a_2\hat{e}_2\right)\cdot k\right)\exp\left(i\pi p\left(-\frac{1}{a_2}\hat{y}\right)\cdot\left(r+a_2\hat{e}_2-qa_1\hat{e}_1\right)\right)\times\\
&\quad\times\exp\left(i\pi p\left(\frac{1}{qa_1}\hat{x}\right)\cdot\left(r-qa_1\hat{e}_1\right)\right)\exp\left(i\pi p\left(\frac{n_1}{a_2}\hat{y}\right)\cdot r\right)u_{\lambda,k}(r)
\end{aligned}$$

and finally the last leg is:

$$\begin{aligned} T_{-a_2\hat{e}_2}T_{-qa_1\hat{e}_1}T_{a_2\hat{e}_2}T_{qa_1\hat{e}_1}\psi(r) &= \exp\left(i\left(r+a_2\hat{e}_2-a_2\hat{e}_2\right)\cdot k\right)\exp\left(i\pi p\left(-\frac{1}{a_2}\hat{y}\right)\cdot\left(r+a_2\hat{e}_2-qa_1\hat{e}_1-a_2\hat{e}_2\right)\right)\times \\ &\times\exp\left(i\pi p\left(\frac{1}{qa_1}\hat{x}\right)\cdot\left(r-qa_1\hat{e}_1-a_2\hat{e}_2\right)\right)\exp\left(i\pi p\left(\frac{n_1}{a_2}\hat{y}\right)\cdot\left(r-a_2\hat{e}_2\right)\right)T_{-a_2\hat{e}_2}u_{\lambda,k}(r) \\ &= \exp\left(i\pi p\left(\frac{1}{qa_1}\hat{x}\right)\cdot\left(-qa_1\hat{e}_1\right)\right)\exp\left(i\pi p\left(\frac{1}{a_2}\hat{y}\right)\cdot\left(-a_2\hat{e}_2\right)\right)\psi(r) \\ &= \exp(-i\pi p)\exp(-i\pi p)\psi(r) \\ &= \exp(-2\pi i p)\psi(r) \end{aligned}$$

- As p depends only on the magnitude of B, $\exp(-2\pi i p)$ is gauge invariant.

□

- Interpreted in this way, we may write $p = \frac{-1}{2\pi}\int d\mathbf{l}\frac{\partial\arg(\psi(r))}{\partial\mathbf{l}}$ where we go in counterclockwise direciton around the boundary of the magnetic unit cell.

CHAPTER 6

The Physical Quantities Corresponding to the Indices

6.1. The TKNN Formula for the Quantum Hall Conductance

Our goal in this section is to show that 1.7.1 actually is equal to the quantum Hall conductance of a bulk system. We follow the presentation in [**Ch95**].

The first thing we do is analyze the linear response formula of Kubo (perturbation theory in quantum mechanics). This will give us the expectation value of an observable in the presence of a perturbation.

- Write $H = H_0 + V(t)$. V is the perturbation. It is written now with time dependence, but ultimately we will assume that long ago in the past it is zero and in the far future it is constant.
- $\rho(t) = \rho_0 + \Delta\rho(t)$ where ρ_0 is a stationary-state of H_0 (that means $\dot{\rho_0} = [\rho_0, H_0] = 0$)
- ρ obeys the Liouville equation $\dot{\rho} = \frac{1}{i\hbar}[H, \rho]$.
- Switch to the interaction picture:
  - $\rho^I(t) := e^{-\frac{1}{i\hbar}H_0 t}\rho e^{\frac{1}{i\hbar}H_0 t}$
  - ${\rho_0}^I = e^{-\frac{1}{i\hbar}H_0 t}\rho_0 e^{\frac{1}{i\hbar}H_0 t} = \rho_0$
  - $\Delta\rho^I(t) = e^{-\frac{1}{i\hbar}H_0 t}\Delta\rho(t) e^{\frac{1}{i\hbar}H_0 t}$
  - ${H_0}^I = e^{-\frac{1}{i\hbar}H_0 t}H_0 e^{\frac{1}{i\hbar}H_0 t} = H_0$

6.1.1. CLAIM. $i\hbar\frac{d}{dt}\Delta\rho^I = \left[V^I, \rho_0\right]$.

PROOF.

- Reverse the definition to get $\rho = e^{\frac{1}{i\hbar}H_0 t}\rho^I(t) e^{-\frac{1}{i\hbar}H_0 t}$.
- Plug this into the Liouville equation to get

$$\begin{aligned}
\frac{d}{dt}\left(e^{\frac{1}{i\hbar}H_0 t}\rho^I(t) e^{-\frac{1}{i\hbar}H_0 t}\right) &= \frac{1}{i\hbar}\left[H, e^{\frac{1}{i\hbar}H_0 t}\rho^I(t) e^{-\frac{1}{i\hbar}H_0 t}\right] \\
\frac{1}{i\hbar}e^{\frac{1}{i\hbar}H_0 t}H_0\rho^I(t) e^{-\frac{1}{i\hbar}H_0 t} &= \frac{1}{i\hbar}\left[H_0 + V, e^{\frac{1}{i\hbar}H_0 t}\rho^I(t) e^{-\frac{1}{i\hbar}H_0 t}\right] \\
-\frac{1}{i\hbar}e^{\frac{1}{i\hbar}H_0 t}\rho^I(t) H_0 e^{-\frac{1}{i\hbar}H_0 t} & \\
+e^{\frac{1}{i\hbar}H_0 t}\left(\frac{d}{dt}\rho^I(t)\right) e^{-\frac{1}{i\hbar}H_0 t} & \\
\frac{1}{i\hbar}\left[H_0, \rho^I(t)\right] + \frac{d}{dt}\rho^I(t) &= \frac{1}{i\hbar}e^{-\frac{1}{i\hbar}H_0 t}\left[H_0 + V, e^{\frac{1}{i\hbar}H_0 t}\rho^I(t) e^{-\frac{1}{i\hbar}H_0 t}\right] e^{\frac{1}{i\hbar}H_0 t} \\
\frac{1}{i\hbar}\left[H_0, \rho^I(t)\right] + \frac{d}{dt}\rho^I(t) &= \frac{1}{i\hbar}\left[(H_0)^I + V^I, \rho^I(t)\right] \\
\frac{d}{dt}\rho^I(t) &= \frac{1}{i\hbar}\left[V^I, \rho^I(t)\right]
\end{aligned}$$

- But $\frac{d}{dt}\left(\rho^I(t)\right) = \frac{d}{dt}\left(\rho_0 + \Delta\rho^I\right) = \frac{d}{dt}\Delta\rho^I$, and $\left[V^I, \Delta\rho^I\right] \propto \mathcal{O}\left(V^2\right)$ (because in perturbation theory $\Delta\rho \propto V$)
- Thus we get $\frac{d}{dt}\Delta\rho^I = \frac{1}{i\hbar}\left[V^I, \rho_0\right]$.

□

- Assume that

$$\lim_{t\to-\infty}\Delta\rho(t) = 0$$

6.1.2. CLAIM. We can integrate the equation of motion to get:

$$\Delta\rho^I = \frac{1}{i\hbar}\int_{-\infty}^{t}\left[V^I(t'), \rho_0\right] dt'$$

PROOF.

- Differentiate this Ansatz to verify its validity.

□

- Let B be some observable.
- Then $\langle B(t)\rangle = \mathrm{Tr}(B\rho(t))$.
  - Due to the cyclicity of the trace we have

$$\begin{aligned}\langle B(t)\rangle &= \mathrm{Tr}\left(Be^{-\frac{i}{\hbar}H_0t}e^{\frac{i}{\hbar}H_0t}\rho(t)\,e^{-\frac{i}{\hbar}H_0t}e^{\frac{i}{\hbar}H_0t}\right)\\ &= \mathrm{Tr}\left(e^{\frac{i}{\hbar}H_0t}Be^{-\frac{i}{\hbar}H_0t}e^{\frac{i}{\hbar}H_0t}\rho(t)\,e^{-\frac{i}{\hbar}H_0t}\right)\\ &= \mathrm{Tr}\left(B^I\rho^I\right)\\ &= \mathrm{Tr}\left(B^I\left((\rho_0)^I+(\Delta\rho)^I\right)\right)\\ &= \mathrm{Tr}\left(B^I(\rho_0)^I\right)+\mathrm{Tr}\left(B^I\Delta\rho^I\right)\end{aligned}$$

- Assume B is such that $\mathrm{Tr}\left(B^I(\rho_0)^I\right)=0$.
- Then

$$\begin{aligned}\langle B(t)\rangle &= \mathrm{Tr}\left(B^I(t)\,\Delta\rho^I(t)\right)\\ &= \mathrm{Tr}\left(B^I(t)\left(\frac{1}{i\hbar}\int_{-\infty}^t\left[V^I(t'),\rho_0\right]dt'\right)\right)\\ &= \frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(B^I(t)\left[V^I(t'),\rho_0\right]\right)dt'\\ &= \frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(B^I(t)\,V^I(t')\,\rho_0-B^I(t)\,\rho_0V^I(t')\right)dt'\\ &= \frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0B^I(t)\,V^I(t')-\rho_0V^I(t')\,B^I(t)\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0V^I(t')\,B^I(t)-\rho_0B^I(t)\,V^I(t')\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0\left[V^I(t'),B^I(t)\right]\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0\left[e^{-\frac{1}{i\hbar}H_0t'}V(t')\,e^{\frac{1}{i\hbar}H_0t'},e^{-\frac{1}{i\hbar}H_0t}Be^{\frac{1}{i\hbar}H_0t}\right]\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0e^{-\frac{1}{i\hbar}H_0t'}V(t')\,e^{\frac{1}{i\hbar}H_0t'}e^{-\frac{1}{i\hbar}H_0t}Be^{\frac{1}{i\hbar}H_0t}-\rho_0e^{-\frac{1}{i\hbar}H_0t}Be^{\frac{1}{i\hbar}H_0t}e^{-\frac{1}{i\hbar}H_0t'}V(t')\,e^{\frac{1}{i\hbar}H_0t'}\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(e^{-\frac{1}{i\hbar}H_0t'}\rho_0V(t')\,e^{\frac{1}{i\hbar}H_0t'}e^{-\frac{1}{i\hbar}H_0t}Be^{\frac{1}{i\hbar}H_0t}-e^{\frac{1}{i\hbar}H_0t'}\rho_0e^{-\frac{1}{i\hbar}H_0t}Be^{\frac{1}{i\hbar}H_0t}e^{-\frac{1}{i\hbar}H_0t'}V(t')\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0V(t')\,e^{\frac{1}{i\hbar}H_0t'}e^{-\frac{1}{i\hbar}H_0t}Be^{\frac{1}{i\hbar}H_0t}e^{-\frac{1}{i\hbar}H_0t'}-\rho_0e^{\frac{1}{i\hbar}H_0t'}e^{-\frac{1}{i\hbar}H_0t}Be^{\frac{1}{i\hbar}H_0t}e^{-\frac{1}{i\hbar}H_0t'}V(t')\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0V(t')\,e^{-\frac{1}{i\hbar}H_0(t-t')}Be^{\frac{1}{i\hbar}H_0(t-t')}-\rho_0e^{-\frac{1}{i\hbar}H_0(t-t')}Be^{\frac{1}{i\hbar}H_0(t-t')}V(t')\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0V(t')\,B^I(t-t')-\rho_0B^I(t-t')\,V(t')\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^t\mathrm{Tr}\left(\rho_0\left[V(t'),B^I(t-t')\right]\right)dt'\end{aligned}$$

- Make a Fourier transform of V as

$$V(t)=\lim_{\eta\to0}\frac{1}{2\pi}\int_{\mathbb{R}}e^{-i(\omega+i\eta)t}\tilde{V}(\omega)\,d\omega$$

where $\eta>0$ is some factor we introduce to insure the boundary condition $\lim_{t\to-\infty}\Delta\rho(t)=0$ is met.

- Then

$$\begin{aligned}\langle B(t)\rangle &= -\frac{1}{i\hbar}\int_{-\infty}^{t}\text{Tr}\left(\rho_0\left[V(t'),B^I(t-t')\right]\right)dt'\\ &= -\frac{1}{i\hbar}\int_{-\infty}^{t}\text{Tr}\left(\rho_0\left[\left(\lim_{\eta\to 0}\frac{1}{2\pi}\int_{\mathbb{R}}e^{-i(\omega+i\eta)t'}\tilde{V}(\omega)\,d\omega\right),B^I(t-t')\right]\right)dt'\\ &= \lim_{\eta\to 0}\frac{1}{2\pi}\int_{\mathbb{R}}\int_{-\infty}^{t}\frac{i}{\hbar}\text{Tr}\left(\rho_0\left[\tilde{V}(\omega),B^I(t-t')\right]\right)e^{-i(\omega+i\eta)t'}dt'd\omega\\ &= \lim_{\eta\to 0}\frac{1}{2\pi}\int_{\mathbb{R}}\int_{-\infty}^{\infty}\frac{i}{\hbar}\text{Tr}\left(\rho_0\left[\tilde{V}(\omega),B^I(t-t')\right]\right)\theta(t-t')\,e^{-i(\omega+i\eta)t'}dt'd\omega\end{aligned}$$

6.1.3. DEFINITION. Define the linear response function

$$\chi_{B\tilde{V}(\omega)}(t):=\frac{i}{\hbar}\text{Tr}\left(\rho_0\left[\tilde{V}(\omega),B^I(t)\right]\right)\theta(t)$$

- Observe we can again change the order to write

$$\begin{aligned}\chi_{B\tilde{V}(\omega)}(t) &\equiv \frac{i}{\hbar}\text{Tr}\left(\rho_0\left[\tilde{V}(\omega),B^I(t)\right]\right)\theta(t)\\ &= \frac{i}{\hbar}\text{Tr}\left(\rho_0\tilde{V}(\omega)B^I(t)-\rho_0B^I(t)\tilde{V}(\omega)\right)\theta(t)\\ &= \frac{i}{\hbar}\text{Tr}\left(\rho_0\tilde{V}(\omega)B^I(t)-\tilde{V}(\omega)\rho_0B^I(t)\right)\theta(t)\\ &= -\frac{i}{\hbar}\text{Tr}\left(\left[\tilde{V}(\omega),\rho_0\right]B^I(t)\right)\theta(t)\end{aligned}$$

Then we find

$$\boxed{\langle B(t)\rangle=\lim_{\eta\to 0}\frac{1}{2\pi}\int_{\mathbb{R}}\int_{-\infty}^{\infty}\chi_{B\tilde{V}(\omega)}(t-t')\,e^{-i(\omega+i\eta)t'}dt'd\omega}$$

which is the linear response formula.

The next step is to employ this in order to find the Hall conductivity. We will start this analysis in the many-body picture:

- Define

$$B_\mu:=-eJ_\mu(r):=-e\left(\frac{1}{2}\sum_{j=1}^{N}\left(v_{j\mu}\delta(r-r_j)+\delta(r-r_j)v_{j\mu}\right)\right)$$

  where $v_{j\mu}$ is the velocity operator of the jth particle along the μth axis.
- Define the operator

$$X_\mu:=\sum_{j=1}^{N}r_{j\mu}$$

- Define

$$\begin{aligned}V(t) &:= \sum_{j=1}^{N}e\sum_{\mu\in\{x,y,z\}}r_{j\mu}E_\mu f(t)\\ &= \sum_{\mu}eX_\mu E_\mu f(t)\end{aligned}$$

  where E_μ is the electric field in the system and $f(t)$ is some attenuation function which goes to zero at $t\to-\infty$ and "turns on" adiabatically.
- Then the linear response is

$$\begin{aligned}\chi_{B_\mu eX_\nu}(t) &:= \frac{i}{\hbar}\text{Tr}\left(\rho_0\left[eX_\nu,-eJ_\mu{}^I(r,t)\right]\right)\theta(t)\\ &= -\frac{ie^2}{\hbar}\text{Tr}\left(\rho_0\left[X_\nu,J_\mu{}^I(r,t)\right]\right)\theta(t)\end{aligned}$$

- By Ohm's law, $j_a=\sigma_{ab}E_b$, that is, σ_{ab} is exactly the response of the current j to the perturbation E, so we expect $\sigma_{\mu\nu}=\chi_{B_\mu eX_\nu}(t)$ somehow, as we shall see below.

- Assume $(|n\rangle)_{n\in\mathbb{N}}$ is an orthonormal complete set of eigenstates of H_0 (the many-body Hamiltonian) with eigenvalues $(E_n)_{n\in\mathbb{N}}$, where we assume $E_0 = \min(\{E_n | n \in \mathbb{N}\})$. In this basis, ρ_0 is diagonal:

$$\begin{aligned}
\rho_0 &= \sum_{n\in\mathbb{N}} |n\rangle \langle n| \rho_0 \sum_{m\in\mathbb{N}} |m\rangle \langle m| \\
&= \sum_{(n,m)\in\mathbb{N}^2} \langle n | \rho_0 | m\rangle |n\rangle \langle m|
\end{aligned}$$

and then $[\rho_0, H_0] = 0$ means

$$\begin{aligned}
\langle m'| [\rho_0, H_0] |n'\rangle &= \langle m'| \left[\sum_{(n,m)\in\mathbb{N}^2} \langle n | \rho_0 | m\rangle |n\rangle \langle m|, H_0 \right] |n'\rangle \\
&= \langle m'| \left(\sum_{(n,m)\in\mathbb{N}^2} \langle n | \rho_0 | m\rangle |n\rangle \langle m| H_0 - \sum_{(n,m)\in\mathbb{N}^2} H_0 \langle n | \rho_0 | m\rangle |n\rangle \langle m| \right) |n'\rangle \\
&= \langle m'| \left(\sum_{(n,m)\in\mathbb{N}^2} \langle n | \rho_0 | m\rangle |n\rangle \langle m| E_m - \sum_{(n,m)\in\mathbb{N}^2} E_n \langle n | \rho_0 | m\rangle |n\rangle \langle m| \right) |n'\rangle \\
&= \langle m'| \sum_{(n,m)\in\mathbb{N}^2} \langle n | \rho_0 | m\rangle |n\rangle \langle m| (E_m - E_n) |n'\rangle \\
&= \langle m' | \rho_0 | n'\rangle (E_{n'} - E_{m'}) \\
&\stackrel{!}{=} 0
\end{aligned}$$

and so if $(E_{n'} - E_{m'}) \neq 0$ then $\langle m' | \rho_0 | n'\rangle = 0$. Assuming we don't have degeneracy, this means $\langle m' | \rho_0 | n'\rangle \propto \delta_{m'n'}$.

- Then

$$\begin{aligned}
\mathrm{Tr}\left(\rho_0 \left[X_\nu, J_\mu{}^I(r,t)\right]\right) &= \sum_{n\in\mathbb{N}} \left\langle n \middle| \rho_0 \left[X_\nu, J_\mu{}^I(r,t)\right] \middle| n \right\rangle \\
&= \sum_{n\in\mathbb{N}} \left\langle n \middle| \sum_{m\in\mathbb{N}} \langle m | \rho_0 | m\rangle |m\rangle \langle m| \left[X_\nu, J_\mu{}^I(r,t)\right] \middle| n \right\rangle \\
&= \sum_{n\in\mathbb{N}} \langle n | \rho_0 | n\rangle \left\langle n \middle| \left[X_\nu, J_\mu{}^I(r,t)\right] \middle| n \right\rangle
\end{aligned}$$

  - In the canonical ensemble,

$$\begin{aligned}
\langle n|\rho_0|n\rangle &= \left\langle n \middle| \left(\frac{e^{-\beta H_0}}{\mathrm{Tr}\left(e^{-\beta H_0}\right)} \right) \middle| n \right\rangle \\
&= \left\langle n \middle| \left(\frac{e^{-\beta E_n}}{Z} \right) \middle| n \right\rangle \\
&= \frac{e^{-\beta E_n}}{Z}
\end{aligned}$$

  - When $T \to 0$, we can make the approximation $\langle n|\rho_0|n\rangle \approx \delta_{n0}$. We also assume that in the ground state there is no current, that is, $\langle 0 | J_\mu(r) | 0\rangle = 0$.

- Thus we have

$$\begin{aligned}
\mathrm{Tr}\left(\rho_0\left[X_\nu, J_\mu{}^I(r,t)\right]\right) &= \sum_{n\in\mathbb{N}} \langle n|\rho_0|n\rangle \left\langle n\middle|\left[X_\nu, J_\mu{}^I(r,t)\right]\middle|n\right\rangle \\
&\approx \left\langle 0\middle|\left[X_\nu, J_\mu{}^I(r,t)\right]\middle|0\right\rangle \\
&= \left\langle 0\middle|X_\nu J_\mu{}^I(r,t)\middle|0\right\rangle - \left\langle 0\middle|J_\mu{}^I(r,t)X_\nu\middle|0\right\rangle \\
&= \left\langle 0\middle|X_\nu \sum_{n\in\mathbb{N}}|n\rangle\langle n|J_\mu{}^I(r,t)\middle|0\right\rangle - \left\langle 0\middle|J_\mu{}^I(r,t)\sum_{n\in\mathbb{N}}|n\rangle\langle n|X_\nu\middle|0\right\rangle \\
&= \sum_{n\in\mathbb{N}} \langle 0|X_\nu|n\rangle \left\langle n\middle|J_\mu{}^I(r,t)\middle|0\right\rangle - \left\langle 0\middle|J_\mu{}^I(r,t)\middle|n\right\rangle \langle n|X_\nu|0\rangle \\
&= \sum_{n\in\mathbb{N}} \langle 0|X_\nu|n\rangle \left\langle n\middle|e^{-\frac{1}{i\hbar}H_0 t}J_\mu(r)e^{\frac{1}{i\hbar}H_0 t}\middle|0\right\rangle - \left\langle 0\middle|e^{-\frac{1}{i\hbar}H_0 t}J_\mu(r)e^{\frac{1}{i\hbar}H_0 t}\middle|n\right\rangle \langle n|X_\nu|0\rangle \\
&= \sum_{n\in\mathbb{N}} \langle 0|X_\nu|n\rangle \left\langle n\middle|e^{-\frac{1}{i\hbar}E_n t}J_\mu(r)e^{\frac{1}{i\hbar}E_0 t}\middle|0\right\rangle - \left\langle 0\middle|e^{-\frac{1}{i\hbar}E_0 t}J_\mu(r)e^{\frac{1}{i\hbar}E_n t}\middle|n\right\rangle \langle n|X_\nu|0\rangle \\
&= \sum_{n\in\mathbb{N}} \langle 0|X_\nu|n\rangle\langle n|J_\mu(r)|0\rangle e^{-\frac{1}{i\hbar}(E_n-E_0)t} - \langle 0|J_\mu(r)|n\rangle\langle n|X_\nu|0\rangle e^{\frac{1}{i\hbar}(E_n-E_0)t}
\end{aligned}$$

- So we find that

$$\lim_{T\to 0}\chi_{B_\mu e X_\nu}(t) \approx -\frac{ie^2}{\hbar}\theta(t)\sum_{n\in\mathbb{N}}\left(\langle 0|X_\nu|n\rangle\langle n|J_\mu(r)|0\rangle e^{-\frac{1}{i\hbar}(E_n-E_0)t} - \langle 0|J_\mu(r)|n\rangle\langle n|X_\nu|0\rangle e^{\frac{1}{i\hbar}(E_n-E_0)t}\right)$$

- Thus the expectation value for the electric current is given by:

$$\begin{aligned}
\lim_{T\to 0}\langle B_\mu(t)\rangle &= \sum_\nu \int_{-\infty}^{\infty}\lim_{T\to 0}\chi_{B_\mu e X_\nu}\left(t-t'\right)E_\nu f\left(t'\right)dt' \\
&= \sum_\nu \underbrace{\int_{-\infty}^{\infty}\lim_{T\to 0}\chi_{B_\mu e X_\nu}\left(t-t'\right)f\left(t'\right)dt'}_{\sigma_{\mu\nu}} E_\nu
\end{aligned}$$

- And as such we found a formula:

$$\begin{aligned}
\lim_{T\to\infty}\sigma_{\mu\nu}(r,t) &= \int_{-\infty}^{\infty}\lim_{T\to 0}\chi_{B_\mu e X_\nu}\left(t-t'\right)f\left(t'\right)dt'd\omega \\
&\approx -\frac{ie^2}{\hbar}\int_{-\infty}^{\infty}\theta\left(t-t'\right)\sum_{n\in\mathbb{N}}\left(\langle 0|X_\nu|n\rangle\langle n|J_\mu(r)|0\rangle e^{-\frac{1}{i\hbar}(E_n-E_0)(t-t')}\right)f\left(t'\right)dt' \\
&\quad -\frac{ie^2}{\hbar}\int_{-\infty}^{\infty}\theta\left(t-t'\right)\sum_{n\in\mathbb{N}}\left(-\langle 0|J_\mu(r)|n\rangle\langle n|X_\nu|0\rangle e^{\frac{1}{i\hbar}(E_n-E_0)(t-t')}\right)f\left(t'\right)dt'
\end{aligned}$$

- The actual conductivity is time independent and so we need to integrate this over time:

$$\sigma_{\mu\nu}(r) = \lim_{\eta\to 0^+}\int_{-\infty}^{\infty}dt e^{-\eta t}\sigma_{\mu\nu}(r,t)$$

  where $e^{-\eta t}$ is a convergence factor with $\eta > 0$.
- Denote by v_μ the total velocity, that is, $v_\mu = \int d^2 r J_\mu(r)$.
- We are interested in the conductivity of the material as a whole, and not just at one particular point, so we should average over space. Thus, if A is the area of the material, the final quantity we are interested

in is

$$\begin{aligned}
\sigma_{\mu\nu} &= \frac{1}{A}\int d^2r \lim_{\eta\to0^+}\int_{-\infty}^{\infty} dte^{-\eta t}\sigma_{\mu\nu}(r,t) \\
&= \frac{1}{A}\int d^2r \lim_{\eta\to0^+}\int_{-\infty}^{\infty} dte^{-\eta t}\int_{-\infty}^{\infty} -\frac{ie^2}{\hbar}\theta(t-t')\times \\
&\times\sum_{n\in\mathbb{N}}\left(\langle 0|X_\nu|n\rangle\langle n|J_\mu(r)|0\rangle e^{-\frac{1}{i\hbar}(E_n-E_0)(t-t')} - \langle 0|J_\mu(r)|n\rangle\langle n|X_\nu|0\rangle e^{\frac{1}{i\hbar}(E_n-E_0)(t-t')}\right) f(t')\,dt' \\
&= e^2\sum_{n\in\mathbb{N}}\left(-\frac{i}{\hbar}\frac{1}{A}\right)\lim_{\eta\to0^+}\int_{-\infty}^{\infty} dte^{-\eta t}\int_{-\infty}^{\infty}\theta(t-t')\times \\
&\times\left(\langle 0|X_\nu|n\rangle\langle n|v_\mu|0\rangle e^{-\frac{1}{i\hbar}(E_n-E_0)(t-t')} - \langle 0|v_\mu|n\rangle\langle n|X_\nu|0\rangle e^{\frac{1}{i\hbar}(E_n-E_0)(t-t')}\right) f(t')\,dt' \\
&= \frac{e^2}{A}\sum_{n\in\mathbb{N}}\frac{\langle 0|X_\nu|n\rangle\langle n|v_\mu|0\rangle + \langle 0|v_\mu|n\rangle\langle n|X_\nu|0\rangle}{E_n-E_0}
\end{aligned}$$

- The last step is to note that the velocity operator is equal to $v_\mu = \dot{X}_\mu$, and of course by the Heisenberg equation of motion we then have $v_\mu = \frac{1}{i\hbar}[X_\mu, H_0]$ or $X_\mu H_0 - H_0 X_0 = i\hbar v_\mu$. As a result,

$$\begin{aligned}
\langle 0|X_\nu|n\rangle &= \frac{E_n-E_0}{E_n-E_0}\langle 0|X_\nu|n\rangle \\
&= \frac{1}{E_n-E_0}\langle 0|(E_n-E_0)X_\nu|n\rangle \\
&= \frac{1}{E_n-E_0}\langle 0|(X_\nu E_n - E_0 X_\nu)|n\rangle \\
&= \frac{1}{E_n-E_0}\langle 0|(X_\nu H_0 - H_0 X_\nu)|n\rangle \\
&= \frac{1}{E_n-E_0}\langle 0|[X_\nu, H_0]|n\rangle \\
&= \frac{1}{E_n-E_0}\langle 0|i\hbar v_\nu|n\rangle \\
&= \frac{i\hbar}{E_n-E_0}\langle 0|v_\nu|n\rangle
\end{aligned}$$

- Thus we can write $\sigma_{\mu\nu}$ with only v's as:

$$\sigma_{\mu\nu} = \frac{ie^2\hbar}{A}\sum_{n\in\mathbb{N}}\frac{\langle 0|v_\nu|n\rangle\langle n|v_\mu|0\rangle - \langle 0|v_\mu|n\rangle\langle n|v_\nu|0\rangle}{(E_n-E_0)^2}$$

which is the many body equivalent of the sum on occupied single-particle states which we had in Eq. (22) (to show this we have to use the formula $v = \frac{1}{\hbar}\frac{\partial E(k)}{\partial k}$, which appears for example in [**As76**] equation E.7).

6.2. The Edge Quantum Hall Conductance

The goal in this section is to show that 1.6.1 actually is equal to the quantum Hall condutance of an edge system. We assume the chemical potential on one edge is μ_+ and μ_- on the other edge, where $\mu_+ \neq \mu_-$ (otherwise the current on one edge cancels out the current on the other edge as they flow in opposite directions). Using the formula

$j = \rho\nu$ where ρ is the density of carriers and ν is the velocity of the carriers, we have

$$\begin{aligned} I &= \frac{1}{2\pi}\sum_j \int_{k_-^j}^{k_+^j} \nu\left(k\right) dk \\ &= \frac{1}{2\pi}\sum_j \int_{k_-^j}^{k_+^j} \frac{1}{h}\frac{\partial E}{\partial k} dk \\ &= \frac{1}{h}\frac{1}{2\pi}\sum_j \left[E\left(k_+^j\right) - E\left(k_-^j\right)\right] \\ &= \frac{1}{h}\frac{1}{2\pi}\sum_j \left[\mu_+ - \mu_-\right] \\ &= \frac{1}{h}\frac{1}{2\pi}\sum_j V \end{aligned}$$

where the sum is on intersection points of either μ_+ or μ_- with the gapless edge states, ν is the velocity, and V is the potential between the two edges. Thus we obtain that for each ascending crossing of the gapless edge mode with either μ_+ or μ_- we must count $+1$ for the conductance (given by $\sigma = \frac{I}{V}$) and -1 for a descending crossing.

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