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Problem 7.1: The sewing matrix expression for the Pfaffian invariant [**Written** | 12 pt(s)]

ID: ex_sewing_matrix_expression_pfaffian_invariant:tqp25

Learning objective

In the lecture, we introduced the Pfaffian invariant as the parity of the vorticity of the Pfaffian in an effective Brillouin zone. This topological $\mathbb{Z}_2$ index characterizes the topological phase of the Kane-Mele model (topological insulator). Here you derive an equivalent expression for the Pfaffian invariant in terms of the *sewing matrix*. This expression is pivotal for the construction of topological insulators in three dimensions.

Let $\{|e_i(\boldsymbol{k})\rangle\}_{i=1\dots 2n}$ be a globally continuous basis of the valence bundle, i.e., the subspace of filled Bloch states $\mathcal{H}_{\boldsymbol{k}}^{\text{filled}}$ over the Brillouin zone T^2. In the lecture, we defined the *Pfaffian index* as

$$I := \frac{1}{2\pi i}\oint_{\partial\text{EBZ}} \mathrm{d}\log P(\boldsymbol{k}) \mod 2 = \frac{1}{2\pi i}\oint_{\partial\text{EBZ}} \nabla\log P(\boldsymbol{k})\cdot \mathrm{d}\boldsymbol{k} \mod 2 \tag{1}$$

with ∂EBZ the boundary of a suitably chosen effective Brillouin zone (EBZ) that does not intersect the vortices of $P(\boldsymbol{k})$. The latter is given as the *Pfaffian* $P(\boldsymbol{k}) := \mathrm{Pf}\,[M(\boldsymbol{k})]$ of the skew-symmetric matrix

$$M_{ij}(\boldsymbol{k}) := \langle e_i(\boldsymbol{k})|\,\tilde{T}_U\,|e_j(\boldsymbol{k})\rangle\ . \tag{2}$$

Here, $\tilde{T}_U = U\mathcal{K}$ is the (antiunitary) *time-reversal operator* with $\tilde{T}_U^2 = -\mathbb{1}$. $\mathcal{K}$ denotes complex conjugation and U is a unitary operator that determines the representation on Bloch space.

Let the *sewing matrix* be defined as

$$w_{ij}(\boldsymbol{k}) := \langle e_i(-\boldsymbol{k})|\,\tilde{T}_U\,|e_j(\boldsymbol{k})\rangle\ . \tag{3}$$

The goal of this exercise is to find an expression for the topological index (1) in terms of the sewing matrix (3). This expression will turn out to be much simpler than Eq. (1) and can straightforwardly be generalized to *three* dimensions.

In the following, $\mathcal{I}$ denotes the set of time-reversal invariant momenta (TRIMs).

a) To warm up, prove the following properties of the sewing matrix for $\boldsymbol{k}\in T^2$ and $\boldsymbol{K}\in\mathcal{I}$: **3**pt(s)

i. $w(\boldsymbol{k})w^\dagger(\boldsymbol{k}) = \mathbb{1}$ $\rightarrow$ Unitarity everywhere on the Brillouin zone

ii. $w^T(\boldsymbol{k}) = -w(-\boldsymbol{k})$ $\rightarrow$ Skew-symmetry at TRIMs

iii. $w(\boldsymbol{K}) = M(\boldsymbol{K})$

iv. $M(-\boldsymbol{k}) = w(\boldsymbol{k})\cdot M^*(\boldsymbol{k})\cdot w^T(\boldsymbol{k})$

v. $\det[w(\boldsymbol{k})] = \frac{P(\boldsymbol{k})}{[P(-\boldsymbol{k})]^*}$

Hint: For $A, B \in \mathbb{C}^{2n\times 2n}$ with A skew-symmetric, it is $\mathrm{Pf}\left[BAB^T\right] = \det(B)\,\mathrm{Pf}\,[A]$.

b) Next, show that $\det[w(\boldsymbol{k})] = \det[w(-\boldsymbol{k})]$ is inversion symmetric on T^2. Use this to prove that 2pt(s)

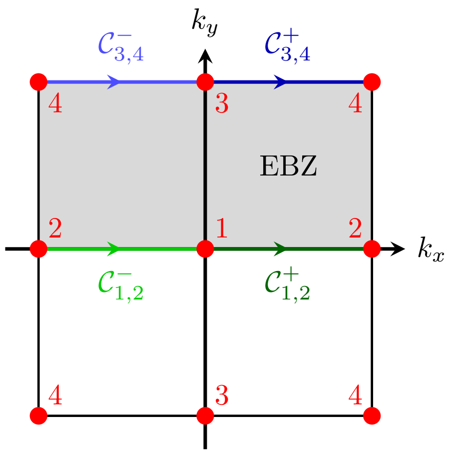
$$\frac{1}{2\pi i}\oint_{\mathcal{C}} \mathrm{d}\log[\det w(\boldsymbol{k})] = 0 \tag{4}$$

vanishes for every closed path $\mathcal{C}$ on the Brillouin zone T^2.

Hint: Note that the *non-contractible* loops around the torus T^2 allow for phase windings even in the absence of vortices. To show that for such loops the above integral vanishes, use that every loop can be continuously deformed into a *time-reversal invariant loop*, i.e., a loop that is mapped onto itself under inversion $\boldsymbol{k} \mapsto -\boldsymbol{k}$.

For a path $\mathcal{C}$ that does not cross zeros of $P(\boldsymbol{k})$, we define $L[\mathcal{C}] := \int_{\mathcal{C}} \mathrm{d}\log P(\boldsymbol{k})$. This allows us to rewrite the Pfaffian index as $I = L[\partial\mathrm{EBZ}]/(2\pi i) \mod 2$ for the closed path $\mathcal{C} = \partial\mathrm{EBZ}$.

In the following, we use $\mathcal{C}_{i,j}$ to label the two disjoint boundary components of the EBZ (each of which passes through two TRIMs $\boldsymbol{K}_i, \boldsymbol{K}_j \in \mathcal{I}$). Each of these paths can be split into two connected components $\mathcal{C}^{\pm}_{i,j}$ that are mapped onto each other under time-reversal:



c) Show that the Pfaffian index is implicitly given by 1pt(s)

$$(-1)^I = \exp\frac{L[\mathcal{C}_{1,2}] - L[\mathcal{C}_{3,4}]}{2} \tag{5}$$

with $L[\mathcal{C}_{i,j}] = 2L[\mathcal{C}^+_{i,j}] + \left(L[\mathcal{C}^-_{i,j}] - L[\mathcal{C}^+_{i,j}]\right)$ for $(i,j) \in \{(1,2),(3,4)\}$.

d) To evaluate Eq. (5), first show that 1pt(s)

$$\exp L[\mathcal{C}^+_{i,j}] = \frac{\mathrm{Pf}\,[w(\boldsymbol{K}_j)]}{\mathrm{Pf}\,[w(\boldsymbol{K}_i)]}\,, \tag{6}$$

e) ... and then show that 2pt(s)

$$L[\mathcal{C}^+_{i,j}] - L[\mathcal{C}^-_{i,j}] = \int_{\mathcal{C}^+_{i,j}} \mathrm{d}\left[\log P(\boldsymbol{k}) - \log P^*(-\boldsymbol{k})\right]\,. \tag{7}$$

Hint: Show that $|P(\boldsymbol{K})| = 1$ at TRIMs $\boldsymbol{K} \in \mathcal{I}$, and that $|P(\boldsymbol{k})| = |P(-\boldsymbol{k})|$ is symmetric. Consider a polar decomposition $P(\boldsymbol{k}) = \rho(\boldsymbol{k})\,e^{i\varphi(\boldsymbol{k})}$ of the Pfaffian.

f) Use Eq. (7) to derive **1**pt(s)

$$\exp\left\{\frac{L[\mathcal{C}_{i,j}^{+}]-L[\mathcal{C}_{i,j}^{-}]}{2}\right\}=\frac{\sqrt{\det w(\boldsymbol{K}_j)}}{\sqrt{\det w(\boldsymbol{K}_i)}}\,. \tag{8}$$

g) Finally, combine your results to prove the expression **2**pt(s)

$$(-1)^I=\prod_{\boldsymbol{K}\in\mathcal{I}}\frac{\mathrm{Pf}\,[w(\boldsymbol{K})]}{\sqrt{\det w(\boldsymbol{K})}}\,. \tag{9}$$

For the validity of Eq. (9) you need the continuity of $\sqrt{\det w(\boldsymbol{k})}$ on T^2 (why?).

Give a reason why such a choice for the square root is possible.

Hint: The identity $\mathrm{Pf}\,[A]^2=\det(A)$ may be useful.

The expression (9) allows for the computation of the Pfaffian invariant I based only on the values of the sewing matrix at the TRIMs (no integration required!). This expression is important because it can be used to generalize the $\mathbb{Z}_2$ invariant to three dimensions. This naturally leads to the concept of *three dimensional topological insulators* (which have been experimentally realized) and *weak topological insulators*[1].

Problem 7.2: Edge modes of the Su-Schrieffer-Heeger chain [**Oral** | 9 pt(s)]

ID: ex_edge_modes_su_schrieffer_heeger_chain:tqp25

> **Learning objective**
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> In the lecture, we claimed (and numerically demonstrated) that the ground state space degeneracy of the open-boundary SSH chain is due to exponentially localized *edge modes* which are present everywhere in the topological phase – even in the presence of sublattice-symmetric disorder. Here you substantiate this claim analytically.

The many-body Hamiltonian of the SSH chain reads for open boundary conditions

$$\hat{H}_{\mathrm{SSH}}=t\sum_{i=1}^{L}(a_i^\dagger b_i+b_i^\dagger a_i)+w\sum_{i=1}^{L-1}(b_i^\dagger a_{i+1}+a_{i+1}^\dagger b_i)\,, \tag{10}$$

with real, uniform hopping strengths $t>0$ and $w>0$. Here $a_i^{(\dagger)}$ and $b_i^{(\dagger)}$ are the fermionic annihilation (creation) operators of the i-th unit cell.

a) Show that the operators **1**pt(s)

$$\tilde{a}_l:=\mathcal{N}\sum_{i=1}^{L}(-x)^{i-1}\,a_i\qquad\text{and}\qquad\tilde{b}_r:=\mathcal{N}\sum_{i=1}^{L}(-x)^{i-1}\,b_{L-i+1} \tag{11}$$

with $x=\frac{t}{w}$ describe two fermionic modes and determine their normalizing factor $\mathcal{N}$.

b) In the thermodynamic limit ($L \to \infty$), and if the system is in the topological phase ($x < 1$), prove that the ground state space of $\hat{H}_{\text{SSH}}$ is four-fold degenerate by showing that **2pt(s)**

$$\left[\tilde{a}_l, \hat{H}_{\text{SSH}}\right] = \mathcal{O}\left(x^L\right) \qquad \text{and} \qquad \left[\tilde{b}_r, \hat{H}_{\text{SSH}}\right] = \mathcal{O}\left(x^L\right) . \tag{12}$$

Show that the energy splitting of the edge modes vanishes *exponentially* with the system size.

Your final goal is to demonstrate that these results are *robust* to disorder that breaks translational invariance, particle-hole symmetry and time-reversal symmetry (but *not* sublattice symmetry!). To this end, consider the *generalized SSH chain* Hamiltonian from the lecture

$$\hat{H}'_{\text{SSH}} = \sum_{i=1}^{L}(t_i\, a_i^\dagger b_i + t_i^*\, b_i^\dagger a_i) + \sum_{i=1}^{L-1}(w_i\, a_{i+1}^\dagger b_i + w_i^*\, b_i^\dagger a_{i+1})\,, \tag{13}$$

with site-dependent, complex coupling constants $t_i, w_i \in \mathbb{C}$.

We define the local ratio $x_i = \frac{t_i}{w_i}$ for $i \in \{1, \dots, L-1\}$ and assume that the moduli $|x_i|$ are *independent and identically distributed* (i.i.d.) random variables with probability density $P(x)$ for $x \in [0, \infty)$. For a given realization of couplings $\{x_i\}$, we define the generalized edge mode operators

$$\tilde{a}_l := \mathcal{N} \sum_{i=1}^{L} X_i\, a_i \qquad \text{and} \qquad \tilde{b}_r := \mathcal{N} \sum_{i=1}^{L} X_i^*\, b_{L-i+1} \tag{14}$$

with $X_i := \prod_{1 \le j < i}(-x_j)$ and $X_1 := 1$.

c) Verify that all algebraic statements from subtask a) remain valid, i.e., that $\tilde{a}_l$ and $\tilde{b}_r$ constitute two fermion modes. **1pt(s)**

Determine again their normalizing factor $\mathcal{N}$.

d) Focus only on the left edge mode $\tilde{a}_l$ and show that **3pt(s)**

$$\left[\tilde{a}_l, \hat{H}'_{\text{SSH}}\right] = \mathcal{N} X_L t_L\, b_L\,. \tag{15}$$

Derive a condition on the probability distribution P such that $X_L \in \mathcal{O}(e^{-\lambda L})$ for some $\lambda > 0$.

Hint: Strictly speaking, the limit $L \to \infty$ is to be taken in a stochastic sense: Use the (strong) *law of large numbers* to convert X_L into an integral over $P(x)$ in the limit $L \to \infty$ (this limit is a so called "almost sure" convergence).

For the sake of concreteness, assume that the moduli $|x_i| \sim \mathcal{U}(\delta, \tilde{x})$ are *uniformly distributed* random variables in the interval $[\delta, \tilde{x}]$. The lower cutoff $0 < \delta \ll 1$ is a regularization of no physical importance; the upper cutoff $\tilde{x} > \delta$ is the parameter of the model.

e) Show that for $\tilde{x} < 1$, the ground state space of $\hat{H}'_{\text{SSH}}$ is four-fold degenerate in the thermodynamic limit – despite the disorder in the hoppings! **2pt(s)**

Hint: Use your result from d).

In this exercise, you have shown explicitly that the topological phase of the SSH chain (indicated by the presence of degenerate edge modes) does *not* rely on translation invariance, even though the topological index derived in the lecture requires a translation invariant formulation to be well-defined.

[1] L. Fu, C. L. Kane, and E. J. Mele, Topological Insulators in Three Dimensions, PRL **98**, 106803 (2007)

Problem 7.3: The Zak phase

[**Oral** | 3 pt(s)]

ID: ex_zak_phase:tqp25

Learning objective

In the lecture, we have shown that the two quantum phases of the SSH chain can be characterized by the *winding number* of the Bloch vector around the origin in the $d_x d_y$-plane. In this exercise, you show that the two quantum phases can also be distinguished by the Berry phase collected over the Brillouin zone. This phase is known as the *Zak phase*[a] and has already been measured in experiments[b].

[a] J. Zak, Berry's phase for energy bands in solids, PRL **62**, 2747 (1989)
[b] M. Atala et al., Direct measurement of the Zak phase in topological Bloch bands, Nature Physics **9**, 795 (2013)

The Bloch Hamiltonian of the SSH chain is given by $H(k) = \vec{d}(k) \cdot \vec{\sigma}$ with Bloch vector

$$\vec{d}(k) = \begin{pmatrix} t + w \cos k \\ w \sin k \\ 0 \end{pmatrix} \tag{16}$$

for $k \in S^1 \equiv [0, 2\pi)$ and $t, w > 0$. Here, $\vec{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)^T$ is the vector of Pauli matrices.

a) Diagonalize the Bloch Hamiltonian and compute its eigenstates $|u_\pm(k)\rangle$. 1 pt(s)

b) Compute the *Zak phase* via the integral of the Berry connection over the Brillouin zone: 1 pt(s)

$$\varphi_{\text{Zak}} = \int_0^{2\pi} i \langle u_\pm(k)|\partial_k u_\pm(k)\rangle \, \mathrm{d}k \,. \tag{17}$$

Show that $\varphi_{\text{Zak}} = \pi \mod 2\pi$ in the topological phase (for $t < w$) and $\varphi_{\text{Zak}} = 0 \mod 2\pi$ in the trivial phase (for $t > w$).

c) Consider a *continuous* gauge transformation $|u_\pm(k)\rangle \mapsto e^{i\varphi_k} |u_\pm(k)\rangle$ and compute the Berry connection and the Zak phase after the transformation. 1 pt(s)

Does the gauge affect the distinction between topological and trivial phase?