Some properties of class-D Hamiltonians

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Abstract

1 Preliminaries

The purpose of this note is to prove that the Chern number satisfies $ch_1 \in 2\mathbb{Z}$ when a gapped two-dimensional Hamiltonian $H(\boldsymbol{k})^\dagger = H(\boldsymbol{k})$, with $\boldsymbol{k} = (k_x, k_y)$, satisfies the class-D symmetry at each point,

$$U_C H(\boldsymbol{k})^T U_C^\dagger = -H(\boldsymbol{k}), \quad U_C^T = U_C. \tag{1}$$

Since the symmetry does not change momentum, it is the symmetry C_2C, namely the combination of a C_2 rotation and PHS. In general, the above U_C depends on $\boldsymbol{k}$, but for simplicity we assume that U_C is independent of $\boldsymbol{k}$. Let $H(\boldsymbol{k})$ be a $2n \times 2n$ matrix.

We assume that the Hamiltonian has been flattened, that is, that its eigenvalues have been adiabatically deformed to ± 1.

Since U_C is a complex symmetric matrix, it can be written as $U_C = UU^T$ with U unitary. After changing basis by this U, the symmetry of the Hamiltonian becomes

$$H(\boldsymbol{k})^T = -H(\boldsymbol{k}). \tag{2}$$

Introduce $A(\boldsymbol{k}) = iH(\boldsymbol{k})$. Then $A(\boldsymbol{k})$ is a real antisymmetric matrix:

$$A(\boldsymbol{k})^* = A(\boldsymbol{k}), \quad A(\boldsymbol{k})^T = -A(\boldsymbol{k}). \tag{3}$$

The matrix $A(\boldsymbol{k})$ can be written using an orthogonal matrix $Q(\boldsymbol{k})$ as

$$A(\boldsymbol{k}) = Q(\boldsymbol{k}) i\tau_y Q(\boldsymbol{k})^T, \quad Q(\boldsymbol{k}) \in \mathrm{O}(2n). \tag{4}$$

There is gauge ambiguity in $Q(\boldsymbol{k})$:

$$Q(\boldsymbol{k}) \mapsto Q(\boldsymbol{k})V(\boldsymbol{k}). \tag{5}$$

Here $V(\boldsymbol{k}) \in \mathrm{O}(2n)$ and satisfies

$$[i\tau_y, V(\boldsymbol{k})] = 0. \tag{6}$$

Solving this condition gives

$$V(\boldsymbol{k}) = \begin{pmatrix} a(\boldsymbol{k}) & b(\boldsymbol{k}) \\ -b(\boldsymbol{k}) & a(\boldsymbol{k}) \end{pmatrix}, \quad a(\boldsymbol{k}), b(\boldsymbol{k}) \in \mathrm{Mat}_{n\times n}(\mathbb{R}), \tag{7}$$

$$a(\boldsymbol{k})a(\boldsymbol{k})^T + b(\boldsymbol{k})b(\boldsymbol{k})^T = 1_n, \quad a(\boldsymbol{k})b(\boldsymbol{k})^T - b(\boldsymbol{k})a(\boldsymbol{k})^T = 0. \tag{8}$$

If

$$U(\boldsymbol{k}) = a(\boldsymbol{k}) + ib(\boldsymbol{k}), \tag{9}$$

this is equivalent to $U(\boldsymbol{k})U(\boldsymbol{k})^\dagger = 1_n$. Conversely, given a $\mathrm{U}(n)$ matrix U, if we set $a = \mathrm{Re}\, U = (U+U^*)/2$ and $b = \mathrm{Im}\, U = (U - U^*)/(2i)$, then the above properties are satisfied. Therefore the gauge freedom is the group $\mathrm{U}(n)$. Explicitly, the embedding $\mathrm{U}(n) \to \mathrm{O}(2n)$ is

$$\mathrm{U}(n) \ni U \mapsto \begin{pmatrix} \mathrm{Re}\, U & \mathrm{Im}\, U \\ -\mathrm{Im}\, U & \mathrm{Re}\, U \end{pmatrix} \in \mathrm{SO}(2n). \tag{10}$$

Notice that $V(\boldsymbol{k}) \in \mathrm{SO}(2n)$.

2 Gauge freedom and the Chern number

Set $U_C = 1$. Let

$$A(\boldsymbol{k}) = Q(\boldsymbol{k}) i\tau_y Q(\boldsymbol{k})^T. \tag{11}$$

The Hamiltonian is

$$H(\boldsymbol{k}) = -iA(\boldsymbol{k}) = Q(\boldsymbol{k})\tau_y Q(\boldsymbol{k})^T, \tag{12}$$

and the occupied states are locally given by

$$\mathcal{U}_-(\boldsymbol{k}) = Q(\boldsymbol{k})\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}. \tag{13}$$

Then the $U(1)$ connection is

$$\mathcal{A} = \mathrm{tr}\,[\mathcal{U}_-^\dagger d\mathcal{U}_-] = \frac{1}{2}\mathrm{tr}\,[(1-\tau_y)Q^T dQ] = \frac{1}{2}\mathrm{tr}\,[Q^T dQ] - \frac{1}{2}\mathrm{tr}\,[\tau_y Q^T dQ] \tag{14}$$

$$= \frac{1}{2} d\log\det Q - \frac{1}{2}\mathrm{tr}\,[\tau_y Q^T dQ] = -\frac{1}{2}\mathrm{tr}\,[\tau_y Q^T dQ]. \tag{15}$$

Under the gauge transformation $Q \mapsto QV$,

$$\mathcal{A} \mapsto \mathcal{A} - \frac{1}{2}\mathrm{tr}\,[\tau_y V^T dV]. \tag{16}$$

Substituting

$$V = \begin{pmatrix} \mathrm{Re}\,U & \mathrm{Im}\,U \\ -\mathrm{Im}\,U & \mathrm{Re}\,U \end{pmatrix}, U \in \mathrm{U}(n), \tag{17}$$

we find

$$-\frac{1}{2}\mathrm{tr}\,[\tau_y V^T dV] = -i\mathrm{tr}\,[(\mathrm{Re}\,U)^T d\mathrm{Im}\,U - (\mathrm{Im}\,U)^T d\mathrm{Re}\,U] = -d\log\det U. \tag{18}$$

Thus the Chern number on the sphere S^2 is

$$ch_1 = \frac{1}{2\pi i}\oint d\log\det U, \tag{19}$$

where $U(\phi) \in \mathrm{U}(n)$ is the gauge transformation on the equator.

3 Proof that $ch_1 \in 2\mathbb{Z}$

The fact that $ch_1 \in 2\mathbb{Z}$ is proved as follows.

By the long exact sequence of homotopy groups, for $n \geq 2$,

$$0 \to \pi_2[O(2n)/U(n)] \xrightarrow{2} \pi_1[U(n)] \xrightarrow{\mathrm{mod}\ 2} \pi_1[O(2n)] \to 0. \tag{20}$$

Therefore it is enough to show that the loop determined by

$$\mathrm{U}(n) \ni U \mapsto V = \begin{pmatrix} \mathrm{Re}\,U & \mathrm{Im}\,U \\ -\mathrm{Im}\,U & \mathrm{Re}\,U \end{pmatrix} \in O(2n) \tag{21}$$

belongs to the trivial fundamental-group class. Indeed, if

$$V'(\phi,\theta) := Q_S(\pi-\theta,\phi)^T Q_N(\theta,\phi), \quad \theta \in [0, \frac{\pi}{2}], \tag{22}$$

then $V(\phi)$ is homotopic to the single point $V'(0,\phi) = Q_S(\pi,\phi)^T Q_N(0,\phi)$.[1]

[1] This proof was explained to me by Kubota.

Next consider the torus case. Since $\pi_0[O(2n)] = \mathbb{Z}_2$, it is characterized by $\det Q \in \pm 1$, and the absence of gapless points means that $\det Q$ is constant over the whole T^2. Thus for any loop C on T^2, $Q(\phi) \in O(n)$, $\phi \in C$, is defined. Take a gauge that is continuous over the whole $k_x \in S^1$ in the k_x direction. In the k_y direction one can take a gauge continuous on the interval $k_y \in [0, 2\pi]$. Then the transition function

$$V(k_x) = Q(k_x, 0)^T Q(k_x, 2\pi), \quad k_x \in S^1, \tag{23}$$

is determined. As an element of $\pi_1[O(2n)]$, we then have $[V] = -[Q(k_y = 0)] + [Q(k_y = 2\pi)]$.[2] Since $Q(k_x, k_y)$ gives a homotopy equivalence $Q(k_y = 0) \sim Q(k_y = 2\pi)$, we have $[V] = 0$. Therefore $V(k_x)$ is null-homotopic.

4 Model

Consider a Dirac model. Mutually anticommuting matrices satisfying $\gamma^* = \gamma$ and $\gamma^T = -\gamma$ consist of only one matrix, $i\tau_y$, in dimension 2×2, whereas in dimension 4×4 there are three, $i\sigma_y$, $i\sigma_x\tau_y$, and $i\sigma_z\tau_y$. Therefore the minimal matrix dimension for a Dirac model on S^2 is 4×4.

The model is

$$H(\boldsymbol{n}) = \boldsymbol{n} \cdot (\sigma_x\tau_y, \sigma_y, \sigma_z\tau_y) = e^{-i\phi\sigma_z\tau_y/2} e^{-i\theta\sigma_y/2} \sigma_z\tau_y e^{i\theta\sigma_y/2} e^{i\phi\sigma_z\tau_y/2}. \tag{24}$$

Then

$$A(\boldsymbol{n}) = iH(\boldsymbol{n}) = e^{-i\phi\sigma_z\tau_y/2} e^{-i\theta\sigma_y/2} \sigma_z\tau_y e^{i\theta\sigma_y/2} e^{i\phi\sigma_z\tau_y/2} \tag{25}$$

$$= e^{-i\phi\sigma_z\tau_y/2} e^{-i\theta\sigma_y/2} (\tau_0 \oplus \tau_z)(1 \otimes i\tau_y)(\tau_0 \oplus \tau_z) e^{i\theta\sigma_y/2} e^{i\phi\sigma_z\tau_y/2}. \tag{26}$$

Therefore

$$Q(\boldsymbol{n}) \sim e^{-i\phi\sigma_z\tau_y/2} e^{-i\theta\sigma_y/2} (\tau_0 \oplus \tau_z). \tag{27}$$

This expression is not continuous at $\theta = 0, \pi$. Using a $U(2)$ gauge transformation, continuous $Q_N(\boldsymbol{n})$ and $Q_S(\boldsymbol{n})$ on the northern and southern hemispheres are, respectively,

$$Q_N(\boldsymbol{n}) = e^{-i\phi\sigma_z\tau_y/2} e^{-i\theta\sigma_y/2} (\tau_0 \oplus \tau_z) e^{i\phi\tau_y/2} = \begin{pmatrix} \cos\frac{\theta}{2} & -e^{-i\phi\tau_y}\sin\frac{\theta}{2}\tau_z \\ e^{i\phi\tau_y}\sin\frac{\theta}{2} & \cos\frac{\theta}{2}\tau_z \end{pmatrix}_\sigma, \tag{28}$$

$$Q_S(\boldsymbol{n}) = e^{-i\phi\sigma_z\tau_y/2} e^{-i\theta\sigma_y/2} (\tau_0 \oplus \tau_z) e^{-i\phi\tau_y/2} = \begin{pmatrix} e^{-i\phi\tau_y}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2}\tau_z \\ \sin\frac{\theta}{2} & e^{i\phi\tau_y}\cos\frac{\theta}{2}\tau_z \end{pmatrix}_\sigma. \tag{29}$$

The transition function at the equator is

$$V_{NS}(\phi) = Q_S(\theta = \frac{\pi}{2}, \phi)^T Q_N(\theta = \frac{\pi}{2}, \phi) = e^{i\phi\tau_y} = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}_\sigma. \tag{30}$$

Therefore the $U(2)$ matrix is

$$U(\phi) = e^{i\phi} 1_2, \tag{31}$$

and its winding number is 2.

Let us also compute the connection.

$$Q_N^T \partial_\phi Q_N = i\sigma_0\tau_y \sin^2\frac{\theta}{2} - i\sigma_y\tau_x e^{i\phi\tau_y} \cos\frac{\theta}{2}\sin\frac{\theta}{2}. \tag{32}$$

Taking the trace only over the τ space gives

$$\mathrm{tr}_\tau[\frac{1-\tau_y}{2} Q_N^T \partial_\phi Q_N] = -i\sigma_0 \sin^2\frac{\theta}{2}. \tag{33}$$

[2] Can this be proved only in the range of stable homotopy groups? One has $Q_1 Q_2 \oplus 1_{2n} \sim Q_1 \oplus Q_2$, but...

Thus the $U(1)$ connection is

$$\mathcal{A}_{N,\phi} = -2i \sin^2 \frac{\theta}{2}. \tag{34}$$

Then the Berry phase is

$$\gamma(\theta) = \arg e^{\oint \mathcal{A}_N} = -4\pi \sin^2 \frac{\theta}{2}, \tag{35}$$

so the winding of the Berry phase is even.

Now, can $\gamma(\theta)/2$ be made well-defined?

5 Berry phase

Let $H(\phi) = Q(\phi)\tau_y Q(\phi)^T$ be a Hamiltonian homotopic to a point. Take a homotopy $Q(\phi, t \in [0,1])$. Let the curvature on D^2 be

$$\mathcal{F} = d\mathcal{A}, \quad \mathcal{A} = \mathrm{tr}\,[\frac{1-\tau_y}{2} Q^T dQ]. \tag{36}$$

If the Berry phase is defined by

$$e^{i\gamma} = e^{\frac{1}{2}\int_{D^2} d\mathcal{A}} \in U(1), \tag{37}$$

then it is independent of the choice of homotopy and hence well-defined.

I would like to compute this from discrete Hamiltonian data.

To be continued.

6 On the decomposition $U_C = UU^T$

At each point the Takagi decomposition $U_C = UU^T$ can be performed, but in general there can be an obstruction to decomposing a parameter family $U_C(\boldsymbol{k})$ over the whole parameter space.

Let $U_C \in U(n)$ be a symmetric matrix, $U_C^T = U_C$. The decomposition $U_C = UU^T$ is invariant under the transformation

$$U \mapsto UO, \quad O \in O(n). \tag{38}$$

Write the equivalence class as

$$[U] \in U(n)/O(n). \tag{39}$$

A global section

$$U(n)/O(n) \to U(n), \quad [U] \mapsto U \tag{40}$$

can be chosen only when the $O(n)$ bundle determined by $U_C \mapsto [U]$ is trivial.

There can be cases where a global $U(\boldsymbol{k})$ does not exist. Indeed, since

$$\pi_1[U(n)] = \mathbb{Z} \to \pi_1[U(n)/O(n)] = \mathbb{Z} \tag{41}$$

is the multiplication-by-two map, a $U_C(\boldsymbol{k})$ corresponding to an odd element of $\pi_1[U(n)/O(n)] = \mathbb{Z}$ does not admit a continuous decomposition $U(\boldsymbol{k})$. The simplest example is the 1×1 matrix on S^1

$$U_C(k \in S^1) = e^{ik}. \tag{42}$$

At each point $k \in S^1$, one can decompose it as

$$U_C(k) = e^{ik/2} e^{ik/2}, \tag{43}$$

but no $U(k)$ continuous over the whole S^1 exists.

Let us consider the constraint on the Hamiltonian when $U_C(k) = e^{ik}$. The condition

$$U_C(k)H(k)^*U_C(k)^\dagger = -H(k) \tag{44}$$

is

$$H(k)^* = -H(k), \tag{45}$$

but since we are now considering a 1×1 model, it follows that $H(k) = 0$ at every point $k \in S^1$. The same result holds for $U_C(k) = 1$. This point can be understood in the real-space picture. Since the antiunitary symmetry $U_C(\boldsymbol{k})$ does not change momentum, it is the combination of inversion and a local PHS. For a 1×1 model, there are two possible inversion centers, $x = 0$ and $x = 1/2$, corresponding to $U_C = 1$ and e^{ik}, respectively. Because a PHS-type symmetry exists at the inversion center, the Hamiltonian is pinned to 0.

On the other hand, if one is interested in a gapped Hamiltonian $H(\boldsymbol{k})$, then there is the constraint that $U_C(\boldsymbol{k})$ exchanges occupied and unoccupied states. For this reason, it is expected that the $O(n)$ bundle $U_C(\boldsymbol{k}) \to [U(\boldsymbol{k})]$ is trivial. As an example, consider the case of one spatial dimension, where $U_C(k)$ is defined for localized orbitals in real space. If the inversion center is 0, then

$$U_C(k) = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}. \tag{46}$$

On the other hand, if the inversion center is $x = 1/2$, then

$$U_C(k) = e^{-ik}\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}. \tag{47}$$

At first sight the latter seems not to admit a global $U(k)$, but the winding number of $U_C(k)$ is 2, and hence a global $U(k)$ exists. Indeed, it is enough to take

$$U(k) = \begin{pmatrix} 1 & \\ & e^{-ik} \end{pmatrix} e^{\frac{\pi}{4}i\tau_x} e^{-\frac{\pi}{4}i}. \tag{48}$$

Conjecture:

- If the $O(n)$ bundle determined by $U_C(\boldsymbol{k}) \mapsto [U(\boldsymbol{k})]$ is nontrivial, then a Hamiltonian $H(\boldsymbol{k})$ with the symmetry $U_C(\boldsymbol{k})H(\boldsymbol{k})^*U_C(\boldsymbol{k})^\dagger = -H(\boldsymbol{k})$ cannot be fully gapped.

7 Computation memo: real-space AHSS

Although the argument is rough, real-space AHSS can be used to show $ch_1 \in 2\mathbb{Z}$. For the second differential $d^2_{2,-2} : \mathbb{Z} \to \mathbb{Z}_2$, it is enough to check whether a class-A Dirac Hamiltonian on a 2-cell,

$$H = \begin{pmatrix} & -i\Delta e^{i\theta(x,y)}(\partial_x - i\partial_y) \\ -i\Delta e^{-i\theta(x,y)}(\partial_x + i\partial_y) & \end{pmatrix} + m\sigma_z, \tag{49}$$

is forced to have a zero mode when $(C_2C)^2 = 1$. For example, if $C_2C = \sigma_x$, then the symmetry condition imposed on the phase $e^{i\theta(x,y)}$ is

$$e^{i\theta(-x,-y)} = -e^{i\theta(x,y)}. \tag{50}$$

Thus a π vortex is forced, so $d^2_{2,-2}$ is nontrivial and $ch_1 \in 2\mathbb{Z} - 1$ cannot be realized.