On the Kane–Mele $\mathbb{Z}_2$ Invariant

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Abstract

This is a memo on the definition of the $\mathbb{Z}_2$ invariant by Kane and Mele [1], and on the gauge-invariant expression given in Ref. [2].

1 The Kane–Mele $\mathbb{Z}_2$ Invariant

Write $k = (k_x, k_y)$. Consider a gapped $2N \times 2N$ Hamiltonian $H_k = H_k^\dagger$ on the two-dimensional momentum space T^2, satisfying

$$U_T H_k^* U_T^\dagger = H_{-k}, \quad U_T^\top = -U_T, \tag{1}$$

where U_T is an antisymmetric unitary matrix. Let $\Phi_k = (u_{1,k}, \dots, u_{2n,k})$ be the matrix whose columns are the negative-energy eigenstates of H_k. It has gauge ambiguity

$$\Phi_k \mapsto \Phi_k W_k, \quad W_k \in U(2n). \tag{2}$$

For any $2N \times 2m$ matrix Ψ, the matrix

$$\Psi^\dagger U_T \Psi^* \tag{3}$$

is antisymmetric, so the Pfaffian

$$\mathrm{Pf}\,[\Psi^\dagger U_T \Psi^*] \in \mathbb{C} \tag{4}$$

is defined.

Consider the Pfaffian of the antisymmetric matrix determined by H_k,

$$M_k = \Phi_k^\dagger U_T \Phi_k^*, \quad P_k = \mathrm{Pf}\,[M_k]. \tag{5}$$

The Pfaffian P_k is not gauge invariant; it transforms as

$$P_k \mapsto P_k \det W_k^*. \tag{6}$$

However, $|P_k|$ is gauge invariant. In particular, the points at which $|P_k| = 0$ are gauge independent. Kane and Mele introduced the $\mathbb{Z}_2$ invariant as the parity of the vorticity of P_k:

$$I = \frac{1}{2\pi i} \oint_{\partial\tau} d \log P_k \mod 2. \tag{7}$$

Here τ is one half of momentum space. See Fig. 1(a). Since the winding number of $\det W_k^*$ coming from a gauge transformation can in general be odd, it may look as if I is only well-defined modulo 1 and therefore no $\mathbb{Z}_2$ number is defined. For example, a gauge transformation whose $\det W_k^*$ winds nontrivially around an arbitrary point k_0 contributes to the vorticity I; at the same time, Φ_k becomes discontinuous at $k = k_0$.

To identify zeros and vortices of P_k one-to-one, it is enough to choose Φ_k continuously, meaning that limits from arbitrary directions agree with the value at the point. There is no obstruction along an S^1 direction, since transition functions take values in $U(2n)$, so a continuous gauge exists on τ. In fact, because the Chern number vanishes, one can choose Φ_k continuously on the whole T^2. For I to be well-defined, one also needs $|P_k| > 0$ on the boundary $\partial\tau$.

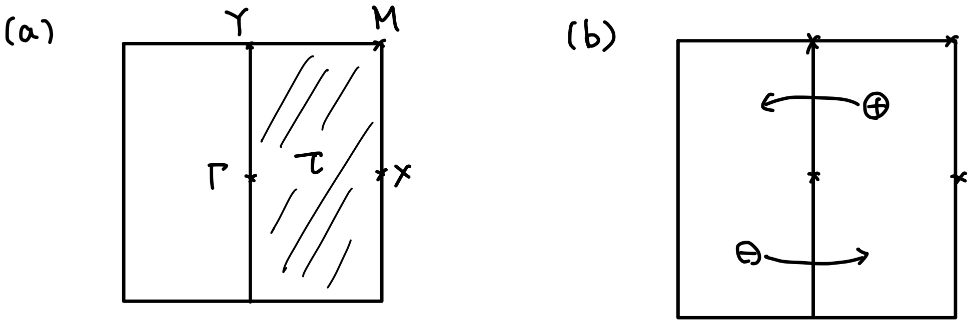

Figure 1:

- If Φ_k is continuous on τ and $|P_k| > 0$ on $\partial\tau$, then I is gauge invariant as an integer.

Indeed,

$$I = \frac{1}{2\pi i}\left[\oint_{-\pi}^{\pi} d_{k_y} \log P_{0,k_y} - \oint_{-\pi}^{\pi} d_{k_y} \log P_{\pi,k_y}\right]. \tag{8}$$

Under a gauge transformation,

$$I \mapsto I + \frac{1}{2\pi i}\left[\oint_{-\pi}^{\pi} d_{k_y} \log W^*_{0,k_y} - \oint_{-\pi}^{\pi} d_{k_y} \log W_{\pi,k_y}\right]. \tag{9}$$

The continuity of Φ_k implies that the phase winding numbers of W_{k_x,k_y} at $k_x = 0$ and $k_x = \pi$ are equal, hence I is gauge invariant.

- During a continuous deformation of H_k preserving the gap, one may have $|P_k| = 0$ on the boundary $\partial\tau$, but the parity of I is preserved.

By symmetry, one can write $\Phi_{-k} = U_T \Phi_k^* V_k$. Then $P_{-k} = P_k^* \det V_k^*$. If P_k has a zero of vorticity i at $k = k_*$, then any nonzero winding of $\det V_k^*$ would contradict the continuity of Φ_k; hence $\det V_k^*$ has zero winding, and P_k has a zero of vorticity $-i$ at $k = -k_*$. At time-reversal-invariant momenta one has $|P_k| = 1$, so vortices do not occur there. Therefore the parity of the total vorticity inside τ is preserved.

2 A Gauge-Invariant Expression

The expression (7) assumes a continuous choice of Φ_k over all of τ, and is therefore inconvenient for computation. Ref. [2] introduced a gauge-fixing-free expression, which we record here. Define the following complex-valued gauge invariant:

$$g(k_y) = \det\left[\prod_{k_x=0}^{\pi-\delta k_x} \Phi^\dagger_{k_x+\delta k_x,k_y} \Phi_{k_x,k_y}\right] \times \frac{\mathrm{Pf}\,[\Phi^\dagger_{0,k_y} U_T \Phi^*_{0,k_y}]}{\mathrm{Pf}\,[\Phi^\dagger_{\pi,k_y} U_T \Phi^*_{\pi,k_y}]} \in \mathbb{C}. \tag{10}$$

This quantity is gauge invariant. As long as $|P_k| > 0$ on $\partial\tau$, one has $g(k_y) \neq 0$, so its phase is well-defined. In a parallel-transport gauge, the Wilson-line contribution disappears, and

$$g(k_y) = P_{0,k_y}/P_{\pi,k_y}. \tag{11}$$

Thus

$$I = \frac{1}{2\pi i}\oint d\log g(k_y). \tag{12}$$

3 Comments

As already noted in Ref. [1], when an additional symmetry is present, P_k may become real. Then the region where $P_k = 0$ can appear as closed curves, and zeros of P_k on the boundary $\partial\tau$ can be unavoidable. Ref. [1] proposed defining

$$I = \frac{1}{2\pi i} \oint_{\partial\tau} d\log[P_k + i\delta] \tag{13}$$

and stated that, in this case, this expression determines the Z_2 index as one half of the number of sign changes along the path, provided the convergence factor δ is included; the sign of I depends on the sign of δ, but I modulo 2 does not. The statement that the $\mathbb{Z}_2$ invariant is given by one half of the number of sign changes of P_k is correct. However, if δ is a constant, the winding number is identically zero. Therefore the claim that this prescription extends the expression for I to the case where P_k is real seems incorrect.

A well-defined expression for the $\mathbb{Z}_2$ invariant in general situations is given in Ref. [3].

References

[1] C. L. Kane and E. J. Mele, "Z2 Topological Order and the Quantum Spin Hall Effect," arXiv:cond-mat/0506581.

[2] Heqiu Li and Kai Sun, "Topological insulators and higher-order topological insulators from gauge-invariant 1D lines," arXiv:2004.05504.

[3] Liang Fu and C. L. Kane, "Time Reversal Polarization and a Z2 Adiabatic Spin Pump," arXiv:cond-mat/0606336.