On the Construction of a Real Berry Connection in Band Theory

Ken Shiozaki

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Consider a PT symmetry

$$U_{\boldsymbol{k}} H_{\boldsymbol{k}}^* U_{\boldsymbol{k}}^\dagger = H_{\boldsymbol{k}}, \quad U_{\boldsymbol{k}} U_{\boldsymbol{k}}^* = 1_N. \tag{1}$$

Assume that the Hamiltonian $H_{\boldsymbol{k}}$ is periodic on the Brillouin zone,

$$H_{\boldsymbol{k}+\boldsymbol{G}} = H_{\boldsymbol{k}}, \tag{2}$$

and that $U_{\boldsymbol{k}}$ is also periodic and globally defined on the Brillouin zone. Let

$$\operatorname{sgn}(H_{\boldsymbol{k}})\Phi_{\boldsymbol{k}} = -\Phi_{\boldsymbol{k}}, \quad \Phi_{\boldsymbol{k}} \in \mathrm{Mat}_{N\times n}(\mathbb{C}), \tag{3}$$

$$\Phi_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}} = 1_n \tag{4}$$

be a frame of the occupied states of $H_{\boldsymbol{k}}$. The frame $\Phi_{\boldsymbol{k}}$ is only locally continuous. Let $\{\mathcal{U}_\alpha\}_\alpha$ be a good cover of the Brillouin zone. On each patch $\mathcal{U}_\alpha$, choose the occupied-state frame so that it satisfies the gauge condition

$$U_{\boldsymbol{k}} (\Phi_{\boldsymbol{k}}^\alpha)^* = \Phi_{\boldsymbol{k}}^\alpha, \quad \boldsymbol{k} \in \mathcal{U}_\alpha. \tag{5}$$

Then the patch transition functions are $O(n)$ matrices:

$$\Phi_{\boldsymbol{k}}^\beta = \Phi_{\boldsymbol{k}}^\alpha T_{\boldsymbol{k}}^{\alpha\beta}, \quad T_{\boldsymbol{k}}^{\alpha\beta} \in O(n), \quad \boldsymbol{k} \in \mathcal{U}_{\alpha\beta} := \mathcal{U}_\alpha \cap \mathcal{U}_\beta. \tag{6}$$

The naive Berry connection

$$A_{\boldsymbol{k}}^\alpha = (\Phi_{\boldsymbol{k}}^\alpha)^\dagger d\Phi_{\boldsymbol{k}}^\alpha \tag{7}$$

is not a real connection because of the $\boldsymbol{k}$ dependence of the PT symmetry matrix $U_{\boldsymbol{k}}$. A correction term appears. Using

$$(\Phi_{\boldsymbol{k}}^\alpha)^* = U_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha, \tag{8}$$

we find

$$(A_{\boldsymbol{k}}^\alpha)^* = (U_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha)^\dagger d(U_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha) \tag{9}$$

$$= A_{\boldsymbol{k}}^\alpha + (\Phi_{\boldsymbol{k}}^\alpha)^\dagger U_{\boldsymbol{k}} dU_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha. \tag{10}$$

The correction term changes sign under complex conjugation:

$$\left[(\Phi_{\boldsymbol{k}}^\alpha)^\dagger U_{\boldsymbol{k}} dU_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha\right]^* = (U_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha)^\dagger U_{\boldsymbol{k}}^* dU_{\boldsymbol{k}}^\top (U_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha) \tag{11}$$

$$= (\Phi_{\boldsymbol{k}}^\alpha)^\dagger dU_{\boldsymbol{k}} U_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha \tag{12}$$

$$= -(\Phi_{\boldsymbol{k}}^\alpha)^\dagger U_{\boldsymbol{k}} dU_{\boldsymbol{k}}^\dagger \Phi_{\boldsymbol{k}}^\alpha. \tag{13}$$

Therefore, redefining the Berry connection by

$$\widetilde{A}^{\alpha}_{\boldsymbol{k}} = A^{\alpha}_{\boldsymbol{k}} + \frac{1}{2}(\Phi^{\alpha}_{\boldsymbol{k}})^{\dagger} U_{\boldsymbol{k}} dU^{\dagger}_{\boldsymbol{k}} \Phi^{\alpha}_{\boldsymbol{k}}, \tag{14}$$

we obtain a real connection.

It remains to check whether this connection satisfies the desired patch transformation rule. The two terms transform as

$$A^{\beta}_{\boldsymbol{k}} = (T^{\alpha\beta}_{\boldsymbol{k}})^{\top}(A^{\alpha}_{\boldsymbol{k}} + d)T^{\alpha\beta}_{\boldsymbol{k}}, \tag{15}$$

$$(\Phi^{\beta}_{\boldsymbol{k}})^{\dagger} U_{\boldsymbol{k}} dU^{\dagger}_{\boldsymbol{k}} \Phi^{\beta}_{\boldsymbol{k}} = (T^{\alpha\beta}_{\boldsymbol{k}})^{\top} \left[(\Phi^{\alpha}_{\boldsymbol{k}})^{\dagger} U_{\boldsymbol{k}} dU^{\dagger}_{\boldsymbol{k}} \Phi^{\alpha}_{\boldsymbol{k}}\right] T^{\alpha\beta}_{\boldsymbol{k}}. \tag{16}$$

Thus

$$\begin{aligned}
\widetilde{A}^{\beta}_{\boldsymbol{k}} &= A^{\beta}_{\boldsymbol{k}} + \frac{1}{2}(\Phi^{\beta}_{\boldsymbol{k}})^{\dagger} U_{\boldsymbol{k}} dU^{\dagger}_{\boldsymbol{k}} \Phi^{\beta}_{\boldsymbol{k}} && (17)\\
&= (T^{\alpha\beta}_{\boldsymbol{k}})^{\top}(A^{\alpha}_{\boldsymbol{k}} + d)T^{\alpha\beta}_{\boldsymbol{k}} + \frac{1}{2}(T^{\alpha\beta}_{\boldsymbol{k}})^{\top}\left[(\Phi^{\alpha}_{\boldsymbol{k}})^{\dagger} U_{\boldsymbol{k}} dU^{\dagger}_{\boldsymbol{k}} \Phi^{\alpha}_{\boldsymbol{k}}\right] T^{\alpha\beta}_{\boldsymbol{k}} && (18)\\
&= (T^{\alpha\beta}_{\boldsymbol{k}})^{\top}\left[A^{\alpha}_{\boldsymbol{k}} + \frac{1}{2}(\Phi^{\alpha}_{\boldsymbol{k}})^{\dagger} U_{\boldsymbol{k}} dU^{\dagger}_{\boldsymbol{k}} \Phi^{\alpha}_{\boldsymbol{k}} + d\right] T^{\alpha\beta}_{\boldsymbol{k}} && (19)\\
&= (T^{\alpha\beta}_{\boldsymbol{k}})^{\top}(\widetilde{A}^{\alpha}_{\boldsymbol{k}} + d)T^{\alpha\beta}_{\boldsymbol{k}}. && (20)
\end{aligned}$$

Hence $\widetilde{A}^{\alpha}_{\boldsymbol{k}}$ has the expected transformation law as an $O(n)$ connection associated with the principal $O(n)$ bundle defined by $T^{\alpha\beta}_{\boldsymbol{k}}$.

As far as I know, a reference in which the redefined connection $\widetilde{A}^{\alpha}_{\boldsymbol{k}}$ appears is [1].

References

[1] Seishiro Ono and Ken Shiozaki, *Towards complete characterization of topological insulators and superconductors: a systematic construction of topological invariants based on Atiyah-Hirzebruch spectral sequence*, arXiv:2311.15814.