Supplemental Material to: Universal higher-order bulk-boundary correspondence of triple nodal points

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I. QUATERNION CHARGE IN DIFFERENT BRILLOUIN ZONES

In this supplement we prove the following conjecture:

Conjecture 1. We assume an N-band system with $\mathcal{PT}$-symmetry squaring to $+\mathbb{1}$, described in the orbital basis by a Hermitian Bloch Hamiltonian $\mathcal{H}(\mathbf{k})$. Let $\gamma : t \in [0,1] \mapsto \gamma(t)$ be a closed contour without any band degeneracies on it that lies in the (first) BZ starting at the *base point* $P = \gamma(0) = \gamma(1)$, and let be $\mathbf{b}$ a reciprocal lattice vector. We define the following three paths:

(*i*) the shifted contour $\gamma'(t) \equiv \gamma(t) + \mathbf{b}$,

(*i*) the path $\gamma_{P,\mathbf{b}}$ along $\mathbf{b}$ connecting the base point P to $P' \equiv \gamma'(0)$ (assuming once more that there are no band degeneracies along it), and

(*iii*) their concatenation (read from left to right)

$$\tilde{\gamma} = \gamma_{P,\mathbf{b}} \circ \gamma' \circ \gamma_{P,\mathbf{b}}^{-1}, \tag{1}$$

which is a closed contour with the same base point P as γ.

Then, the quaternion invariants on γ and $\tilde{\gamma}$ (computed with the same gauge choice for the real eigenstates at P, cf. Sec. I D) are related by

$$\mathfrak{q}(\tilde{\gamma}) = \overline{F_{P,\mathbf{b}}}\,\mathfrak{q}(\gamma)\,\overline{F_{P,\mathbf{b}}}^{-1}, \tag{2}$$

where

$$\overline{F_{P,\mathbf{b}}} \equiv \prod_{i\,:\,e^{i\phi_i}=-1} \epsilon_i \tag{3}$$

with ϕ_i the Berry phase of band i along $\mathbf{b}$ and $\{\epsilon_i\}_{i=1}^N$ the generators ($\epsilon_i\epsilon_j + \epsilon_j\epsilon_i = -2\delta_{ij}$) of the Clifford algebra $C\ell_{0,N}$ as used in the construction of $\mathsf{Spin}(N)$ [cf. Sec. I B 2]. (Let us emphasize that this is *different* from the Clifford algebra $C\ell_{0,N-1}$, the particular subset $\overline{P}_N$ of which corresponds to the generalized quaternion charge [1]; cf. Sec. I B 3.) Note that the ordering of the factors in Eq. (3) does not affect Eq. (2) as long as the same ordering is used in both occurrences of $\overline{F_{P,\mathbf{b}}}$. Nevertheless, for concreteness, we fix the ordering such that factors with smaller subscript i appear to the right inside the product.

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Before proving the above conjecture, let us briefly restate the corollary from Appendix E and referred to in Sec. III B:

Corollary 1. Assume an N-band system with $\mathcal{PT}$-symmetry squaring to $+\mathbb{1}$ described in the orbital basis by a Hermitian Bloch Hamiltonian $\mathcal{H}(\mathbf{k})$. Let $\gamma : t \in [0,1] \mapsto \gamma(t)$ be a closed contour with no band degeneracies located inside the (first) BZ. The path starts at the *base point* $P = \gamma(0) = \gamma(1)$ and we decompose

$$\mathfrak{q}(\gamma) = s \prod_{j\in J} g_j \tag{4}$$

with $s \in \{\pm 1\}$, g_j the generators defined in Refs. [1, 2] and $J \subseteq \{1, 2, \ldots, N-1\}$ a subset of the energy gaps of the N-band Hamiltonian (factors with smaller subscript j appearing to the right). Then, the quaternion charge on the corresponding contour $\tilde{\gamma}$ with the same base point and enclosing the same band inversions but in the BZ shifted by the reciprocal lattice vector $\mathbf{b}$ [cf. Fig. 25] is

$$\mathfrak{q}(\tilde{\gamma}) = (-1)^m \mathfrak{q}(\gamma), \tag{5}$$

where m is the number of elements of the set

$$\left\{ j \in J \,\middle|\, \phi_j \neq \phi_{j+1} \right\} \tag{6}$$

with $\phi_j \in \{0, \pi\}$ the Berry phase of the j^{th} band in the direction $\mathbf{b}$. [Note that in the conditioning in Eq. (6) the label $j+1$ may not be in the set J.]

Proof. Given Conjecture 1, the only thing to show is that Eq. (2) reduces to Eq. (5) given Eq. (4). The generators g_j of the generalized quaternion group can be defined in terms of the generators ϵ_i of $C\ell_{0,N}$ [see Eq. (51)] as

$$g_1 = -\epsilon_1\epsilon_2, \quad g_{j\geq 2} = \epsilon_j\epsilon_{j+1}. \tag{7}$$

The above two expressions can be jointly encoded as $g_j = (-1)^{\delta_{j1}}\epsilon_j\epsilon_{j+1}$. By combining Eqs. (2) and (4), we first find (through a repeated insertion of the identity $\overline{F_{P,\mathbf{b}}}^{-1}\overline{F_{P,\mathbf{b}}} = 1$ into the product over $j \in J$) that

$$\begin{aligned}\mathfrak{q}(\tilde{\gamma}) &= s\left(\prod_{i\,:\,e^{i\phi_i}=-1}\epsilon_i\right)\left(\prod_{j\in J} g_j\right)\left(\prod_{i\,:\,e^{i\phi_i}=-1}\epsilon_i\right)^{-1} \\ &= s\prod_{j\in J}\left[\left(\prod_{i\,:\,e^{i\phi_i}=-1}\epsilon_i\right)(-1)^{\delta_{j1}}\epsilon_j\epsilon_{j+1}\left(\prod_{i\,:\,e^{i\phi_i}=-1}\epsilon_i\right)^{-1}\right].\end{aligned} \tag{8}$$

Observe that for every $j \in J$, the conjugation with $\overline{F_{P,\mathbf{b}}} = \prod_{i:\,\mathrm{e}^{\mathrm{i}\phi_i}=-1} \epsilon_i$ results in an overall minus sign if and only if exactly one of ϵ_j and ϵ_{j+1} is present in $\overline{F_{P,\mathbf{b}}}$; otherwise, the conjugation does not affect the factor $\epsilon_j\epsilon_{j+1}$. Therefore, the number of -1 factors picked up through the conjugation is equal to the number of $j \in J$ where $\mathrm{e}^{\mathrm{i}\phi_j} \neq \mathrm{e}^{\mathrm{i}\phi_{j+1}}$. This is equal to the order m of the set in Eq. (6), implying Eq. (5). □

In preparation for the proof of Conjecture 1, we prove several lemmas. For that we proceed as follows. In Sec. I A we discuss the form and the (non-)periodicity of a $\mathcal{PT}$-symmetric Bloch Hamiltonian in the extended momentum space (i.e., beyond the first Brillouin zone). In Secs. I B and I C we first revisit the construction of the double covers of $\mathsf{SO}(N)$ and of its subgroup P_N, and then show how to lift elements of $\mathsf{SO}(N)$ close to the identity after being conjugated by elements in $\mathsf{P}_{Nh} < \mathsf{O}(N)$. Armed with the derived lemmas, we continue by discussing (*i*) the quaternion charge on the various paths involved in the conjecture in Sec. I D and (*ii*) the Berry phases of the contour winding around the Brillouin zone torus in Sec. I E. Finally, we use the derived lemmas and results to prove the conjecture 1 in Sec. I F.

A. Bloch Hamiltonian

Before analyzing the quaternion charges, we review in the present section several properties of Bloch Hamiltonians in $\mathcal{PT}$-symmetric systems. Note that we adopt the Bloch convention which takes into account the positions of the orbitals within the unit cell when forming the Bloch basis, see Eq. (13). This is the convention in which the Berry curvature respects the symmetries of the lattice [3, 4] and the Zak phase of energy bands is in one-to-one correspondence with their electric polarization [5]. The prize to pay for this physical interpretability is that the resulting Bloch Hamiltonian may be non-periodic in reciprocal-lattice vectors.

Recall [6] that, due to $(\mathcal{PT})^2 = +\mathbb{1}$, for each $\mathbf{k}$, there is a change of basis given by a unitary matrix $V_\mathbf{k}$ such that $\mathcal{PT}$ is represented by complex conjugation $\mathcal{K}$:

$$V_\mathbf{k}\overline{D}_\mathbf{k}(\mathcal{PT})\mathcal{K}V_\mathbf{k}^\dagger = \mathcal{K} \tag{9}$$

(here the unitary matrix $\overline{D}_\mathbf{k}(\mathcal{PT})$ is the *corepresentation* $\mathcal{PT}$). It follows that

$$V_\mathbf{k}\mathcal{H}(\mathbf{k})V_\mathbf{k}^\dagger \equiv \mathcal{H}_\mathrm{R}(\mathbf{k}) \tag{10}$$

is a real symmetric matrix. Note that $V_\mathbf{k}$ is not unique, but any $W_\mathbf{k}V_\mathbf{k}$ for $W_\mathbf{k} \in \mathsf{O}(N)$ defines another such basis.

Given a real symmetric Hamiltonian $\mathcal{H}_\mathrm{R}(\mathbf{k})$, it is natural to write its eigenstates in a real gauge; if we additionaly order the eigenstates as columns from left to right according to increasing energy, we obtain the *eigenframe* $\mathsf{u} \in \mathsf{O}(N)$, and

$$\mathcal{H}_\mathrm{R}(\mathbf{k}) = \mathsf{u}(\mathbf{k})\mathcal{E}(\mathbf{k})\mathsf{u}(\mathbf{k})^\top. \tag{11}$$

However, the orthogonal eigenframe is not unique, but exhibits a gauge degree of freedom, $\mathsf{u} \mapsto \mathsf{u}F$, where $F \in \mathsf{P}_{Nh} \cong \mathbb{Z}_2^N$ is a diagonal matrix of ±1's. In particular, note that $F^2 = FF^\top = \mathbb{1}$.

It is important to note that while the eigenenergies are periodic in momentum space, the Bloch Hamiltonian $\mathcal{H}(\mathbf{k})$ in general is only periodic up to a unitary transformation,

$$\mathcal{H}(\mathbf{k}+\mathbf{b}) = U_\mathbf{b}\mathcal{H}(\mathbf{k})U_\mathbf{b}^\dagger, \tag{12}$$

where $\mathbf{b}$ is a reciprocal lattice vector, and the unitary matrix is defined up to an overall multiplication by a phase factor.

In the context of a tight-binding model with orbital α placed at position $\mathbf{r}_\alpha$ relative to the unit cell with origin at $\mathbf{R}$ and Hamiltonian $\hat{\mathcal{H}}$, we define the Bloch basis

$$|\mathbf{k},\alpha\rangle = \sum_\mathbf{R} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_\alpha)}\,|\mathbf{R},\alpha\rangle\,, \tag{13}$$

where $|\mathbf{R},\alpha\rangle$ forms the tight-binding basis, and the sum is over Bravais lattice vectors $\mathbf{R}$. Then, the Bloch Hamiltonian $\mathcal{H}(\mathbf{k})$ is the matrix with components $\mathcal{H}^{\alpha\beta}(\mathbf{k})$ defined by

$$\langle\mathbf{k},\alpha|\hat{\mathcal{H}}|\mathbf{k}',\beta\rangle = \mathcal{H}^{\alpha\beta}(\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'}. \tag{14}$$

and the unitary transformation in Eq. (12) is given by

$$U_\mathbf{b}^{\alpha\beta} = \mathrm{e}^{-\mathrm{i}\mathbf{b}\cdot\mathbf{r}_\alpha}\delta_{\alpha\beta} \tag{15}$$

in the orbital basis $|\mathbf{R},\alpha\rangle$.

In the basis, where the Hamiltonian is real, we have the following lemma:

Lemma A.1. *In the context of an N-orbital tight-binding model with $\mathcal{PT}$ symmetry, $U_{\mathbf{b},\mathrm{R}} \equiv V_\mathbf{k}U_\mathbf{b}V_\mathbf{k}^\dagger \in \mathsf{O}(N)$ and $U_{\mathbf{b},\mathrm{R}}$ is independent of $\mathbf{k}$.*

Proof. In real space $\mathcal{PT}$ acts like inversion, mapping a position vector $\mathbf{r}$ (relative to the center of the unit cell) to $-\mathbf{r}$. If $\mathcal{PT}$ is a symmetry of the system, then there are two options for each tight-binding orbital α: (1) it is mapped to itself (potentially to a Bravais-translation-related copy of itself in another unit cell) or (2) it is exchanged with another orbital. This implies that, in the orbital basis $|\mathbf{R},\alpha\rangle$, the corepresentation matrix $\overline{D}_\mathbf{k}(\mathcal{PT})$ is block-diagonal with one- and two-dimensional blocks. Below we consider both cases (1) and (2) to explicitly construct $V_\mathbf{k}$ such that

$$V_\mathbf{k}\,\overline{D}_\mathbf{k}(\mathcal{PT})V_\mathbf{k}^\top = \mathbb{1}, \tag{16}$$

i.e., the unitary rotation from the orbital basis to the basis in which $\mathcal{PT}$ is represented by complex conjugation [cf. Eq. (9)].

Let us first consider option (1). For the orbital α to be mapped to itself under $\mathcal{PT}$, its position $\mathbf{r}_\alpha$ must be an inversion-symmetric point, i.e., $-\mathbf{r}_\alpha = \mathbf{r}_\alpha + \mathbf{R}_\alpha$ for some Bravais lattice vector $\mathbf{R}_\alpha$. Then, $\mathbf{r}_\alpha = -\frac{1}{2}\mathbf{R}_\alpha$, and the corresponding block of the corepresentation matrix must take the form

$$\overline{D}_\mathbf{k}(\mathcal{PT}) = \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_\alpha+\mathrm{i}\varphi_\alpha} \tag{17}$$

with some phase $\varphi_\alpha \in \mathbb{R}$. One trivially verifies that $\overline{D}_\mathbf{k}(\mathcal{PT})\overline{D}_\mathbf{k}(\mathcal{PT})^* = \mathbb{1}$, as expected for spinless bands. We next observe that the corresponding block of $V_{\mathbf{k}}$ satisfying Eq. (16) is

$$V_{\mathbf{k}} = \mathrm{e}^{-\frac{1}{2}(-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_\alpha+\mathrm{i}\varphi_\alpha)}. \quad (18)$$

Therefore $U_{\mathbf{b}}$ defined in Eq. (15) is transformed to

$$U_{\mathbf{b},R} = V_{\mathbf{k}}\mathrm{e}^{-\mathrm{i}\mathbf{b}\cdot\mathbf{r}_\alpha}V_{\mathbf{k}}^\dagger = \mathrm{e}^{\mathrm{i}\frac{1}{2}\mathbf{b}\cdot\mathbf{R}}. \quad (19)$$

Note that $\mathbf{b}$ is a reciprocal lattice vector and $\mathbf{R}$ a Bravais lattice vector, such that $\frac{1}{2}\mathbf{b}\cdot\mathbf{R}$ is 0 or π (modulo 2π) and $U_{\mathbf{b},R} = \pm 1 \in \mathsf{O}(1)$ is independent of $\mathbf{k}$.

Next, we consider option (2). For concreteness let us assume that the orbitals α and β are mapped to each other, then the corresponding block of the (unitary) corepresentation matrix must be off-diagonal,

$$\overline{D}_{\mathbf{k}}(\mathcal{PT}) = \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}\varphi_{\alpha\beta}} \\ \mathrm{e}^{\mathrm{i}\varphi_{\alpha\beta}} & 0 \end{pmatrix}, \quad (20)$$

where the phases of the off-diagonal matrix elements must be equal in order to satisfy $\overline{D}_{\mathbf{k}}(\mathcal{PT})\overline{D}_{\mathbf{k}}(\mathcal{PT})^* = \mathbb{1}$. Again we construct the corresponding block of $V_{\mathbf{k}}$ satisfying Eq. (16):

$$V_{\mathbf{k}} = \frac{\mathrm{e}^{-\mathrm{i}\frac{1}{2}\varphi_{\alpha\beta}}}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ \mathrm{i} & -\mathrm{i} \end{pmatrix}. \quad (21)$$

The fact that orbitals α and β are mapped to each other under $\mathcal{PT}$ implies that $-\mathbf{r}_\alpha = \mathbf{r}_\beta$ and thus

$$U_{\mathbf{b}} = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\mathbf{b}\cdot\mathbf{r}_\alpha} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\mathbf{b}\cdot\mathbf{r}_\alpha} \end{pmatrix}. \quad (22)$$

In the transformed basis, we therefore end up with

$$U_{\mathbf{b},R} = V_{\mathbf{k}}U_{\mathbf{b}}V_{\mathbf{k}}^\dagger = \begin{pmatrix} \cos(-\mathbf{b}\cdot\mathbf{r}_\alpha) & \sin(-\mathbf{b}\cdot\mathbf{r}_\alpha) \\ -\sin(-\mathbf{b}\cdot\mathbf{r}_\alpha) & \cos(-\mathbf{b}\cdot\mathbf{r}_\alpha) \end{pmatrix} \in \mathsf{O}(2), \quad (23)$$

which is independent of $\mathbf{k}$.

We have shown that the full $V_{\mathbf{k}}$ is block-diagonal and because $U_{\mathbf{b}}$ is diagonal [cf. Eq. (15)] this implies that $U_{\mathbf{b},R}$ is also block diagonal with $\mathbf{k}$-independent blocks either in $\mathsf{O}(1)$ or $\mathsf{O}(2)$. Therefore, $U_{\mathbf{b},R} \in \mathsf{O}(N)$ is $\mathbf{k}$-independent as well. □

B. Double covers of $\mathsf{SO}(N)$ and P_N

1. Lie algebra $\mathfrak{so}(N)$

We consider the special orthogonal group $\mathsf{SO}(N)$, whose Lie algebra is denoted $\mathfrak{so}(N)$. A basis for $\mathfrak{so}(N)$ is given by the $N \times N$ matrices

$$L_{ij} = -E_{ij} + E_{ji}, \quad i < j, \quad (24)$$

where $(E_{ij})_{ab} = \delta_{ai}\delta_{bj}$ is the matrix with a single non-zero element 1 at position (i, j). The matrices E_{ij} satisfy

$$E_{ij}E_{k\ell} = \delta_{jk}E_{i\ell}, \quad (25)$$

such that

$$\left[L_{ij}, L_{k\ell}\right] = -\delta_{i\ell}L_{kj} + \delta_{ik}L_{\ell j} - \delta_{j\ell}L_{ik} + \delta_{jk}L_{i\ell}, \quad (26)$$

which defines the Lie algebra.

2. Construction of $\mathsf{Spin}(N)$

The simply-connected double cover of $\mathsf{SO}(N)$, called $\mathsf{Spin}(N)$, can be constructed [7] via the Clifford algebra $C\ell_{0,N}$ with generators ϵ_i satisfying

$$\epsilon_i\epsilon_j + \epsilon_j\epsilon_i = -2\delta_{ij}. \quad (27)$$

We note that the quadratic elements

$$t_{ij} \equiv -\frac{1}{2}\epsilon_i\epsilon_j, \quad i < j, \quad (28)$$

satisfy the same commutation relation as Eq. (26):

$$\left[t_{ij}, t_{k\ell}\right] = -\delta_{i\ell}t_{kj} + \delta_{ik}t_{\ell j} - \delta_{j\ell}t_{ik} + \delta_{jk}t_{i\ell}, \quad (29)$$

such that we can construct the isomorphism

$$\begin{array}{ccc} \mathfrak{so}(N) & \to & \mathfrak{spin}(N) \\ L_{ij} & \mapsto & \overline{L_{ij}} \equiv t_{ij} = -\frac{1}{2}\epsilon_i\epsilon_j \end{array}. \quad (30)$$

of the two Lie algebras.

Using the exponential map of elements in the Lie algebras, we obtain the corresponding Lie groups:

$$\mathrm{e}^{\sum_{i<j}\alpha_{ij}L_{ij}} \in \mathsf{SO}(N), \qquad \mathrm{e}^{\sum_{i<j}\theta_{ij}t_{ij}} \in \mathsf{Spin}(N). \quad (31)$$

The isomorphism of Lie algebras in Eq. (30) induces a homomorphism of the corresponding Lie groups. In particular, for elements of $\mathsf{SO}(N)$ close to the identity one can construct the *lift map*:

$$\overline{\cdot} : \mathrm{e}^{\sum_{i<j}\alpha_{ij}L_{ij}} \mapsto \mathrm{e}^{\sum_{i<j}\alpha_{ij}t_{ij}}. \quad (32)$$

For $A \in \mathsf{SO}(N)$ close to the identity, we denote the unique lift to $\mathsf{Spin}(N)$ close to the identity, as defined in Eq. (32), by $\overline{A}$.

We proceed to develop an elementary intuition about the lift map $\overline{\cdot} : \mathsf{SO}(N) \to \mathsf{Spin}(N)$ for elements close to the identity.

Because $\mathsf{Spin}(N)$ is the double cover of $\mathsf{SO}(N)$, we have the following short exact sequence of group homomorphisms:

$$1 \longrightarrow \mathbb{Z}_2 = \{\pm 1\} \xrightarrow{\varphi} \mathsf{Spin}(N) \xrightarrow{\sigma} \mathsf{SO}(N) \longrightarrow 1 \quad (33)$$

where $\varphi(\pm 1)$ is in the center of $\mathsf{Spin}(N)$, and σ is a two-to-one projection map. Let as clarify in some detail what the sequence in Eq. (33) entails. Since φ is a group homomorphism, we have

$$1 = \varphi(1) = \varphi((-1)(-1)) = \varphi(-1)\varphi(-1), \quad (34)$$

thus we identify $\varphi(-1) = -1 \in \mathsf{Spin}(N)$, i.e., as the non-trivial element of $\mathsf{Spin}(N)$ that commutes with all other elements of $\mathsf{Spin}(N)$. The exactness of the above sequence implies that

$$1 = (\sigma \circ \varphi)(\pm 1) = \sigma(\pm 1), \quad (35)$$

i.e., the center $\pm 1 \in \mathsf{Spin}(N)$ projects onto the identity element $1 \in \mathsf{SO}(N)$.

Now consider $M_1, M_2 \in \mathsf{Spin}(N)$ with $\sigma(M_1) = \sigma(M_2)$, then

$$\sigma(M_1 M_2^{-1}) = \sigma(M_1)\sigma(M_2)^{-1} = 1, \qquad (36)$$

i.e., $M_1 M_2^{-1}$ is in the kernel of σ, which due to the exactness of the sequence is the image of φ; therefore

$$M_1 M_2^{-1} \in \{\pm 1\} \Rightarrow M_1 = \pm M_2. \qquad (37)$$

We also have that

$$\sigma\left(\overline{A}\right) = A \qquad (38)$$

(i.e., the lift map followed by the projection map is equivalent to the identity operation) for all elements $A \in \mathsf{SO}(N)$ close to identity.

One should bear in mind that we use the same symbol '$^{-}$' for two different (but closely related) maps: (1) the isomorphism of the Lie algebras [Eq. (30)], and the lift map of Lie-group elements close to the identity [Eq. (32)]. These maps are canonically related, because the Lie algebra $\mathfrak{g}$ corresponds to the tangent space of the Lie group G at the identity.

Lemma B.1. *Let $A \in \mathsf{SO}(N)$ be close to the identity, A^{-1} its inverse (which is also close to the identity). Let us denote their (unique) lifts to $\mathsf{Spin}(N)$, according to Eq. (32), as $\overline{A}$ and $\overline{A^{-1}}$. Then:*

$$\overline{A}^{-1} = \overline{A^{-1}}. \qquad (39)$$

Proof. Set $M_1 := \overline{A}^{-1}$, $M_2 := \overline{A^{-1}}$, then

$$\sigma(M_1) = \sigma\left(\overline{A}^{-1}\right) = \sigma\left(\overline{A}\right)^{-1} = A^{-1} = \sigma(M_2), \qquad (40)$$

where we used that σ is a group homomorpshim. It follows, according to Eq. (37), that

$$\overline{A} \cdot \overline{A^{-1}} = \pm 1. \qquad (41)$$

However, because the left hand side is a product of elements close to the identity, the right hand side has to be close to the identity as well, such that it can only be 1 (and not -1). Thus, $\overline{A}^{-1} = \overline{A^{-1}}$, i.e., for elements $A \in \mathsf{SO}(N)$ close to the identity, the lift map commutes with the matrix inverse map. □

3. The group P_N and its double cover

We proceed to discuss the generalized quaternion charges, as introduced in the supplementary material of Ref. 1. Consider elements of the discrete subgroup,

$$\mathsf{P}_N = \left\langle \left\{ e^{\pi L_{ij}} \right\}_{i<j} \right\rangle < \mathsf{SO}(N), \qquad (42)$$

where the angular brackets denote the group generated by taking products of the elements of the set inside the brackets. Note that

$$L_{ij}^n = \begin{cases} \mathbb{1}, & n = 0 \\ (-1)^k L_{ij}, & n = 2k+1, k \in \mathbb{N}_0 \\ (-1)^k (E_{ii} + E_{jj}), & n = 2k, k \in \mathbb{N}_{>0} \end{cases}, \qquad (43)$$

resulting in

$$e^{\alpha L_{ij}} = \mathbb{1} + \sin(\alpha) L_{ij} + (\cos(\alpha) - 1)(E_{ii} + E_{jj}). \qquad (44)$$

For the elements of P_N we thus have

$$e^{\pi L_{ij}} = \mathbb{1} - 2(E_{ii} + E_{jj}), \qquad (45)$$

i.e., diagonal matrices with $+1$ on the diagonal except for the i^{th} and j^{th} element, which are -1. Note that $e^{-\pi L_{ij}} = e^{\pi L_{ij}} = (e^{-\pi L_{ij}})^{-1}$. (Let us also remark that throughout this supplemental material we do *not* use the Einstein summation convention, i.e., there is no implicit summation over repeated indices.)

The double cover of P_N, denoted $\overline{\mathsf{P}}_N < \mathsf{Spin}(N)$, can be constructed starting from the generators of P_N: $e^{\alpha_{ij} L_{ij}}$ and applying the algebra isomorphism in the exponent, then

$$\overline{\mathsf{P}}_N = \left\langle \left\{ e^{\pi t_{ij}} \right\}_{i<j} \right\rangle. \qquad (46)$$

Since for $i \neq j$, $t_{ij}^2 = -\frac{1}{4}$, we find

$$e^{\theta t_{ij}} = \cos\left(\frac{\theta}{2}\right) + 2t_{ij}\sin\left(\frac{\theta}{2}\right) \qquad (47)$$

such that the generators of $\overline{\mathsf{P}}_N$ are $e^{\pi t_{ij}} = 2t_{ij}$, and

$$\sigma\left(2t_{ij}\right) = e^{\pi L_{ij}}. \qquad (48)$$

The above results allow us to relate the generators $\{e_j\}_{j=1}^{N-1}$ of $\overline{\mathsf{P}}_N$ and of the Clifford algebra $\mathcal{C}\ell_{0,N-1}$ introduced in Ref. 1 to the generators $\{\epsilon_i\}_{i=1}^{N}$ of $\mathcal{C}\ell_{0,N}$ adopted in Sec. I B 2, namely"

$$e_j \equiv 2t_{1,j+1} = -\epsilon_1 \epsilon_{j+1}. \qquad (49)$$

The same reference introduces an alternative, physically motivated set of generators

$$g_j \equiv \begin{cases} e_1, & j = 1 \\ e_{j-1} e_j, & 2 \leq j \leq N-1 \end{cases}. \qquad (50)$$

It follows from combining the preceding equations that

$$g_j = \begin{cases} -\epsilon_1 \epsilon_2, & j = 1 \\ \epsilon_j \epsilon_{j+1}, & 2 \leq j \leq N-1 \end{cases}. \qquad (51)$$

4. The group P_{Nh}

The group P_{Nh} of diagonal matrices with ± 1 on the diagonal is not a subgroup of $\mathsf{SO}(N)$, but a subgroup of $\mathsf{O}(N)$. It can be written as

$$\mathsf{P}_{Nh} = \mathsf{P}_N \cup (\mathbb{1} - 2E_{ii})\mathsf{P}_N \qquad (52)$$

for any $1 \leq i \leq N$. In the following, we will consider conjugation of elements of $\mathsf{SO}(N)$ with elements of P_{Nh}. Since the determinant of a product equals the product of the determinants of its factors, conjugation of an element in $\mathsf{SO}(N)$ with an element of P_{Nh} does not leave $\mathsf{SO}(N)$.

Similarly, the double cover $\overline{\mathsf{P}}_{Nh}$ of P_{Nh} can be constructed as

$$\overline{\mathsf{P}}_{Nh} = \overline{\mathsf{P}}_N \cup \epsilon_i \overline{\mathsf{P}}_N \tag{53}$$

for any $1 \le i \le N$. Based on this and the construction of $\overline{\mathsf{P}}_N$, any $\mathfrak{p} \in \overline{\mathsf{P}}_{Nh}$ can, for example, be written as

$$\mathfrak{p} = \epsilon_1^{p_0} \prod_{i<j} (2t_{ij})^{p_{ij}} \tag{54}$$

for $p_0, p_{ij} \in \{0, 1\}$. In this decomposition, p_0 distinguishes whether $\mathfrak{p}$ lies in the proper subgroup P_N ($p_0 = 0$) or not ($p_0 = 1$). Finally, we remark that

$$\sigma(\mathfrak{p}) = (\mathbb{1} - 2E_{ii})^{p_0} \mathrm{e}^{\pi \sum_{i<j} p_{ij} L_{ij}}. \tag{55}$$

for the projection of any element $\mathfrak{p} \in \overline{P}_{Nh}$.

C. Lift of conjugated elements

Lemma C.1. *We consider two basis elements of $\mathfrak{so}(N)$: L_{ij} ($i < j$) and $L_{k\ell}$ ($k < \ell$). Then $\mathrm{e}^{\pi L_{ij}} L_{k\ell} \mathrm{e}^{-\pi L_{ij}} \in \mathfrak{so}(N)$ and*

$$\overline{\mathrm{e}^{\pi L_{ij}} L_{k\ell} \mathrm{e}^{-\pi L_{ij}}} = \mathrm{e}^{\pi t_{ij}} t_{k\ell} \mathrm{e}^{-\pi t_{ij}} = (2t_{ij}) t_{k\ell} (2t_{ij})^{-1}, \tag{56}$$

which is an element of $\mathfrak{spin}(N)$.

Proof. Using Eqs. (24) and (45), and that

$$\forall i \neq j, k \neq \ell : E_{ii} L_{kl} E_{jj} = \left(-\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}\right) E_{ij}, \tag{57a}$$

$$\forall k \neq \ell : E_{ii} L_{kl} E_{ii} = 0 \tag{57b}$$

we find after some algebra that

$$\begin{aligned} &\mathrm{e}^{\pi L_{ij}} L_{k\ell} \mathrm{e}^{-\pi L_{ij}} \\ &= \left[\mathbb{1} - 2(E_{ii} + E_{jj})\right] L_{k\ell} \left[\mathbb{1} - 2(E_{ii} + E_{jj})\right] \\ &= \left(1 - 2\left(\delta_{ik} + \delta_{i\ell} + \delta_{jk} + \delta_{j\ell}\right) + 4\left(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}\right)\right) L_{k\ell} \\ &\overset{i \neq j}{=} (1 - 2\delta_{ik} - 2\delta_{i\ell})\left(1 - 2\delta_{jk} - 2\delta_{j\ell}\right) L_{k\ell}. \end{aligned} \tag{58}$$

We observe that, since $i < j$ and $k < \ell$, the prefactors in front of $L_{\ell k}$ are ± 1, and thus $\mathrm{e}^{\pi L_{ij}} L_{k\ell} \mathrm{e}^{-\pi L_{ij}} = \pm L_{ij}$ is, up to a sign, one of the basis elements of $\mathfrak{so}(N)$. Applying the algebra isomorphism, this gives

$$\overline{\mathrm{e}^{\pi L_{ij}} L_{k\ell} \mathrm{e}^{-\pi L_{ij}}} = (1 - 2\delta_{ik} - 2\delta_{i\ell})\left(1 - 2\delta_{jk} - 2\delta_{j\ell}\right) t_{k\ell}, \tag{59}$$

which is an element of $\mathfrak{spin}(N)$.

On the other hand, an explicit calculation [e.g., via a repeated application of Eqs. (27) and (28)] reveals that for $i < j$ and $k < \ell$

$$(2t_{ij}) t_{k\ell} (-2t_{ij}) = (1 - 2\delta_{ik} - 2\delta_{i\ell})\left(1 - 2\delta_{jk} - 2\delta_{j\ell}\right) t_{k\ell}, \tag{60}$$

where $t_{k\ell} \in \mathfrak{spin}(N)$ and $\mathrm{e}^{\pi L_{ij}} = 2t_{ij} \in \overline{\mathsf{P}_N}$ Noting that $(2t_{ij})^{-1} = -2t_{ij}$, we observe that the right-hand sides of Eqs. (59) and (60) are equal, such the left-hand sides must be equal as well. □

Lemma C.2. *Let $A \in \mathsf{SO}(N)$ be close to the identity and $D \in \mathsf{P}_N$, then $DAD^{-1} \in \mathsf{SO}(N)$ is close to the identity as well, and*

$$\overline{DAD^{-1}} = \overline{D}\,\overline{A}\,\overline{D}^{-1}, \tag{61}$$

with $\overline{D}$ defined as follows: Any $D \in \mathsf{P}_N$ can be written as

$$D = \prod_{i<j} (\mathrm{e}^{\pi L_{ij}})^{d_{ij}} \tag{62}$$

for a (non-unique) set of $\{d_{ij}\}$, $d_{ij} \in \{0, 1\}$, then

$$\overline{D} \equiv \prod_{i<j} (2t_{ij})^{d_{ij}}, \tag{63}$$

where the ordering of the factors in Eq. (63) matches the ordering in Eq. (62).

Let us remark that while $\overline{A}$ is given by Eq. (32), $\overline{D}$ needs to be defined explicitly, since D is not an element close to the identity.

Proof. Obviously, any $D \in \mathsf{P}_N$ can be written as a (non-unique) product of generators:

$$D = \prod_{i<j} (\mathrm{e}^{\pi L_{ij}})^{d_{ij}}, \tag{64}$$

where $d_{ij} \in \{0, 1\}$. First we consider $L_{k\ell} \in \mathfrak{so}(N)$, then

$$D L_{k\ell} D^{-1} = \mathrm{e}^{\pi L_{i'j'}} \cdots \mathrm{e}^{\pi L_{ij}} L_{k\ell} \mathrm{e}^{-\pi L_{ij}} \cdots \mathrm{e}^{-\pi L_{i'j'}}, \tag{65}$$

where only $\mathrm{e}^{\pi L_{ij}}$ with $i < j$ and $d_{ij} = 1$ appear in the product. This is just consecutive conjugation by generators of P_N and, by Lemma C.1, the result of each conjugation is an element of $\mathfrak{so}(N)$ again, such that $D L_{k\ell} D^{-1} \in \mathfrak{so}(N)$ and

$$\overline{D L_{k\ell} D^{-1}} = \overline{D} t_{k\ell} \overline{D}^{-1}, \tag{66}$$

where

$$\overline{D} \equiv \prod_{i<j} (\mathrm{e}^{\pi t_{ij}})^{d_{ij}} = \prod_{i<j} (2t_{ij})^{d_{ij}}. \tag{67}$$

Now, any $A \in \mathsf{SO}(N)$ close to the identity can be expanded in $\mathfrak{so}(N)$:

$$A \approx \mathbb{1} + \sum_{k<\ell} \alpha_{k\ell} L_{k\ell}. \tag{68}$$

Therefore,

$$DAD^{-1} = \mathbb{1} + \sum_{k<\ell} \alpha_{k\ell} D L_{k\ell} D^{-1} \tag{69}$$

is an element of $\mathsf{SO}(N)$ close to the identity and we can lift it to $\mathsf{Spin}(N)$ following Eq. (32), resulting in

$$\overline{DAD^{-1}} = 1 + \sum_{k<\ell} \alpha_{k\ell} \overline{D} t_{k\ell} \overline{D}^{-1} \tag{70}$$

$$= \overline{D}\left(1 + \sum_{k<\ell} \alpha_{k\ell} t_{k\ell}\right)\overline{D}^{-1} = \overline{D}\,\overline{A}\,\overline{D}^{-1}. \tag{71}$$

It remains to be shown that conjugation with $\overline{D}$ is independent of the choice of $\{d_{ij}\}$ (among the ones that give the same D) and their order. But this follows immediately, because the effect of conjugation with one factor in D amounts to just a single prefactor ± 1 [cf. the text following Eq. (58)] which is identical to the prefactor resulting from the conjugation with the corresponding factor in $\overline{D}$ [cf. Eq. (60)]. If two choices of $\{d_{ij}\}$ represent the same D, then in particular the overall prefactor is the same and thus the results of conjugating with the two versions of $\overline{D}$ match. □

Note that $\overline{D} \in \overline{\mathsf{P}}_N < \mathsf{Spin}(N)$ and it covers D, i.e.,

$$\sigma\left(\overline{D}\right) = D, \tag{72}$$

which follows directly from the definition of $\overline{D}$ and Eq. (48).

We now extend the above results to conjugation with an element of P_{Nh}.

Lemma C.3. *Let $L_{k\ell}$ $(k < \ell)$ be a basis element of $\mathfrak{so}(N)$, then $(\mathbb{1} - 2E_{ii})L_{k\ell}(\mathbb{1} - 2E_{ii}) \in \mathfrak{so}(N)$ and*

$$\overline{(\mathbb{1} - 2E_{ii})L_{k\ell}(\mathbb{1} - 2E_{ii})} = \epsilon_i t_{k\ell} \epsilon_i^{-1} \in \mathfrak{spin}(N), \tag{73}$$

where ϵ_i is the corresponding generator of $C\ell_{0,N}$.

Proof. First observe that

$$(\mathbb{1} - 2E_{ii})L_{k\ell}(\mathbb{1} - 2E_{ii}) = [1 - 2(\delta_{ik} + \delta_{i\ell})] L_{k\ell} \in \mathfrak{so}(N). \tag{74}$$

On the other hand, we find that

$$\epsilon_i t_{k\ell}(-\epsilon_i) = [1 - 2(\delta_{ik} + \delta_{i\ell})] t_{k\ell}, \tag{75}$$

which implies that

$$\overline{(\mathbb{1} - 2E_{ii})L_{k\ell}(\mathbb{1} - 2E_{ii})} = \epsilon_i t_{k\ell}(-\epsilon_i) \in \mathfrak{spin}(N). \tag{76}$$

Note that $\epsilon_i^{-1} = -\epsilon_i$, because $\epsilon_i^2 = -1$. □

Lemma C.4. *Let $A \in \mathsf{SO}(N)$ be close to the identity and $P \in \mathsf{P}_{Nh}$, then $PAP^{-1} \in \mathsf{SO}(N)$ is close to the identity as well, and*

$$\overline{PAP^{-1}} = \overline{P}\,\overline{A}\,\overline{P}^{-1}, \tag{77}$$

where $\overline{P}$ is defined as

$$\overline{P} \equiv \epsilon_1^{(1-\det(P))/2} \overline{D} \tag{78}$$

for $D \equiv (\mathbb{1} - 2E_{11})^{(1-\det(P))/2} P \in \mathsf{P}_N$ and $\overline{D}$ is defined according to Eq. (63).

Note that $\overline{P}$ must be explicitly defined because P is not close to the identity, implying that $\overline{P}$ has a sign ambiguity. This ambiguity is irrelevant for Eq. (77), because the $\pm$ sign appears twice and therefore cancels. Nevertheless, for concreteness we opt to work with the particular choice of sign fixed by Eq. (78).

Proof. Obviously, for any $P \in \mathsf{P}_{Nh}$,

$$D \equiv (\mathbb{1} - 2E_{11})^{(1-\det(P))/2} P \in \mathsf{P}_N, \tag{79}$$

because

$$\det(D) = (-1)^{(1-\det(P))/2} \det(P) = \det(P)^2 = +1. \tag{80}$$

If $\det(P) = +1$, then $D = P$ and the statement of the Lemma C.4 reduces to the already proved Lemma C.2. On the other hand, if $\det(P) = -1$, we have $D = (\mathbb{1} - 2E_{11})P$ and

$$PAP^{-1} = (\mathbb{1} - 2E_{11}) DAD^{-1} (\mathbb{1} - 2E_{11}). \tag{81}$$

Lemma C.2 implies that $B \equiv DAD^{-1} \in \mathsf{SO}(N)$ is close to the identity and $\overline{B} = \overline{D}\,\overline{A}\,\overline{D}^{-1}$, such that we only need to prove that for any $B \in \mathsf{SO}(N)$ close to the identity $(\mathbb{1} - 2E_{11})B(\mathbb{1} - 2E_{11}) \in \mathsf{SO}(N)$ is close to the identity and

$$\overline{(\mathbb{1} - 2E_{11})B(\mathbb{1} - 2E_{11})} = \epsilon_1 \overline{B} \epsilon_1^{-1}. \tag{82}$$

But this follows from Lemma C.3 with analogous arguments as those used in the proof of Lemma C.2 □

Note that given some $P \in \mathsf{P}_{Nh}$ as a matrix

$$P = \mathrm{diag}(p_1, p_2, \ldots, p_N) = \prod_{i\,:\,p_i = -1} (\mathbb{1} - 2E_{ii}) \tag{83}$$

with $p_i \in \{\pm 1\}$ we can use Lemma C.3 to conclude that the $\overline{P}$ defined above has the canonical parametrization

$$\overline{P} = \prod_{i\,:\,p_i = -1} \epsilon_i, \tag{84}$$

which is obtained by replacing each factor of $(\mathbb{1} - 2E_{ii})$ with ϵ_i. The choice of sign mentioned above now corresponds to fixing the ordering of the factors in Eq. (84). Here we choose the convention that in Eqs. (83) and (84) factors with smaller indices appear to the right.

Finally, we consider the conjugation of an element of $\overline{\mathsf{P}}_N$ with an element of $\overline{\mathsf{P}}_{Nh}$.

Lemma C.5. *Let $\mathfrak{d} \in \overline{\mathsf{P}}_N$ and $\mathfrak{p} \in \overline{\mathsf{P}}_{Nh}$, then*

$$\mathfrak{p}\mathfrak{d}\mathfrak{p}^{-1} = s(\mathfrak{d}, \mathfrak{p})\mathfrak{d} \tag{85}$$

with $s(\mathfrak{d}, \mathfrak{p}) \in \{-1, +1\}$.

Proof. First we recall from Sec. I B that any $\mathfrak{d} \in \overline{\mathsf{P}}_N$ can be written as

$$\mathfrak{d} = \prod_{k<\ell} (-\epsilon_k \epsilon_\ell)^{d_{k\ell}} \tag{86}$$

for some (non-unique) $d_{k\ell} \in \{0, 1\}$ and any $\mathfrak{p} \in \overline{\mathsf{P}}_{Nh}$ can be written as

$$\mathfrak{p} = \epsilon_1^{p_0} \prod_{i<j} (-\epsilon_i \epsilon_j)^{p_{ij}} \tag{87}$$

for $p_0 \in \{0,1\}$ and some (non-unique) $p_{ij} \in \{0,1\}$, where $\{\epsilon_i\}_{i=1}^N$ are the generators of $\mathcal{C}\ell_{0,N}$.

Equations (28) and (75) imply that for $k < \ell$

$$\epsilon_i \epsilon_k \epsilon_\ell \epsilon_i^{-1} = [1 - 2(\delta_{ik} + \delta_{i\ell})] \epsilon_k \epsilon_\ell, \tag{88}$$

such that

$$\epsilon_i \mathfrak{d} \epsilon_i^{-1} = \underbrace{\left(\prod_{k<\ell} [1 - 2(\delta_{ik} + \delta_{i\ell})]^{d_{k\ell}} \right)}_{=: s(\mathfrak{d}, \epsilon_i) \in \{-1,+1\}} \mathfrak{d}. \tag{89}$$

Therefore,

$$\begin{aligned} \mathfrak{p} \mathfrak{d} \mathfrak{p}^{-1} &= \epsilon_1^{p_0} \left(\prod_{i<j} \epsilon_i^{p_{ij}} \epsilon_j^{p_{ij}} \right) \mathfrak{d} \left({\prod_{i<j}}' \epsilon_j^{-p_{ij}} \epsilon_i^{-p_{ij}} \right) \epsilon_1^{-p_0} \\ &= \underbrace{\left(s(\mathfrak{d}, \epsilon_1)^{p_0} \prod_{i<j} \left(s(\mathfrak{d}, \epsilon_i) s(\mathfrak{d}, \epsilon_j) \right)^{p_{ij}} \right)}_{=: s(\mathfrak{d}, \mathfrak{p})} \mathfrak{d}, \end{aligned} \tag{90}$$

where the dashed product indicates reversed order of the terms. The prefactor $s(\mathfrak{d}, \mathfrak{p})$ is obviously just a sign, because all the factors $s(\mathfrak{d}, \epsilon_i)$ are just signs. The independence of this conclusion and in particular of the prefactor $s(\mathfrak{d}, \mathfrak{p}) \in \{\pm 1\}$ from the parametrization of $\mathfrak{d}$ and of $\mathfrak{p}$ follows trivially, because the left hand side of the above equation is obviously independent of those parameterizations, and the same is true for the remainder $\mathfrak{d}$ on the right-hand side of the equation. □

D. Quaternion invariant

Recall the definition [1, 6] of the quaternion invariant on a closed path γ (here assumed to be completely contained in the first Brillouin zone) based at point P. We will in the following label the same point as $(0,0)$ (the numbers do not correspond to the **k**-space coordinates). It is assumed that there is no band degeneracy of the N-band real-symmetric Hamiltonian $\mathcal{H}_\mathrm{R}(\mathbf{k})$ along γ. We partition the path into infinitesimally spaced points, which we label $(0,1), (0,2), \ldots, (0, n-1)$. The next point in the sequence is $(0,n) \equiv P$, i.e., the initial point again. (The motivation for the additional 0's in the label for each listed point will become clear in later paragraphs.)

At each point $\mathbf{k}$ on γ we can find the eigenframe [Eq. (11)] $\mathsf{u}(\mathbf{k})$. However, as discussed above, it is not unique and has the gauge freedom $\mathsf{u} \mapsto \mathsf{u}F$, where $F \in \mathsf{P}_{Nh}$. Starting with an initial right-handed eigenframe $\mathsf{u}_{0,0} \in \mathsf{SO}(N)$ of $\mathcal{H}_\mathrm{R}(P)$, we define the eigenframes $\mathsf{u}_{0,j}$ of $\mathcal{H}_\mathrm{R}$ at the subsequent points such that the rotation $\mathsf{u}_{0,j}^\top \mathsf{u}_{0,j+1}$ is close to identity $\mathbb{1} \in \mathsf{SO}(N)$. We will refer to this continuous choice of frame either as a *parallel transport* or *monodromy* of $\mathsf{u}_{0,0}$. In the last step of the closed path γ, we define $\underline{\mathsf{u}}_{0,0}$ such that $u_{0,n-1}^\top \underline{u}_{0,0}$ is close to identity; the underline indicates that the final $\underline{\mathsf{u}}_{0,0}$ is in general different from the initial $\mathsf{u}_{0,0}$ due to the possible presence of Berry phases on γ. We denote the gauge transformation that relates the two eigenframes as $F_\gamma \in \mathsf{P}_N$, i.e.

$$\underline{\mathsf{u}}_{0,0} = \mathsf{u}_{0,0} F_\gamma. \tag{91}$$

The quanternion charge is then defined as

$$\mathfrak{q}(\gamma) = \overline{\mathsf{u}_{0,0}^\top \mathsf{u}_{0,1}} \cdot \overline{\mathsf{u}_{0,1}^\top \mathsf{u}_{0,2}} \cdot \ldots \cdot \overline{\mathsf{u}_{0,n-1}^\top \underline{\mathsf{u}}_{0,0}}, \tag{92}$$

where $\overline{\mathsf{u}_{0,j}^\top \mathsf{u}_{0,j+1}}$ is defined according to Eq. (32), since $\mathsf{u}_{0,j}^\top \mathsf{u}_{0,j+1} \in \mathsf{SO}(N)$ is close to the identity by construction. Note that $\mathfrak{q}(\gamma)$ implicitly depends on both the base point P of the closed path γ as well as on the choice of gauge of the initial eigenframe $\mathsf{u}_{0,0}$.

Let us also establish the notation for the other two paths that we defined in Conjecture 1. We partition $\gamma_{P,\mathbf{b}}$ that connects $P \equiv (0,0)$ to $P + \mathbf{b} \equiv P' \equiv (m,0)$ into infinitesimally spaced points labelled sequentially as $(0,0), (1,0), (2,0), \ldots, (m-1,0), (m,0)$. Note that this path is not closed, $P' \neq P$; in particular, the Hamiltonians $\mathcal{H}(P)$ and $\mathcal{H}(P')$ may differ by the unitary transformation in Eq. (12).

Furthermore, we partition the shifted (closed) contour γ' based at P' into the points $(m,j) = (0,j) + \mathbf{b}$ for $1 \le j \le n$. Note that the energy spectra on γ and γ' are identical, i.e., by our previous assumption there is no band degeneracy on γ'.

Analogously to the case of γ, we define the eigenframes $\mathsf{u}_{i,0}$, $1 \le i \le m$, on $\gamma_{P,\mathbf{b}}$ such that the rotation $\mathsf{u}_{i,0}^\top \mathsf{u}_{i+1,0}$ is close to identity $\mathbb{1} \in \mathsf{SO}(N)$ (i.e., through parallel transport), and similarly for $\mathsf{u}_{m,j}$, $1 \le j \le n$.

The final frame on γ', i.e., at P' *after* traversing γ', is related to the initial frame on γ' via a gauge transformation $F_{\gamma'} \in \mathsf{P}_N$ [cf. Eq. (91)]

$$\underline{\mathsf{u}}_{m,0} = \mathsf{u}_{m,0} F_{\gamma'}. \tag{93}$$

Therefore, the eigenframes on $\gamma_{P,\mathbf{b}}^{-1}$ are not $\mathsf{u}_{i,0}$ and we instead define new eigenframes $\underline{\mathsf{u}}_{i,0}$, $1 \le i \le m$, through parallel transport, i.e., such that $\underline{\mathsf{u}}_{i,0}^\top \underline{\mathsf{u}}_{i-1,0}$ is close to identity $\mathbb{1} \in \mathsf{SO}(N)$ (note the reversed order in the subscript i because the path $\gamma_{P,\mathbf{b}}$ is traversed in reverse). The final frame on $\gamma_{P,\mathbf{b}}^{-1}$, defined via parallel transport as well, is instead denoted by $\underline{\underline{\mathsf{u}}}_{0,0}$ to avoid confusion with the already defined $\underline{\mathsf{u}}_{0,0}$ [however, we will later show that $\underline{\underline{\mathsf{u}}}_{0,0} = \underline{\mathsf{u}}_{0,0}$, cf. Eq. (112)]. All the frames on $\gamma_{P,\mathbf{b}}^{-1}$ are related to the corresponding frames on $\gamma_{P,\mathbf{b}}$ by some gauge transformation $F_{(i,0)} \in \mathsf{P}_N$: for $1 \le i \le m$

$$\underline{\mathsf{u}}_{i,0} = \mathsf{u}_{i,0} F_{(i,0)}, \tag{94a}$$

where $F_{(m,0)} = F_{\gamma'}$; for the last point on $\gamma_{P,\mathbf{b}}^{-1}$ we have

$$\underline{\underline{\mathsf{u}}}_{0,0} = \mathsf{u}_{0,0} F_{(0,0)}. \tag{94b}$$

Lemma D.1. *Under the assumptions of Conjecture 1, $F_{(i,0)}$ defined in Eq. (94) and $F_{\gamma'}$ defined in Eq. (93) are equal,*

$$\forall 0 \le i \le m : F_{(i,0)} = F_{\gamma'}. \tag{95}$$

Proof. The statement follows from Eq. (93) due to the monodromy (flatness) of the parallel transport. We construct an explicit proof via recursion starting from $i = m$ [cf. Eq. (93)]. Assuming $F_{(i+1,0)} = F_\gamma$ for some $0 \le i < m$, the frame $\underline{\mathsf{u}}_{i,0}$ is defined via parallel transport such that

$$\underline{\mathsf{u}}_{i+1,0}^\top \underline{\mathsf{u}}_{i,0} = F_{\gamma'}^\top \mathsf{u}_{i+1,0}^\top \mathsf{u}_{i,0} F_{(i,0)} \tag{96}$$

is close to the identity. On the other hand the frames $\mathsf{u}_{i,0}$, $0 \le i \le m$, are defined such that $\mathsf{u}_{i,0}^\top \mathsf{u}_{i+1,0}$ is close to the identity, which is equivalent to the condition that $\mathsf{u}_{i+1,0}^\top \mathsf{u}_{i,0}$ is close to the identity. Thus, $F_{(i,0)}$ and $F_{\gamma'}$ have to be close, but because the gauge transformations $F_{\gamma'}$ and $F_{(i,0)}$ are diagonal with ± 1's on the diagonal, it follows that $F_{(i,0)} = F_{\gamma'}$. □

Lemma D.2. *Under the assumptions of Conjecture 1, F_γ defined in Eq. (91) and $F_{\gamma'}$ defined in Eq. (93) are equal*

$$F_{\gamma'} = F_\gamma. \tag{97}$$

The physical interpretation of this result is that the Berry phases of the individual bands on closed paths γ and γ' match.

Proof. The gauge transformations F_γ and $F_{\gamma'}$ are defined as gauge transformations at P and P', respectively. We can obtain an eigenframe of $\mathcal{H}(P+\mathbf{b})$ from the initial eigenframe $\mathsf{u}_{0,0}$ of $\mathcal{H}(P)$ in two distinct but canonical ways. On the one hand, through parallel transport we have defined an eigenframe $\mathsf{u}_{m,0}$ at P'. On the other hand, the unitary relation through $U_{\mathbf{b},\mathrm{R}}$ defines the eigenframe $U_{\mathbf{b},\mathrm{R}}\mathsf{u}_{0,0}$ at P'. These two eigenframes in general differ by a gauge transformation $F_{P,\mathbf{b}} \in \mathsf{P}_{Nh}$, so we write

$$U_{\mathbf{b},\mathrm{R}}\mathsf{u}_{0,0} = \mathsf{u}_{m,0} F_{P,\mathbf{b}}. \tag{98}$$

Thus, we have

$$F_{P,\mathbf{b}} = \mathsf{u}_{m,0}^\top U_{\mathbf{b},\mathrm{R}} \mathsf{u}_{0,0}. \tag{99}$$

We emphasize that it is possible for $F_{P,\mathbf{b}}$ to have a negative determinant. This happens when an odd number of bands carry non-trivial Berry phase π in the $\mathbf{b}$ direction.

It also follows from the monodromy (flatness) of the parallel transport that

$$U_{\mathbf{b},\mathrm{R}}\mathsf{u}_{0,j} = \mathsf{u}_{m,j} F_{P,\mathbf{b}} \tag{100}$$

for all j, such that we can rewrite $\mathsf{u}_{m,j}$ in terms of $\mathsf{u}_{0,j}$:

$$\mathsf{u}_{m,j} = U_{\mathbf{b},\mathrm{R}}\mathsf{u}_{0,j} {F_{P,\mathbf{b}}}^\top. \tag{101}$$

For the same reason, i.e., monodromy, an analogous equation holds for $\underline{\mathsf{u}}_{m,0}$ and $\underline{\mathsf{u}}_{0,0}$, which are defined via parallel transport from $\mathsf{u}_{m,n-1}$ and $\mathsf{u}_{0,n-1}$, respectively:

$$\underline{\mathsf{u}}_{m,0} = U_{\mathbf{b},\mathrm{R}} \underline{\mathsf{u}}_{0,0} F_{P,\mathbf{b}}^\top \tag{102}$$

Together with Eqs. (91) and (101), this gives

$$\begin{aligned}\underline{\mathsf{u}}_{m,0} &= U_{\mathbf{b},\mathrm{R}}\mathsf{u}_{0,0} F_\gamma F_{P,\mathbf{b}}^\top \\ &= \mathsf{u}_{m,0} F_{P,\mathbf{b}} F_\gamma F_{P,\mathbf{b}}^\top.\end{aligned} \tag{103}$$

By comparing Eq. (103) to Eq. (93), we see that $F_{\gamma'} = F_{P,\mathbf{b}} F_\gamma F_{P,\mathbf{b}}^\top$. However, since F_γ, $F_{\gamma'}$ and $F_{P,\mathbf{b}}$ are all elements of P_{Nh} (i.e., diagonal matrices with ±1 on the diagonal) and therefore commute with each other, we immediately find $F_{\gamma'} = F_\gamma$. □

Besides the quaternion charge $\mathfrak{q}(\gamma')$, which is defined analogously to Eq. (92), we now define the total eigenframe rotations along $\gamma_{P,\mathbf{b}}$ and $\gamma_{P,\mathbf{b}}^{-1}$

$$\mathfrak{b}\left(\gamma_{P,\mathbf{b}}\right) = \overline{\mathsf{u}_{0,0}^\top \mathsf{u}_{1,0}} \cdot \overline{\mathsf{u}_{1,0}^\top \mathsf{u}_{2,0}} \cdot \ldots \cdot \overline{\mathsf{u}_{m-1,0}^\top \mathsf{u}_{m,0}}, \tag{104}$$

$$\mathfrak{b}\left(\gamma_{P,\mathbf{b}}^{-1}\right) = \overline{\underline{\mathsf{u}}_{m,0}^\top \underline{\mathsf{u}}_{m-1,0}} \cdot \ldots \cdot \overline{\underline{\mathsf{u}}_{2,0}^\top \underline{\mathsf{u}}_{1,0}} \cdot \overline{\underline{\mathsf{u}}_{1,0}^\top \underline{\underline{\mathsf{u}}}_{0,0}}. \tag{105}$$

With these definitions, we can proceed to prove several relations between the introduced elements in $\mathsf{Spin}(N)$. One should bear in mind that $\mathfrak{b}\left(\gamma_{P,\mathbf{b}}\right)$ depends not only on the base point P but also implicitly on the initial frame $\mathsf{u}_{0,0}$; the quaternion charge $\mathfrak{q}(\gamma')$ depends implicitly on P, $\mathsf{u}_{0,0}$ and the path $\gamma_{P,\mathbf{b}}$, while $\mathfrak{b}\left(\gamma_{P,\mathbf{b}}^{-1}\right)$ additionally depends on the whole path γ. Therefore, the following statement only make sense in the context of Conjecture 1, i.e., when we consider a path $\tilde{\gamma} = \gamma_{P,\mathbf{b}} \circ \gamma' \circ \gamma_{P,\mathbf{b}}^{-1}$ with base point P, fixed initial frame $\mathsf{u}_{0,0}$.

Lemma D.3. *Under the assumptions of Conjecture 1, we have*

$$\mathfrak{q}(\gamma') = \overline{F_{P,\mathbf{b}}}\, \mathfrak{q}(\gamma) \overline{F_{P,\mathbf{b}}}^{-1}, \tag{106}$$

where

$$F_{P,\mathbf{b}} = \mathsf{u}_{m,0}^\top U_{\mathbf{b},\mathrm{R}} \mathsf{u}_{0,0} \in \mathsf{P}_{Nh} \tag{107}$$

and given the above $F_{P,\mathbf{b}}$, $\overline{F_{P,\mathbf{b}}}$ is defined according to Eq. (78).

Proof. Equation (101) allows us to rewrite the factors in the definition of $\mathfrak{q}(\gamma')$ [Eq. (92)]: for $1 \le j < n-1$

$$\begin{aligned}\overline{\mathsf{u}_{m,j}^\top \mathsf{u}_{m,j+1}} &= \overline{F_{P,\mathbf{b}} \mathsf{u}_{0,j}^\top \left(U_{\mathbf{b},\mathrm{R}}\right)^\top U_{\mathbf{b},\mathrm{R}} \mathsf{u}_{0,j+1} F_{P,\mathbf{b}}^\top} \\ &= \overline{F_{P,\mathbf{b}} \mathsf{u}_{0,j}^\top \mathsf{u}_{0,j+1} F_{P,\mathbf{b}}^{-1}} \\ &= \overline{F_{P,\mathbf{b}}} \cdot \overline{\mathsf{u}_{0,j}^\top \mathsf{u}_{0,j+1}} \cdot \overline{F_{P,\mathbf{b}}}^{-1},\end{aligned} \tag{108}$$

where we used that $U_{\mathbf{b},\mathrm{R}}$ and $F_{P,\mathbf{b}}$ are orthogonal and applied Lemma C.4 with $\overline{F_{P,\mathbf{b}}}$ as defined therein. Thus, in $\mathfrak{q}(\gamma')$ all the $\overline{F_{P,\mathbf{b}}}$ between the factors cancel and we are left with

$$\begin{aligned}\mathfrak{q}(\gamma') &= \overline{\mathsf{u}_{m,0}^\top \mathsf{u}_{m,1}} \cdot \overline{\mathsf{u}_{m,1}^\top \mathsf{u}_{m,2}} \cdot \ldots \cdot \overline{\mathsf{u}_{m,n-1}^\top \underline{\mathsf{u}}_{m,0}} \\ &= \overline{F_{P,\mathbf{b}}}\, \mathfrak{q}(\gamma) \overline{F_{P,\mathbf{b}}}^{-1},\end{aligned} \tag{109}$$

as desired. □

Lemma D.4. *Under the assumptions of Conjecture 1, we have*

$$\mathfrak{b}\left(\gamma_{P,\mathbf{b}}^{-1}\right) = \mathfrak{q}(\gamma)^{-1} \mathfrak{b}\left(\gamma_{P,\mathbf{b}}\right)^{-1} \mathfrak{q}(\gamma). \tag{110}$$

Proof. Applying Lemmas D.1 and D.2 to Eq. (94) gives for all $1 \le i \le m$ that

$$\underline{\mathsf{u}}_{i,0} = \mathsf{u}_{i,0} F_\gamma \tag{111}$$

and

$$\underline{\underline{\mathsf{u}}}_{0,0} = \mathsf{u}_{0,0} F_\gamma = \underline{\mathsf{u}}_{0,0}. \tag{112}$$

Substituting Eqs. (111) and (112) into the expression for $\mathfrak{b}\left(\gamma_{P,\mathbf{b}}^{-1}\right)$ in Eq. (105), and applying Lemma C.2, we find for $0 \le i \le m$

$$\begin{aligned}\overline{\underline{\mathsf{u}}_{i,0}^{\top}\underline{\mathsf{u}}_{i-1,0}} &= \overline{F_\gamma^{-1}\mathsf{u}_{i,0}^{\top}\mathsf{u}_{i-1,0}F_\gamma} \\ &= \overline{F_\gamma}^{-1}\cdot\overline{\mathsf{u}_{i,0}^{\top}\mathsf{u}_{i-1,0}}\cdot\overline{F_\gamma},\end{aligned} \tag{113}$$

such that

$$\mathfrak{b}\left(\gamma_{P,\mathbf{b}}^{-1}\right) = \overline{F_\gamma}^{-1}\cdot\overline{\mathsf{u}_{m,0}^{\top}\mathsf{u}_{m-1,0}}\cdot\ldots\cdot\overline{\mathsf{u}_{1,0}^{\top}\mathsf{u}_{0,0}}\cdot\overline{F_\gamma}. \tag{114}$$

Since $\mathsf{u}_{i-1,0}^{\top}\mathsf{u}_{i,0} \in \mathsf{SO}(N)$ is close to the identity, we can apply Lemma B.1 and find

$$\overline{\mathsf{u}_{i-1,0}^{\top}\mathsf{u}_{i,0}}^{-1} = \left(\overline{\mathsf{u}_{i-1,0}^{\top}\mathsf{u}_{i,0}}\right)^{\top} = \overline{\mathsf{u}_{i,0}^{\top}\mathsf{u}_{i-1,0}}. \tag{115}$$

On the other hand, by inverting Eq. (104) we obtain

$$\begin{aligned}\mathfrak{b}\left(\gamma_{P,\mathbf{b}}\right)^{-1} &= \overline{\mathsf{u}_{m-1,0}^{\top}\mathsf{u}_{m,0}}^{-1}\cdot\ldots\cdot\overline{\mathsf{u}_{1,0}^{\top}\mathsf{u}_{2,0}}^{-1}\cdot\overline{\mathsf{u}_{0,0}^{\top}\mathsf{u}_{1,0}}^{-1} \\ &\overset{\text{Eq. (115)}}{=} \overline{\mathsf{u}_{m,0}^{\top}\mathsf{u}_{m-1,0}}\cdot\ldots\cdot\overline{\mathsf{u}_{2,0}^{\top}\mathsf{u}_{1,0}}\cdot\overline{\mathsf{u}_{1,0}^{\top}\mathsf{u}_{0,0}}\end{aligned} \tag{116}$$

and by comparing to Eq. (114) find that

$$\mathfrak{b}\left(\gamma_{P,\mathbf{b}}^{-1}\right) = \overline{F_\gamma}^{-1}\mathfrak{b}\left(\gamma_{P,\mathbf{b}}\right)^{-1}\overline{F_\gamma}. \tag{117}$$

Additionally, recall that $\overline{F_\gamma}$ satisfies

$$\sigma\left(\overline{F_\gamma}\right) = F_\gamma \tag{118}$$

and by the definition of the quaternion invariant in Eq. (92),

$$\sigma(\mathfrak{q}(\gamma)) = \mathsf{u}_{0,0}^{\top}\mathsf{u}_{0,1}\mathsf{u}_{0,1}^{\top}\mathsf{u}_{0,2}\ldots\mathsf{u}_{0,n-1}^{\top}\underline{\mathsf{u}}_{0,0} = \mathsf{u}_{0,0}^{\top}\underline{\mathsf{u}}_{0,0} = F_\gamma, \tag{119}$$

such that, according to Eq. (37),

$$\mathfrak{q}(\gamma) = \pm\overline{F_\gamma}. \tag{120}$$

Thus,

$$\mathfrak{b}\left(\gamma_{P,\mathbf{b}}^{-1}\right) = \mathfrak{q}(\gamma)^{-1}\mathfrak{b}\gamma_{P,\mathbf{b}}^{-1}\mathfrak{q}(\gamma), \tag{121}$$

because the inverse $\mathfrak{q}(\gamma)^{-1}$ comes with the same sign as $\mathfrak{q}(\gamma)$ and consequently the overall sign ambiguity cancels. □

E. Berry Phases

Lemma E.1. *The gauge transformation relating the eigenframes at P and $P+\mathbf{b}$ with the reciprocal lattice vector $\mathbf{b}$,*

$$F_{P,\mathbf{b}} = \mathsf{u}_{m,0}^{\top}U_{\mathbf{b},\mathrm{R}}\mathsf{u}_{0,0} \in \mathsf{P}_{Nh}, \tag{122}$$

is given by the Berry phases ϕ_i of the bands $1 \le i \le N$ in the direction $\mathbf{b}$:

$$F_{P,\mathbf{b}} = \operatorname{diag}\left(e^{i\phi_1}, e^{i\phi_2}, \ldots, e^{i\phi_N}\right). \tag{123}$$

Proof. Recall the construction of the eigenframes following the path $\gamma_{P,\mathbf{b}}$. At each of the infinitesimally spaced points $(0,0),(1,0),\ldots,(m,0)$, we find a right-handed eigenframe $\hat{\mathsf{u}}_{i+1,0} \in \mathsf{SO}(N)$. At P we fix an arbitrary gauge

$$\mathsf{u}_{0,0} := \hat{\mathsf{u}}_{0,0} \in \mathsf{SO}(N) \tag{124}$$

and then recursively choose the right gauge as follows: given $\mathsf{u}_{i-1,0}$ the next eigenframe (in the right gauge) is

$$\mathsf{u}_{i,0} = \hat{\mathsf{u}}_{i,0}F_i \tag{125}$$

with $F_i \in \mathsf{P}_N$ such that

$$\mathsf{u}_{i-1,0}^{\top}\mathsf{u}_{i,0} = \mathsf{u}_{i-1,0}^{\top}\hat{\mathsf{u}}_{i,0}F_i \tag{126}$$

is close to the identity. The latter is equivalent to

$$\operatorname{sign}\operatorname{diag}\left(\mathsf{u}_{i-1,0}^{\top}\hat{\mathsf{u}}_{i,0}F_i\right) = \mathbb{1}, \tag{127}$$

where, given a matrix M, $\operatorname{sign}\operatorname{diag}(M)$ is the matrix with entries

$$(\operatorname{sign}\operatorname{diag}(M))_{ij} = \operatorname{sign}(M_{ii})\delta_{ij}. \tag{128}$$

Obviously, for any matrix $D \in \mathsf{P}_{Nh}$,

$$[\operatorname{sign}\operatorname{diag}(M)]D = \operatorname{sign}\operatorname{diag}(MD), \tag{129a}$$
$$D[\operatorname{sign}\operatorname{diag}(M)] = \operatorname{sign}\operatorname{diag}(DM), \tag{129b}$$

such that from Eqs. (127) and (129a) we get

$$F_i^{\top} = \operatorname{sign}\operatorname{diag}\left(\mathsf{u}_{i-1,0}^{\top}\hat{\mathsf{u}}_{i,0}\right). \tag{130}$$

Expressing $\mathsf{u}_{i,0}^{\top}$ from Eq. (125) and using Eq. (129b), we further obtain

$$F_i^{\top} = F_{i-1}^{\top}\operatorname{sign}\operatorname{diag}\left(\hat{\mathsf{u}}_{i-1,0}^{\top}\hat{\mathsf{u}}_{i,0}\right), \tag{131}$$

which constitutes a recursion relation for the gauge transformations F_i.

With $F_0 = \mathbb{1}$ [cf.Eq. (124)], the above recursion relation has solution

$$F_j = \prod_{i=1}^{j}\operatorname{sign}\operatorname{diag}\left(\hat{\mathsf{u}}_{i,0}^{\top}\hat{\mathsf{u}}_{i-1,0}\right), \tag{132}$$

where factors with smaller i appear to the *right* (note also the reversed ordering of the $\hat{\mathsf{u}}_{i,0}$ in each factor due to the transposition). Then, according to Eq. (125)),

$$\mathsf{u}_{m,0} = \hat{\mathsf{u}}_{m,0}\left(\prod_{i=1}^{m}\operatorname{sign}\operatorname{diag}\left(\hat{\mathsf{u}}_{i,0}^{\top}\hat{\mathsf{u}}_{i-1,0}\right)\right), \tag{133}$$

such that

$$F_{P,\mathbf{b}} = \left(\prod_{i=1}^{m}\operatorname{sign}\operatorname{diag}\left(\hat{\mathsf{u}}_{i-1,0}^{\top}\hat{\mathsf{u}}_{i,0}\right)\right)\hat{\mathsf{u}}_{m,0}^{\top}U_{\mathbf{b},\mathrm{R}}\hat{\mathsf{u}}_{0,0}. \tag{134}$$

where factors with smaller i appear to the *left*. Note that $F_{P,\mathbf{b}} \in \mathsf{P}_{Nh}$, such that we can apply Eq. (129a) with $M = \hat{\mathsf{u}}_{m-1,0}^\top \hat{\mathsf{u}}_{m,0}$ and $D = F_{P,\mathbf{b}}$ and obtain

$$F_{P,\mathbf{b}} = \left(\prod_{i=1}^{m-1} \operatorname{sign}\operatorname{diag}\left(\hat{\mathsf{u}}_{i-1,0}^\top \hat{\mathsf{u}}_{i,0}\right)\right) \times \times \operatorname{sign}\operatorname{diag}\left(\hat{\mathsf{u}}_{m-1,0}^\top \hat{\mathsf{u}}_{m,0} \hat{\mathsf{u}}_{m,0}^\top U_{\mathbf{b},\mathrm{R}} \hat{\mathsf{u}}_{0,0}\right). \quad (135)$$

Orthogonality of $\hat{\mathsf{u}}_{m,0}$ finally gives

$$F_{P,\mathbf{b}} = \left(\prod_{i=1}^{m-1} \operatorname{sign}\operatorname{diag}\left(\hat{\mathsf{u}}_{i-1,0}^\top \hat{\mathsf{u}}_{i,0}\right)\right) \operatorname{sign}\operatorname{diag}\left(\hat{\mathsf{u}}_{m-1,0}^\top U_{\mathbf{b},\mathrm{R}} \hat{\mathsf{u}}_{0,0}\right), \quad (136)$$

where again factors with smaller i appear to the *left*.

Next, we consider the Berry phase ϕ_j of the j^{th} band along $\gamma_{P,\mathbf{b}}$. It can be defined in terms of the Wilson operator $\mathcal{W}_j$ as follows. Let $\mathbf{u}_j^{(i)}$ be the j^{th} column of the eigenframe $\hat{\mathsf{u}}_{i,0}$, i.e., the j^{th} eigenvector of the real Bloch Hamiltonian at the point $(i, 0)$ (in an arbitrary gauge), then

$$\mathcal{W}_j(\gamma_{P,\mathbf{b}}) = \frac{\left(U_{\mathbf{b},\mathrm{R}}\mathbf{u}_j^{(0)}\right)^\top}{\left|\left(U_{\mathbf{b},\mathrm{R}}\mathbf{u}_j^{(0)}\right)^\top \mathbf{u}_j^{(m-1)}\right|} \left(\prod_{i=1}^{m-1} \frac{\mathbf{u}_j^{(i)}\left(\mathbf{u}_j^{(i)}\right)^\top}{\left|\left(\mathbf{u}_j^{(i)}\right)^\top \mathbf{u}_j^{(i-1)}\right|}\right) \mathbf{u}_j^{(0)} \quad (137)$$

where factors with smaller i appear to the right, and we continue to assume the limit of a partitioning into infinitesimal steps. Rearranging the terms, we arrive at (factors with smaller i still appear to the right)

$$\mathcal{W}_j(\gamma_{P,\mathbf{b}}) = \frac{\left(U_{\mathbf{b},\mathrm{R}}\mathbf{u}_j^{(0)}\right)^\top \mathbf{u}_j^{(m-1)}}{\left|\left(U_{\mathbf{b},\mathrm{R}}\mathbf{u}_j^{(0)}\right)^\top \mathbf{u}_j^{(m-1)}\right|} \left(\prod_{i=1}^{m-1} \frac{\left(\mathbf{u}_j^{(i)}\right)^\top \mathbf{u}_j^{(i-1)}}{\left|\left(\mathbf{u}_j^{(i)}\right)^\top \mathbf{u}_j^{(i-1)}\right|}\right). \quad (138)$$

Since $\mathcal{W}$ is a number, it is its own transpose and we find

$$\mathcal{W}_j(\gamma_{P,\mathbf{b}}) = \left(\prod_{i=1}^{m-1} \frac{\left(\mathbf{u}_j^{(i-1)}\right)^\top \mathbf{u}_j^{(i)}}{\left|\left(\mathbf{u}_j^{(i-1)}\right)^\top \mathbf{u}_j^{(i)}\right|}\right) \frac{\left(\mathbf{u}_j^{(m-1)}\right)^\top U_{\mathbf{b},\mathrm{R}}\mathbf{u}_j^{(0)}}{\left|\left(\mathbf{u}_j^{(m-1)}\right)^\top U_{\mathbf{b},\mathrm{R}}\mathbf{u}_j^{(0)}\right|}, \quad (139)$$

where factors with smaller i now appear to the *left* because of the transposition. Each factor is just a phase, and because the eigenvectors are real (by assumption) this implies that it is a just a sign. Assuming that the points along the path are sufficiently close, the denominators are all close to 1 and we can rewrite the Wilson operator as

$$\mathcal{W}_j(\gamma_{P,\mathbf{b}}) = \left(\prod_{i=1}^{m-1} \operatorname{sign}\left(\left(\mathbf{u}_j^{(i-1)}\right)^\top \mathbf{u}_j^{(i)}\right)\right) \times \times \operatorname{sign}\left(\left(\mathbf{u}_j^{(m-1)}\right)^\top U_{\mathbf{b},\mathrm{R}}\mathbf{u}_j^{(0)}\right). \quad (140)$$

We observe that

$$\left(\hat{\mathsf{u}}_{i-1,0}^\top \hat{\mathsf{u}}_{i,0}\right)_{jj} = \left(\mathbf{u}_j^{(i-1)}\right)^\top \mathbf{u}_j^{(i)}, \quad (141)$$

such that

$$(F_{P,\mathbf{b}})_{ij} = \mathcal{W}_i \delta_{ij}. \quad (142)$$

With the definition of the Berry phase, $\mathcal{W}_i = \mathrm{e}^{\mathrm{i}\phi_i}$, the desired Eq. (123) follows. □

F. Proof of Conjecture 1

We can finally prove Conjecture 1.

Proof. By definition, the quaternion charge of $\tilde{\gamma}$ is

$$\mathfrak{q}(\tilde{\gamma}) = \mathfrak{b}(\gamma_{P,\mathbf{b}})\, \mathfrak{q}(\gamma')\mathfrak{b}\left(\gamma_{P,\mathbf{b}}^{-1}\right) \quad (143)$$

and using Lemmas C.5, D.3 and D.4, this gives

$$\begin{aligned}
\mathfrak{q}(\tilde{\gamma}) &= \mathfrak{b}(\gamma_{P,\mathbf{b}}) \underbrace{\overline{F_{P,\mathbf{b}}}\mathfrak{q}(\gamma)\overline{F_{P,\mathbf{b}}}^{-1}}_{=s\left(\mathfrak{q}(\gamma),\overline{F_{P,\mathbf{b}}}\right)\mathfrak{q}(\gamma)} \mathfrak{q}(\gamma)^{-1}\mathfrak{b}(\gamma_{P,\mathbf{b}})^{-1}\mathfrak{q}(\gamma) \\
&= \mathfrak{b}(\gamma_{P,\mathbf{b}})\, s\left(\mathfrak{q}(\gamma), \overline{F_{P,\mathbf{b}}}\right) \underbrace{\mathfrak{q}(\gamma)\mathfrak{q}(\gamma)^{-1}}_{=1} \mathfrak{b}(\gamma_{P,\mathbf{b}})^{-1}\mathfrak{q}(\gamma) \\
&= \underbrace{\mathfrak{b}(\gamma_{P,\mathbf{b}})\, \mathfrak{b}(\gamma_{P,\mathbf{b}})^{-1}}\, \underbrace{s\left(\mathfrak{q}(\gamma), \overline{F_{P,\mathbf{b}}}\right)\mathfrak{q}(\gamma)}_{=\overline{F_{P,\mathbf{b}}}\mathfrak{q}(\gamma)\overline{F_{P,\mathbf{b}}}^{-1}} \\
&= \overline{F_{P,\mathbf{b}}}\mathfrak{q}(\gamma)\overline{F_{P,\mathbf{b}}}^{-1}
\end{aligned} \quad (144)$$

with $\overline{F_{P,\mathbf{b}}}$ defined according to Eq. (78), given

$$F_{P,\mathbf{b}} = \mathsf{u}_{m,0}^\top U_{\mathbf{b},\mathrm{R}} \mathsf{u}_{0,0} \in \mathsf{P}_{Nh}. \quad (145)$$

But according to Lemma E.1

$$F_{P,\mathbf{b}} = \operatorname{diag}\left(\mathrm{e}^{\mathrm{i}\phi_1}, \mathrm{e}^{\mathrm{i}\phi_2}, \ldots, \mathrm{e}^{\mathrm{i}\phi_N}\right). \quad (146)$$

where $\phi_i \in \{0, \pi\}$ is the Berry phase of the i^{th} band in the direction $\mathbf{b}$ and, according to Eq. (84),

$$\overline{F_{P,\mathbf{b}}} = \overline{\prod_{i\,:\,\mathrm{e}^{\mathrm{i}\phi_i}=-1} (\mathbb{1} - 2E_{ii})} = \prod_{i\,:\,\mathrm{e}^{\mathrm{i}\phi_i}=-1} \epsilon_i, \quad (147)$$

as desired. The ordering of the product in Eq. (147) is fixed by the convention in Lemma E.1 such that ϵ_i with smaller i appear to the right. Without fixing the ordering in the product, there would be a sign ambiguity in $\overline{F_{P,\mathbf{b}}}$, because $F_{P,\mathbf{b}}$ is not close to the identity. However, note that in Eq. (144) $\overline{F_{P,\mathbf{b}}}$ appears twice, such that result holds for both choices of the sign. □

[1] Q. Wu, A. A. Soluyanov, and T. Bzdušek, Science **365**, 1273 (2019).
[2] P. M. Lenggenhager, X. Liu, S. S. Tsirkin, T. Neupert, and T. Bzdušek, Phys. Rev. B **103**, L121101 (2021).
[3] M. Fruchart, D. Carpentier, and K. Gawedzki, EPL **106**, 10.1209/0295-5075/106/60002 (2014).
[4] E. Dobardžić, M. Dimitrijević, and M. V. Milovanović, Phys. Rev. B **91**, 125424 (2015).
[5] A. Nelson, T. Neupert, A. Alexandradinata, and T. Bzdušek, preprint (2021), arXiv:2111.09365.
[6] A. Bouhon, Q. Wu, R.-J. Slager, H. Weng, O. V. Yazyev, and T. Bzdušek, Nat. Phys. **16**, 1137 (2020).
[7] P. Woit, Lecture notes: Clifford algebras and Spin groups, `http://www.math.columbia.edu/%7Ewoit/LieGroups-2012/cliffalgsandspingroups.pdf#page=6` (2012), [Online; accessed 15-Feb-2022].