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Symmetry-protected $\mathbb{Z}_2$-quantization and quaternionic Berry connection with Kramers degeneracy

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Abstract. As for a generic parameter-dependent Hamiltonian with time reversal (TR) invariance, a non-Abelian Berry connection with Kramers (KR) degeneracy is introduced by using a quaternionic Berry connection. This quaternionic structure naturally extends to the many-body system with KR degeneracy. Its topological structure is explicitly discussed in comparison with the one without KR degeneracy. Natural dimensions to have nontrivial topological structures are discussed by presenting explicit gauge fixing. Minimum models to have accidental degeneracies are given with/without KR degeneracy, which describe the monopoles of Dirac and Yang. We have shown that the Yang monopole is literally a quaternionic Dirac monopole.

The generic Berry phases with/without KR degeneracy are introduced by the complex/quaternionic Berry connections. As for the symmetry-protected $\mathbb{Z}_2$-quantization of these general Berry phases, a sufficient condition of the $\mathbb{Z}_2$-quantization is given as the inversion/reflection equivalence.

Topological charges of the SO(3) and SO(5) nonlinear σ-models are discussed in relation to the Chern numbers of the CP^1 and HP^1 models as well.

Contents

1. Introduction

Topological numbers have been important in physics, especially in quantum phenomena. They give a conceptual foundation of quantizations for various elementary degrees of freedom such as charges, fluxes, vortices and monopoles [1, 2]. One of the milestones of the emerging topological numbers is a quantization of the Hall conductance where a response function is directly related to the topological quantum number as the first Chern number [3]–[7]. Its fundamental physical meaning has become clear by introducing an idea of the geometrical concept, which is known as the Berry connection today [8]. For quantum Hall (QH) states, the bulk is gapped and does not have any characteristic symmetry breaking. It results in the absence of a local order parameter and no low-energy excitations as Goldstone bosons. A class of such featureless systems is the (gapped) quantum liquid and the spin liquid. A possible effective field theory for gapped quantum liquids is topological field theory, where topological quantities play a central role. Then a corresponding new idea to describe the system is topological order [9, 10]. It should be compared with the standard Ginzburg–Landau–Wilson scenario, where a local field theory to describe the fluctuation of a local order parameter is essential. As for a bulk topological ordered state, the degeneracy of the ground state depends on the topology of the physical space [9]. However, there were not so many quantities to describe the topological order. As an extension of the success for the QH state, we have successfully used the Berry connections and related topological quantities for characterization of the topological ordered states [11]–[17]. Also note that although the bulk QH state is featureless, the system with boundaries has characteristic localized states as the edge states [18, 19]. Extending this observation, we propose an idea of the bulk–edge correspondence which says that although the bulk is gapped and only characterized by topological quantities, there exist characteristic boundary states that reflect the topologically nontrivial bulk for the system with boundaries [7, 20]. This 'bulk–edge correspondence' seems to be a universal feature of topological ordered states such as QH states, quantum spins [13, 17, 21], graphene [22], photonic crystals [23], cold atoms [24], characterization of localizations [25] and quantum spin Hall (QSH) systems [26]–[28].

The QSH state is an analogous state to the QH state, but it respects time reversal (TR) symmetry with the help of spins [26, 27]. Then, it is natural that the Berry connection and TR invariance play fundamental roles. There have been substantial amounts of works on the topic [25]–[39]. In this paper, we present a self-contained description of Berry connections and related topological quantities with/without Kramers (KR) degeneracy. Especially we focus on its quaternioninc structure. Quaternions are fundamental in the description of the TR invariant system with KR degeneracy, which was first pointed out by Dyson a long time ago [29, 30, 40, 41]. There is more than an analogy between the system with/without KR degeneracy. One can make a mapping between them by replacing the complex number by the quaternions [41]. We explicitly demonstrate this for topological quantities by introducing canonical minimum models, which are related to monopoles and accidental degeneracies.

As for topological quantities, there can be two classes. One includes topological invariants by their definition. Quantization for them is automatically guaranteed only by stability and a regularity of the Berry connections. Examples are Chern numbers, winding numbers and the Pontrjagin index. Additionally, we introduce a new class of quantized quantities as a generalization of the $\mathbb{Z}_2$ Berry phase [13], which is geometrical. However, as for the quantization, one needs an additional symmetry requirement. We give a sufficient condition for this symmetry-protected $\mathbb{Z}_2$-quantization.

As for the application of a gauge-invariant description of Chern numbers, a relation between Chern numbers and topological charges of the SO(3) and SO(5) nonlinear σ-models is also presented.

2. TR and quaternions

Let us first introduce a quaternion notation for a TR-invariant bi-linear system [40]. Introducing D parameters $x = (x^1, \ldots, x^\mu, \ldots, x^D) \in V_D$, $\dim V_D = D$, let us consider a bi-linear $2N$-fermion Hamiltonian $\mathcal{H}(x) = c_m^\dagger H_{mn}(x) c_n$, $c_n^\dagger = (c_{n\uparrow}^\dagger, c_{n\downarrow}^\dagger)$, where H_{mn} is a 2×2 complex matrix and c_n $(n = 1, \ldots, N)$ is a spinor, a pair of fermion annihilation operators (summation over doubled indexes is assumed and $n = 1, \ldots, N$). Further let us impose an invariance under the TR operation Θ for the Hamiltonian $\mathcal{H}$. Since Θ operates as $c_{n\sigma} \to (-)^{(\sigma-1)/2} c_{n-\sigma}$ $(\uparrow = +1$ and $\downarrow = -1$, $c_{n\uparrow} \to c_{n\downarrow}$ and $c_{n\downarrow} \to -c_{n\uparrow})$ and taking a complex conjugate $\mathcal{K}$, we have $\widetilde{J} H_{mn}^* J = -J H_{mn}^* J = H_{mn}$ $(J = \mathrm{i}\sigma_y)$, where $\sigma_{x,y,z}$ are the Pauli matrices ($\widetilde{\ }$ is a matrix transpose). As for the bi-linear Hamiltonian here, it is expressed as $[H, \Theta_b] = 0$, where $\{H\}_{mn} = H_{mn}$ and $\Theta_b = -\mathcal{K} J$ (J operates subblock of H_{mn}). Now let us expand this 2×2 matrix H_{mn} as $H_{mn} = h_{mn}^0 + h_{mn}^1 I + h_{mn}^2 J + h_{mn}^3 K$, where $I = \mathrm{i}\sigma_z = -I^* = -I^\dagger$, $J = \mathrm{i}\sigma_y = J^* = -J^\dagger$ and $K = \mathrm{i}\sigma_x = -K^* = -K^\dagger$. Then TR invariance implies $h_{mn}^\alpha \in \mathbb{R}$ $(\alpha = 0, \ldots, 3)$, that is, H_{mn} is identified as a quaternion $\mathbb{H} \ni h_{mn}$ by a standard equivalence $I \cong i_{\mathbb{H}}$, $J \cong j_{\mathbb{H}}$, $K \cong k_{\mathbb{H}}$, $i_{\mathbb{H}}, j_{\mathbb{H}}, k_{\mathbb{H}} \in \mathbb{H}$, ${i_{\mathbb{H}}}^2 = {j_{\mathbb{H}}}^2 = {k_{\mathbb{H}}}^2 = i_{\mathbb{H}} j_{\mathbb{H}} k_{\mathbb{H}} = -1$, since $-J H_{mn}^* J = (h_{mn}^0)^*(-JJ) + (h_{mn}^1)^*(-J(-I)J) + (h_{mn}^2)^*(-J(J)J) + (h_{mn}^3)^*(-J(-K)J) \cong (h_{mn}^0)^* + (h_{mn}^1)^* i_{\mathbb{H}} + (h_{mn}^2)^* j_{\mathbb{H}} + (h_{mn}^3)^* k_{\mathbb{H}}$. Hermiticity of the $\mathcal{H}$, $H^\dagger = H$, implies four conditions for the *real* matrices, h^α, $\widetilde{h}^0 = h^0$,

$\widetilde{h}^\alpha = -h^\alpha$ $(\alpha = 1, 2, 3)$, where $(h^\alpha)_{mn} \equiv h^\alpha_{mn}$. It gives a Hermite quaternionic matrix $h^{\mathbb{H}} = h^0 + h^1 i_{\mathbb{H}} + h^1 i_{\mathbb{H}} + h^2 j_{\mathbb{H}} + h^3 k_{\mathbb{H}} \cong H = h^0 + h^1 I + h^2 J + h^3 K$ expressed as $(h^{\mathbb{H}})^\dagger = h^{\mathbb{H}}$.

As for a normalized eigenstate,

$$\psi_\ell = \begin{bmatrix} \psi_{\ell\uparrow} \\ \psi_{\ell\downarrow} \end{bmatrix} \qquad (\psi_\ell^\dagger \psi_\ell = 1),$$

of the $2N$-dimensional Hamiltonian H $(H\psi_\ell = \epsilon_\ell \psi_\ell)$, it is degenerate with

$$\psi_\ell^\Theta = \Theta\psi_\ell = \begin{bmatrix} -\psi^*_{\ell\downarrow} \\ \psi^*_{\ell\uparrow} \end{bmatrix},$$

which is the KR degeneracy. Its orthogonality, $\psi_\ell^\dagger \psi_\ell^\Theta = 0$, is trivial here (generically, there are N KR pairs, $\ell = 1, \ldots, N$). Let us write this KR pair as

$$\begin{aligned} \Psi_\ell = (\psi_\ell, \Theta\psi_\ell) &= \psi_\ell^0 \otimes E_2 + \psi_\ell^1 \otimes I + \psi_\ell^2 \otimes J + \psi_\ell^3 \otimes K \\ &= \begin{bmatrix} \psi_\ell^0 + \mathrm{i}\psi_\ell^1 & \psi_\ell^2 + \mathrm{i}\psi_\ell^3 \\ -\psi_\ell^2 + \mathrm{i}\psi_\ell^3 & \psi_\ell^0 - \mathrm{i}\psi_\ell^1 \end{bmatrix} \cong \psi_\ell^{\mathbb{H}} \in \mathbb{H}^N, \end{aligned}$$

where $\psi_\ell^0 = \mathrm{Re}\,\psi_\ell^\uparrow$, $\psi_\ell^1 = \mathrm{Im}\,\psi_\ell^\uparrow$, $\psi_\ell^2 = -\mathrm{Re}\,\psi_{\ell\downarrow}$, $\psi_\ell^3 = \mathrm{Im}\,\psi_\ell^\downarrow$, $\psi_\ell^\alpha \in \mathbb{R}^N$ and E_2 is a two-dimensional unit matrix. Here $\psi_\ell^{\mathbb{H}}$ is a quaternion vector of dimension N.

A linear canonical transformation of the fermions $\{c_n\} \to \{d_\ell\}$, $c_n = U_{n\ell} d_\ell$, which is consistent with the TR invariance (written in $\{d_\ell\}$), requires that the 2×2 matrix $U_{n\ell}$ does commute with the TR, that is, $\tilde{J} U^*_{n\ell} J = U_{n\ell} \cong u^{\mathbb{H}}_{n\ell} \in \mathbb{H}$. Supplementing the unitarity of this matrix $U^\dagger U = U U^\dagger = E_{2N}$, $(U)_{n\ell} = U_{n\ell}$, $U \in U(2N, \mathbb{C})$, which guarantees the fermion anticommutation relations of the $\{d_{\sigma\ell}\}$'s, this $2N \times 2N$ matrix U satisfies $\widetilde{U} J_{2N} U = J_{2N}$, $J_{2N} = J \otimes E_N$ $(U \in \mathrm{Sp}(2N, \mathbb{C}))$. It implies $U \in \mathrm{Sp}(N) = U(2N, \mathbb{C}) \cap \mathrm{Sp}(2N, \mathbb{C})$ as a $2N$-dimensional matrix. By standard equivalence, we also have an N-dimensional quaternion matrix $u^{\mathbb{H}} \in M_N(\mathbb{H})$, $(u^{\mathbb{H}})_{n\ell} = u^{\mathbb{H}}_{n\ell} \in \mathbb{H}$. It is constructed from all of the orthonormalized eigenstates (KR pairs), $\{\psi_\ell^{\mathbb{H}}\}$, as $u^{\mathbb{H}} = (\psi_1^{\mathbb{H}}, \ldots, \psi_N^{\mathbb{H}})$, $H\psi_\ell = \epsilon_\ell \psi_\ell$ $(\epsilon_\ell \neq \epsilon_{\ell'}, \ell \neq \ell')$.

3. Quaternionic structure of the many-body system with KR degeneracy

The quaternionic structure introduced in section 2 is directly extended to the Fock space of the fermion many-body states as far as the total number of particles is conserved, since the TR operation Θ commutes with the $\mathrm{Sp}(N)$ unitary transformation among the fermion spinors $\{\boldsymbol{c}_n^\dagger\} \to \{\boldsymbol{d}_n^\dagger\}$ and the TR operation Θ, $\boldsymbol{c}_{i\uparrow} \to \boldsymbol{c}_{i\downarrow}$, $\boldsymbol{c}_{i\downarrow} \to -\boldsymbol{c}_{i\uparrow}$ and taking the complex conjugate, has a basis independent meaning. Then, it is also applicable for the $S = \frac{1}{2}$ quantum spins by the standard representation $\boldsymbol{S}_i = \frac{1}{2}\boldsymbol{c}_i^\dagger \boldsymbol{\sigma} \boldsymbol{c}_i$ (extension to the general spins is trivial by introducing Hund coupling).

Now let us consider a TR-invariant many-body Hamiltonian $\mathcal{H}$, $[\mathcal{H}, \Theta] = 0$. When the state $|\Psi\rangle$ is an eigen state of the Hamiltonian, its TR pair $|\Psi^\Theta\rangle = \Theta|\Psi\rangle$ is also an eigenstate. As mentioned before, we assume that the Hamiltonian preserves the total fermion number. Then one may discuss an M-particle sector separately. The TR operation for this M-particle sector then satisfies $\Theta^2|\psi\rangle = (-)^M|\psi\rangle$.

Let us further assume that the number of total fermions ($\frac{1}{2}$ spins) M is odd to have KR degeneracy. Then we have the following fundamental relation:

$$\Theta^2|\psi\rangle = -|\psi\rangle.$$

A generic M-particle state is spanned by the Fock basis as

$$|\psi\rangle = \sum \left[\psi_O(i)|O(i)\rangle + \psi_E(i)|E(i)\rangle\right],$$

where $|O(i)\rangle$ and $|E(i)\rangle$ represent a basis with an odd (even) number of spin-up fermions:

$$|O(i)\rangle = c^\dagger_{m_1\uparrow}\cdots c^\dagger_{m_{M_u}\uparrow}c^\dagger_{m_1\downarrow}\cdots c^\dagger_{m_{M_d}\downarrow}|0\rangle \qquad (M_u: \text{odd},\ M_d: \text{even}),$$
$$|E(i)\rangle = c^\dagger_{m_1\uparrow}\cdots c^\dagger_{m_{M_u}\uparrow}c^\dagger_{m_1\downarrow}\cdots c^\dagger_{m_{M_d}\downarrow}|0\rangle \qquad (M_u: \text{even},\ M_d: \text{odd}).$$

They are orthonormalized as

$$\langle O(i)|O(j)\rangle = \langle E(i)|E(j)\rangle = \delta_{ij}, \quad \langle O(i)|E(j)\rangle = 0,$$

where $i = 1, \ldots, D_{\mathrm{F}}$ is a label of the Fock states. Since the total number of particles is odd, the basis with even up spins $|E(i)\rangle$ is given by that of the odd as

$$|E(i)\rangle = \Theta|O(i)\rangle.$$

Therefore, one has (also it is confirmed directly)

$$\Theta|E(i)\rangle = \Theta^2|O(i)\rangle = -|O(i)\rangle.$$

As for the generic state $|\psi\rangle$, the TR operation is given as

$$\Theta|\psi\rangle = |\psi^\Theta\rangle = \sum(-\psi^*_E(i)|O(i)\rangle + \psi^*_O(i)|E(i)\rangle).$$

Using this setup, one can directly extend the discussion in section 2. As for the eigenstate

$$\psi = \begin{bmatrix}\psi_O\\ \psi_E\end{bmatrix}, \quad \psi_O = \begin{bmatrix}\psi_O(1)\\ \vdots \\ \psi_O(D_F)\end{bmatrix}, \quad \psi_E = \begin{bmatrix}\psi_E(1)\\ \vdots \\ \psi_E(D_F)\end{bmatrix},$$

the KR multiplet of the many-body state is given as

$$\Psi = (\psi, \Theta\psi) \equiv \begin{bmatrix}\psi_O & -\psi^*_E\\ \psi_E & \psi^*_O\end{bmatrix} = \psi^0 E + \psi^1 I + \psi^2 J + \psi^3 K,$$

where $\psi^0 = \mathrm{Re}\,\psi_O$, $\psi^1 = \mathrm{Im}\,\psi_O$, $\psi^2 = -\mathrm{Re}\,\psi_E$, $\psi^3 = \mathrm{Im}\,\psi_E$. The orthogonality of the KR pair is also trivial. Similar to the discussion in section 2, we identity the KR multiplet as a single state of the quaternion as

$$\Psi \cong \psi^{\mathbb{H}} = \psi^0 + \psi^1 i_{\mathbb{H}} + \psi^2 j_{\mathbb{H}} + \psi^3 k_{\mathbb{H}}.$$

Then all of the discussion is trivially transformed into a discussion of the many-body states. For example, the quaternionic Berry connection for the many-body state is defined as $a^{\mathbb{H}} = (\psi^{\mathbb{H}})^\dagger \mathrm{d}\psi^{\mathbb{H}}$. All of the discussion in the paper can be applicable to the many-body system. Applications for electronic systems with electron–electron interaction will be given elsewhere.

4. Minimum dimensions for nontrivial Berry connections

To have a nontrivial topological structure with the Berry connection generically, there are some requirements for the dimension of the parameter space D, which we describe here. Let us first start from a generic consideration of the normalized m-dimensional multiplet $\Psi = (\Psi_1, \ldots, \Psi_m)$, $\Psi^\dagger \Psi = E_m$ and the corresponding m-dimensional non-Abelian Berry connection $A = \Psi^\dagger \mathrm{d}\Psi = \Psi^\dagger \partial_\mu \Psi \mathrm{d}x^\mu$, which transforms under a gauge transformation $\Psi_g = \Psi g$, $g \in U(m)$, as $A_g = g^{-1} A g + g^{-1} \mathrm{d}g$ [8, 42]. The nth Chern number C_n of this connection is defined as

$$C_n = \left(\frac{\mathrm{i}}{2\pi}\right)^n \frac{1}{n!} \int_{M_{2n}} \mathrm{Tr}\, F^n, \quad F = \mathrm{d}A + A^2,$$

where M_{2n} is a $2n$-dimensional manifold without boundaries $\partial M_{2n} = 0$ [43, 44]. Although the field strength F gets modified by the above gauge transformation as $F_g = g^{-1} F g$, the Chern number is invariant. As for the explicit discussion of the Berry connection, Zumino's generic construction of the topological quantities is quite useful. We summarize a part of them which we require in this paper [43, 44]. They read as

$$\mathrm{Tr}\, F = \mathrm{d}\omega_1(A), \quad \mathrm{Tr}\, F^2 = \mathrm{d}\omega_3(A),$$
$$\omega_1(A) = \mathrm{Tr}\, A, \quad \omega_3(A) = \mathrm{Tr}(A\mathrm{d}A + \tfrac{2}{3}A^3) = \mathrm{Tr}(AF - \tfrac{1}{3}A^3).$$

The transformation properties are given as

$$\omega_1(A_g) = \omega_1(A) + \mathrm{Tr}(g^{-1}\mathrm{d}g), \quad \omega_3(A_g) = \omega_3(A) - \tfrac{1}{3}\,\mathrm{Tr}(g^{-1}\mathrm{d}g)^3 + \mathrm{d}\alpha_2,$$

where $\alpha_2 = \mathrm{Tr}(A\mathrm{d}g g^{-1})$. Although Zumino's construction is general for $\mathrm{Tr} F^n = \mathrm{d}\omega_{2n-1}(A)$, we just need $n = 1$ and 2, which one can explicitly confirm by a direct calculation.

The Chern number is gauge invariant and is explicitly given by the gauge-invariant projection $P = \Psi\Psi^\dagger$. It is given for the first Chern number [45], but is also given for the higher ones. By taking a differential of P, we have $\mathrm{d}P = \mathrm{d}\Psi\Psi^\dagger + \Psi\mathrm{d}\Psi^\dagger$. Then the following direct calculation gives a useful formula for gauge-invariant quantities as

$$\Psi F \Psi^\dagger = P\mathrm{d}P^2 P, \quad \mathrm{Tr}\,(P\mathrm{d}P^2)^n = \mathrm{Tr}\, F^n.$$

It obeys the following observation:

$$
\begin{aligned}
(\mathrm{d}P)^2 &= \mathrm{d}\Psi\Psi^\dagger \mathrm{d}\Psi\Psi^\dagger + \Psi\mathrm{d}\Psi^\dagger \mathrm{d}\Psi\Psi^\dagger + \mathrm{d}\Psi\Psi^\dagger\Psi\mathrm{d}\Psi^\dagger + \Psi\mathrm{d}\Psi^\dagger\Psi\mathrm{d}\Psi^\dagger \\
&= -\mathrm{d}\Psi\mathrm{d}\Psi^\dagger\Psi\Psi^\dagger + \Psi\mathrm{d}\Psi^\dagger\mathrm{d}\Psi\Psi^\dagger + \mathrm{d}\Psi\mathrm{d}\Psi^\dagger - \Psi\Psi^\dagger\mathrm{d}\Psi\mathrm{d}\Psi^\dagger \\
&= -\mathrm{d}\Psi\mathrm{d}\Psi^\dagger P + \Psi\mathrm{d}\Psi^\dagger\mathrm{d}\Psi\Psi^\dagger + \mathrm{d}\Psi\mathrm{d}\Psi^\dagger - P\mathrm{d}\Psi\mathrm{d}\Psi^\dagger, \\
P(\mathrm{d}P)^2P &= -P\mathrm{d}\Psi\mathrm{d}\Psi^\dagger P + P\Psi\mathrm{d}\Psi^\dagger\mathrm{d}\Psi\Psi^\dagger P + P\mathrm{d}\Psi\mathrm{d}\Psi^\dagger P - P\mathrm{d}\Psi\mathrm{d}\Psi^\dagger P \\
&= -P\mathrm{d}\Psi\mathrm{d}\Psi^\dagger P + P\Psi\mathrm{d}\Psi^\dagger\mathrm{d}\Psi\Psi^\dagger P \\
&= -\Psi\Psi^\dagger\mathrm{d}\Psi\mathrm{d}\Psi^\dagger\Psi\Psi^\dagger + \Psi\Psi^\dagger\Psi\mathrm{d}\Psi^\dagger\mathrm{d}\Psi\Psi^\dagger\Psi\Psi^\dagger \\
&= \Psi\Psi^\dagger\mathrm{d}\Psi\Psi^\dagger\mathrm{d}\Psi\Psi^\dagger + \Psi\mathrm{d}\Psi^\dagger\mathrm{d}\Psi\Psi^\dagger \\
&= \Psi\big[\mathrm{d}\Psi^\dagger\mathrm{d}\Psi + (\Psi^\dagger\mathrm{d}\Psi)^2\big]\Psi^\dagger = \Psi F\Psi^\dagger,
\end{aligned}
$$

where the normalization $\Psi^\dagger\Psi = E_M$ implies $\Psi^\dagger\mathrm{d}\Psi = -\mathrm{d}\Psi^\dagger\Psi$, $P^2 = P$ and $\mathrm{d}A = \mathrm{d}\Psi^\dagger\mathrm{d}\Psi$. Then the Chern number is written as an explicit gauge-invariant form as

$$
C_n = \left(\frac{\mathrm{i}}{2\pi}\right)^n \frac{1}{n!}\int_{M_{2n}} \mathrm{Tr}\big[P(\mathrm{d}P)^2P\big]^n = \left(\frac{\mathrm{i}}{2\pi}\right)^n \frac{1}{n!}\int_{M_{2n}} \mathrm{Tr}\big[P(\mathrm{d}P)^2\big]^n.
$$

As for the TR-invariant system with KR degeneracy, we identify the multiplet of dimension $2M$ to the quaternionic one with dimension M as $\Psi = (\Psi_1, \ldots, \Psi_M) \cong \psi^{\mathbb{H}}$. Then a gauge transformation $\psi^{\mathbb{H}}_g = \psi^{\mathbb{H}} g$, $g \in \mathrm{Sp}(M)$ preserves the TR-invariant linear space spanned by $\psi^{\mathbb{H}}$. Now the quaternionic Berry connection $a^{\mathbb{H}} = (\psi^{\mathbb{H}})^\dagger \mathrm{d}\psi^{\mathbb{H}}$ and corresponding field strength $f^{\mathbb{H}} = \mathrm{d}a^{\mathbb{H}} + (a^{\mathbb{H}})^2$ are defined as usual. Their transformation properties are also standard as $a^{\mathbb{H}}_g = (\psi^{\mathbb{H}}_g)^\dagger \mathrm{d}\psi^{\mathbb{H}}_g = g^{-1}a^{\mathbb{H}}g + g^{-1}\mathrm{d}g$ and $f^{\mathbb{H}}_g = \mathrm{d}a^{\mathbb{H}}_g + (a^{\mathbb{H}}_g)^2 = g^{-1}f^{\mathbb{H}}g$. The nth Chern number with *even* n, C_n, is defined as (since C_n is intrinsically integer, it suggests vanishing C_n for odd n)

$$
C_n = \left(\frac{-1}{4\pi^2}\right)^{n/2} \frac{1}{n!}\int_{M_n} \mathrm{Tr}_M\, T\,(f^{\mathbb{H}})^n = \left(\frac{-1}{4\pi^2}\right)^{n/2} \frac{1}{n!}\int_{M_n} \mathrm{Tr}_M\, T\,[p^{\mathbb{H}}(\mathrm{d}p^{\mathbb{H}})^2]^n,
$$

where $Tx^{\mathbb{H}} = x + \bar{x} = 2x^0 \in \mathbb{R}$ for a quaternion $x = x^0 + x^1 i_{\mathbb{H}} + x^2 j_{\mathbb{H}} + x^3 k_{\mathbb{H}}$ and the quateronic projection is $p^{\mathbb{H}} = \psi^{\mathbb{H}}(\psi^{\mathbb{H}})^\dagger$. In the following, we omit the symbol $^{\mathbb{H}}$ and simply use the lower character for quaternionic notation if the situation is clear.

Since the multiplet and the Berry connection have a gauge freedom, one needs to fix it for the connection to be well defined. As for the generic multiplet without KR degeneracy, the gauge is specified by an arbitrary but given multiplet Φ as $\Psi_\Phi = P\Phi N_\Phi^{-1/2}$, where P is a gauge-independent projection, and the normalization matrix $N_\Phi = \Phi^\dagger P\Phi$, which is also gauge invariant and semi-positive definite [11]. When one can use this single gauge over the whole parameter space, the Berry connection is trivial. Generically, however, the normalization matrix may have zero eigen values as $\det N_\Phi({}^\exists x_\Phi) = 0$. Then near this zero, x_Φ, this gauge is singular since one can not normalize. One needs to use the other gauge, say $\psi_{\Phi'}$, by taking Φ'. Since $\det N_{\Phi'}(x_\Phi) \neq 0$, generically, one can express the projection by the multiplet explicitly as $P = \Psi_{\psi'}\Psi^\dagger_{\psi'}$ and the normalization matrix is factorized as $N_\Phi = \Phi^\dagger P\Phi = \eta^\dagger_{\Phi'\Phi}\eta_{\Phi'\Phi}$, $\eta_{\Phi'\Phi} \equiv \Psi^\dagger_{\Phi'}\Phi$.

One may write it as $\eta_\Phi = \Psi^\dagger \Phi$ when one does not need to specify the gauge. Now it is clear that the singularity is specified by

$$\det \eta_{\Phi'\Phi} = 0 \rightleftarrows \mathrm{Re}\,(\det \eta_{\Phi'\Phi}) = \mathrm{Im}\,(\det \eta_{\Phi'\Phi}) = 0$$

since this determinant is complex, $\det \eta_\Phi(x) \in \mathbb{C}$. Generically one does not have zeros when the dimension of the parameter space is too low and the Berry connection is trivial. To have a non-trivial topological structure, the dimension of the parameter space has to satisfy $D \geqslant D_{\min} = 2$, since the condition to have the singularities is given by two real equations. A two-dimensional magnetic Brillouin zone to discuss the Hall conductance as the first Chern number is this minimum space where the singularities occur in points [6]. Note that the gauge transformation between the two gauges by taking Φ and Φ', $\Psi_{\Phi'} = \Psi_\Phi g_{\Phi\Phi'}$, is explicitly given by

$$\begin{aligned}\Psi_\Phi &= \Psi_{\Phi'} \Psi_{\Phi'}^\dagger \Phi N_\Phi^{-1/2} = \Psi_{\Phi'} g_{\Phi'\Phi},\\ g_{\Phi'\Phi} &= \Psi_{\Phi'}^\dagger \Phi N_\Phi^{-1/2} = (N_{\Phi'})^{-1/2} \Phi'^\dagger P \Phi (N_\Phi)^{-1/2} \in U(M).\end{aligned}$$

The unitarity is confirmed as

$$\begin{aligned}g_{\Phi'\Phi} g_{\Phi'\Phi}^\dagger &= (N_{\Phi'})^{-1/2} \Phi'^\dagger P \Phi (N_\Phi)^{-1} \Phi^\dagger P \Phi' (N_{\Phi'})^{-1/2}\\ &= (N_{\Phi'})^{-1/2} \eta_{\Phi'}^\dagger \eta_\Phi (N_\Phi)^{-1} \eta_\Phi^\dagger \eta_{\Phi'} (N_{\Phi'})^{-1/2} = (N_{\Phi'})^{-1/2} \eta_{\Phi'}^\dagger \eta_{\Phi'} (N_{\Phi'})^{-1/2} = E_M,\end{aligned}$$

and $g_{\Phi'\Phi}^\dagger g_{\Phi'\Phi} = E_M$ similarly.

As for a system with KR pairs, let us consider the simplest $M = 1$ case. Now starting from the gauge-invariant projection p into the degenerate KR space, the gauge is fixed by an arbitrary quaternion vector $\phi \in \mathbb{H}^N$ as

$$\psi_\phi = p\phi N_\phi^{-1/2}, \quad N_\phi = \phi^\dagger p \phi = N(\eta_\phi) \in \mathbb{R}, \quad \eta_\phi = \psi^\dagger \phi \in \mathbb{H},$$

where $N(x) = \bar{x}x = (x^0)^2 + (x^1)^2 + (x^2)^2 + (x^3)^2$ is a norm of a quaternion $x \in \mathbb{H}$. This gauge is again well defined only if $N_\phi \neq 0$. Note that although η_ϕ itself is gauge dependent, the norm $N(\eta_\phi)$ is gauge invariant as $N(\psi_g^\dagger \phi) = N(\bar{g}\psi^\dagger \phi) = N(g)N(\psi^\dagger \phi) = N(\psi^\dagger \phi)$ ($\psi_g = \psi g$, $g \in \mathrm{Sp}(1)$). Therefore, we do not need to specify the gauge for $N(\eta_\phi)$.

Near the singular point of this gauge, one needs to use the other gauge by taking ϕ'. Then the condition of the vanishing norm $N_\phi = N(\eta_{\phi'\phi})$ is expressed as

$$\eta_{\phi'\phi} = 0 \rightleftarrows T(\eta_{\phi'\phi}) = T(i_{\mathbb{H}} \eta_{\phi'\phi}) = T(j_{\mathbb{H}} \eta_{\phi'\phi}) = T(k_{\mathbb{H}} \eta_{\phi'\phi}) = 0.$$

It clearly shows that the singularity may occur in the parameter space of the dimension $D \geqslant D_{\min}^{\mathrm{KR}} = 4$. The gauge transformation is also given as

$$\psi_\phi = \psi_{\phi'} g_{\phi'\phi}, \qquad g_{\phi'\phi} = [N(\phi')]^{-1/2} (\phi')^\dagger p \phi [N(\phi)]^{-1/2} \in \mathrm{Sp}(1).$$

When the dimension of the parameter space is less than this minimum dimension, one can generically take a single patch over the whole parameter space. Since the base space to define the Chern numbers is assumed to be without boundaries, this implies that the Chern number is vanishing for $\dim M_{2n} = 2n < D^{\mathrm{KR}}_{\mathrm{min}} = 4$. Then the natural quantities to have nontrivial topological structure by the Chern numbers are C_1 for the generic case and C_2 for the system with KR degeneracy.

Also note that the normalization of the KR pair in quaternion notation $\psi^\dagger\psi = 1$ gives $0 = \psi^\dagger \mathrm{d}\psi + \mathrm{d}\psi^\dagger\psi = \psi^\dagger \mathrm{d}\psi + \widetilde{\mathrm{d}\psi^\dagger\psi} = \psi^\dagger \mathrm{d}\psi + \tilde{\psi}\mathrm{d}\bar{\psi} = T(\psi^\dagger \mathrm{d}\psi) = T(a)$. This implies that the first Chern number vanishes, which is consistent with the generic argument [29, 46]. Now let us focus on the second Chern number with KR degeneracy.

5. Degeneracies and monopoles with/without KR degeneracy

As pointed out by Berry, the generic degeneracy of a complex Hamiltonian has a co-dimension $\mathrm{d}_C = 3$ [8]. That is, the minimum Hamiltonian ($N = 2$) to describe the degeneracy (at $E = \mathrm{Tr}\, H_{\mathbb{C}} = 0$) is a complex Hermite 2×2 matrix $H_{\mathbb{C}}$ that is expanded by the Pauli matrix with three-dimensional real coefficients $\boldsymbol{R}(x) = (R_1(x), R_2(x), R_3(x)) \in \mathbb{R}^3$ as

$$H_{\mathbb{C}}(x) = \begin{bmatrix} R_3 & z \\ \bar{z} & -R_3 \end{bmatrix}, \quad z = R_1 - \mathrm{i}R_2,$$

where $R_3 = R_3(x) \in \mathbb{R}$, $z = z(x) \in \mathbb{C}$. Similarly, the system with KR degeneracy has a co-dimension $\mathrm{d}_H = 5$, as pointed out by Avron *et al* [29, 46]. Then the minimum model ($N = 2$, $E = \mathrm{Tr}\, H_{\mathbb{H}} = 0$) is realized by the following quaternionic Hermite Hamiltonian:

$$H_{\mathbb{H}}(x) = \begin{bmatrix} Q_5 & q \\ \bar{q} & -Q_5 \end{bmatrix}, \quad q = q_0 + q_1 i_{\mathbb{H}} + q_2 j_{\mathbb{H}} + q_3 k_{\mathbb{H}},$$

where $Q_5 = Q_5(x) \in \mathbb{R}$, $q_i(x) \in \mathbb{R}$ $(i = 1, 2, 3)$ and $q = q(x) \in \mathbb{H}$. These $\boldsymbol{Q} = (Q_1, Q_2, Q_3, Q_4, Q_5) \in \mathbb{R}^5$ $(Q_1 = q_1,\ Q_2 = q_2,\ Q_3 = q_3,\ Q_4 = q_0)$ form five-dimensional parameters of the minimum model with KR degeneracy.

The above observation suggests a strong analogy between systems with and without KR degeneracy, which we pursue in this paper. There is also topological correspondence, as discussed below (see figure 1). Actually, it is more than analogy and there exists a mapping by $R_3 \to Q_5$ and $z(\in \mathbb{C}) \to q(\in \mathbb{H})$, as one can see. The origins of the parameter spaces $\boldsymbol{R} = 0$ and $\boldsymbol{Q} = 0$ give degeneracies that bring singularities for each of the Berry connections. They are the Dirac monopole [1] and the Yang monopole [27], [30]–[32], [47]–[49]. The Yang monopole is literally a quaternionic Dirac monopole up to its topological structure.

5.1. Dirac monopole and the first Chern number

Owing to a simple observation, $H_{\mathbb{C}}^2 = R^2 E_2$, $R = |\boldsymbol{R}|$, the energies of $H_{\mathbb{C}}$ are $\pm R = \sqrt{|z|^2 + R_3^2}$. Then degeneracy occurs at the origin in the three-dimensional $\boldsymbol{R}$ space $\mathbb{R}^3$. Away from this degeneracy, the eigenstate of the energy $\pm R$ subspace is well defined by the projection $P_\pm = \frac{1}{2}(1 \pm H_{\mathbb{C}}/R)$. As for the base manifold to define the first Chern number, for simplicity let us take the two-sphere $S^2 = \{\boldsymbol{R} | R = 1\} \subset \mathbb{R}^3$ as for M_{2n}, $n = 1$ (figure 1). Then the possible singularities of the Berry connection can be points on S^2 by the generic consideration before. When

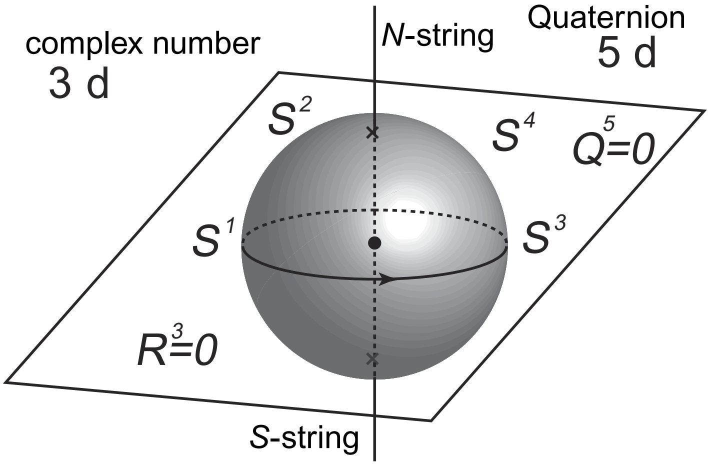

Figure 1. Topological objects and singularities for the Dirac monopole and the Yang monopole.

one considers a generic base space in $\mathbb{R}^3$, these singularities form lines, which correspond to Dirac strings [50]. The gauge-invariant projection into each eigen subspace is explicitly given as

$$P_\pm = \frac{1}{2}\begin{bmatrix} 1 \pm R_3 & \pm z \\ \pm \bar{z} & 1 \mp R_3 \end{bmatrix}.$$

In the following, let us consider a positive energy subspace $P = P_+$. Taking a gauge by

$$\Phi_N = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

the normalized state on S^2 ($|z|^2 + R_3^2 = 1$) is given as $\Psi_N = P\Phi_N N_N^{-1/2}$, with $N_N = \Phi_N^\dagger P \Phi_N = \frac{1}{2}(1 + R_3)$. Since this gauge is only singular at the south pole $R_3 = -1$, we can safely use

$$\Psi_N = \frac{1}{\sqrt{2}}\begin{bmatrix} (1 + R_3)^{+1/2} \\ \bar{z}(1 + R_3)^{-1/2} \end{bmatrix}$$

for the north hemisphere S_N^2 ($R_3 \geqslant 0$). For the south hemisphere, we need to use the other gauge, say, by taking

$$\Phi_S = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Then the normalized state is given similarly as

$$\Psi_S = P\Phi_S N_S^{-1/2} = \frac{1}{\sqrt{2}}\begin{bmatrix} z(1 - R_3)^{-1/2} \\ (1 - R_3)^{+1/2} \end{bmatrix}, \qquad N_S = \Phi_S^\dagger P \Phi_S = \tfrac{1}{2}(1 - R_3),$$

which is regular everywhere on the south hemisphere S_S^2 ($R_3 \leqslant 0$).

The gauge transformation, $g_{SN}^{\mathbb{C}}$, between them, $\Psi_N = \Psi_S g_{SN}^{\mathbb{C}}$, is given by the generic formula before as

$$g_{SN}^{\mathbb{C}} = N_S^{-1/2}\Phi_S^\dagger P \Phi_N N_N^{-1/2} = \bar{z}/|z|.$$

This is regular except for the north and south poles $R_3 = \pm 1$.

The first Chern number of the Berry connection is easily evaluated using these two gauges and the gauge transformation, $A_N = g_{SN}^{-1} A_S g_{SN} + g_{SN}^{-1} \mathrm{d} g_{SN}$,

$$C_1 = \frac{\mathrm{i}}{2\pi} \int_{S^2} \mathrm{Tr}\, F = \frac{\mathrm{i}}{2\pi} \int_{S^2} \mathrm{d}\omega_1(A) = \frac{\mathrm{i}}{2\pi} \left(\int_{S_N^2} \mathrm{d}\omega_1(A_N) + \int_{S_S^2} \mathrm{d}\omega_1(A_S) \right)$$
$$= \frac{\mathrm{i}}{2\pi} \left(\int_{\partial S_N^2} \omega_1(A_N) + \int_{\partial S_S^2} \omega_1(A_S) \right) = \frac{\mathrm{i}}{2\pi} \int_{S^1 = \partial S_N^2} (\omega_1(A_N) - \omega_1(A_S))$$
$$= W_{S^1}(g_{SN}^{\mathbb{C}}),$$

where $S^1 = \partial S_N^2 = \partial S_S^2$ is an equator $S^1 = \{\boldsymbol{R} | R = 1, R_3 = 0\}$ and $W_{S^1}(g_{SN}^{\mathbb{C}})$ is a winding number of the map from the one-sphere (circle) $S^1 = \{(R_1, R_2) | R_1^2 + R_2^2 = 1\}$ to $U(1) \cong S^1 = \{z | |z|^2 = 1\} \in \mathbb{C}$ as

$$W_{S^1}(g_{SN}^{\mathbb{C}}) = \frac{\mathrm{i}}{2\pi} \int_{S^1} (g_{SN}^{\mathbb{C}})^{-1} \mathrm{d} g_{SN}^{\mathbb{C}} = -1.$$

This winding number can be evaluated in several ways. Since it is invariant against a rotation in S^1 ($g \to \mathrm{e}^{\mathrm{i}\theta} g$), we write it in a local coordinate near $R_1 = 0$ and $R_2 = 1$ as $g = +\mathrm{i}$, $\mathrm{d}g = -\mathrm{d}R_1$ as $W_{S^1}(g_{SN}^{\mathbb{C}}) = (\mathrm{i}/2\pi)(-) \int_{S^1} \mathrm{d}R_1/(+\mathrm{i}) = -\int_{S^1} \mathrm{d}R_1/(2\pi) = -1$, where $\int_{S^1} \mathrm{d}R_1 = 2\pi$ is a volume (length) of the circle S^1. Also using the explicit form $g_{SN}^{\mathbb{C}} = \mathrm{e}^{\mathrm{i}\mathrm{Arg}\,(R_1 + \mathrm{i}R_2)}$, we have $\int_{S^1} g^{-1} \mathrm{d}g = \mathrm{i} \int_{S^1} \mathrm{d}\,\mathrm{Arg}\,(R_1 + \mathrm{i}R_2) = 2\pi \mathrm{i}$.

Considering S^2 as a boundary of the solid sphere V_3 ($\partial V_3 = S^2$), naive application of the Stokes (Gauss) theorem, $C_1 = \int_{V_3} \mathrm{d}F$, suggests that $\frac{\mathrm{i}}{2\pi} \mathrm{d}F = -\delta^{(3)}(\boldsymbol{R})$ since $\mathrm{d}F = \mathrm{d}^2 A = 0$ as far as the Berry connection is well defined except at the origin. This is the *Dirac monopole* at the origin of the three-dimensional $\boldsymbol{R}$ space where the degeneracy of the generic complex Hamiltonian occurs [1].

5.2. *Yang monopole as a quaternionic Dirac monopole*

The discussion with KR degeneracy can be done analogously. Let us again start from a simple observation $H_{\mathbb{H}}^2 = Q^2 E_5$, $Q = |\boldsymbol{Q}|$, which implies that eigen energies of the KR multiplets are $\pm Q = \pm\sqrt{|q|^2 + Q_5^2}$, $|q| = \sqrt{N(q)} \in \mathbb{R}$, and the additional degeneracy to KR degeneracy occurs at the origin in the five-dimensional $\boldsymbol{Q}$ space $\mathbb{R}^5$ (figure 1). A projection into the positive energy KR multiplet is defined as $p = \frac{1}{2}(1 + H_{\mathbb{H}}/Q)$. Similar to the discussion above, let us take a four-sphere $S^4 = \{\boldsymbol{Q} | Q = 1\} \subset \mathbb{R}^5$ as the base space $M_{2n} (n = 2)$ to define the second Chern number C_2. Then the generic singularities of the KR multiplet are again points on S^4, which make lines in $\mathbb{R}^5$ when one considers a generic four-dimensional surface as a base space ('Yang' strings). To be more specific, let us take a gauge by taking a quaternion vector with two components $\phi_N = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \in \mathbb{H}^2$. Then the normalized KR multiplet is given, in the north pole gauge (regular in the northern hemisphere $S_N^4 (Q_5 \geqslant 0)$), as

$$\psi_N = p \phi_N N_N^{-1/2} = \frac{1}{\sqrt{2}} \begin{bmatrix} (1 + Q_5)^{+1/2} \\ \bar{q}(1 + Q_5)^{-1/2} \end{bmatrix}$$

where $N_N = \phi_N^\dagger p \phi_N = \frac{1}{2}(1+Q_5)$. This gauge is only singular at the south pole $Q_5 = -1$ on S^4. The other gauge by

$$\phi_S = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

also defines the multiplet (in the south pole gauge)

$$\psi_S = p\phi_S N_S^{-1/2} = \frac{1}{\sqrt{2}} \begin{bmatrix} q(1-Q_5)^{-1/2} \\ (1-Q_5)^{+1/2} \end{bmatrix},$$

where $N_S = \phi_S^\dagger p \phi_S = \frac{1}{2}(1-Q_5)$. This is regular in the southern hemisphere $S_S^4(Q_5 \leqslant 0)$. The gauge transformation between them is also calculated as

$$\psi_S^{\mathbb{H}} = g_{SN}^{\mathbb{H}} \psi_N^{\mathbb{H}}, \quad g_{SN}^{\mathbb{H}} = \bar{q}/|q| \in \mathrm{Sp}(1) = \{g \in \mathbb{H} | N(g) = 1\}$$

Now let us calculate the second Chern number in quaternionic notation as

$$\begin{aligned} C_2 &= -\frac{1}{8\pi^2} \int_{S^4} T f^2 = -\frac{1}{8\pi^2} \int_{S^4} \mathrm{d}\omega_3(a) = -\frac{1}{8\pi^2} \left(\int_{S_N^4} \mathrm{d}\omega_3(a_N) + \int_{S_S^4} \mathrm{d}\omega_3(a_S) \right) \\ &= -\frac{1}{8\pi^2} \int_{S^3} (\omega_3(a_N) - \omega_3(a_S)) = \frac{1}{24\pi^2} \int_{S^3} T((g_{SN}^{\mathbb{H}})^{-1} \mathrm{d} g_{SN}^{\mathbb{H}})^3 \\ &\equiv W_{S^3}(g_{SN}^{\mathbb{H}}) = -1 \end{aligned}$$

where $S^3 = S^4|_{Q_5=0} = \{(q_1, q_2, q_3, q_0) | |q| = 1\}$ is an equator, $\omega_3(a) = T(a\mathrm{d}a + \frac{2}{3}a^3)$ and $W_{S^3}(g_{SN}^{\mathbb{H}})$ is the Pontrjagin number of the map $S^3 \to \mathrm{Sp}(1) \cong S^3$ that is a covering degree, which is intrinsically integer. Here we used $\int_{S^3} \mathrm{d}\alpha_2 = \int_{\partial S^3} \alpha_2 = 0$ since the gauge is regular on S^3, which does not have boundaries. This Pontrjagin number is explicitly evaluated [51]. Since it is invariant for the change $q \to q\xi$, $|\xi| = 1$ that induces a rotation of S^3, it is enough to evaluate it near $q = 1$ ($q_0 = 1, q_1 = q_2 = q_3 = 0$), where $T(q^{-1}\mathrm{d}q)^3 = 3!T(i_{\mathbb{H}} j_{\mathbb{H}} k_{\mathbb{H}}) \mathrm{d}q_1 \mathrm{d}q_2 \mathrm{d}q_3 = -12 \mathrm{d}q_1 \mathrm{d}q_2 \mathrm{d}q_3$. Then we have $C_2(\boldsymbol{Q}) = W_{S^3}(g_{SN}^{\mathbb{H}}) = \frac{1}{24\pi^2}(-12 \times 2\pi^2) = -1$, where $2\pi^2$ is a volume of S^3.

Again writing S^4 as a surface of a five-dimensional solid sphere $V_5 = \{\boldsymbol{Q} | |\boldsymbol{Q}| \leqslant 1\}$, $\partial V_5 = S^4$, one may write symbolically $\mathrm{d}T(f^2) = -\delta^{(5)}(\boldsymbol{Q})$ by a simple application of the Stokes theorem $\int_{V_5} \mathrm{d}T(f^2) = \int_{\partial V_5} T(f^2) = -1$, since $\mathrm{d}T(f^2) = \mathrm{d}^2\omega_3 = 0$ away from the origin where the singularity exists. The origin of the five-dimensional $\boldsymbol{Q}$ space, $\boldsymbol{Q} = 0$, is a singular point for the Berry connection due to the additional degeneracy (four-fold) and it induces the Yang monopole in five dimensions [47], which locates at $\boldsymbol{Q} = 0$ (the charge is -1). This explicitly demonstrates that *the Yang monopole is a quaternioninc Dirac monopole.*

5.3. Chiral symmetry and topological stability of the doubled Dirac cones

For simplicity, we have assumed the two-sphere and the four-sphere as parameter spaces M_2 and M_4. In a generic situation, let us consider the Chern numbers of models $H_{\mathbb{C}}(\boldsymbol{R}(x))$ ($x \in M_2$) and $H_{\mathbb{H}}(\boldsymbol{Q}(x))$ ($x \in M_4$). Assuming that the energy gaps never collapse, images $\boldsymbol{R}(M_2) \subset \mathbb{R}^3$ and $\boldsymbol{Q}(M_4) \subset \mathbb{R}^5$ are deformed into spheres S^2 and S^4 without changing the Chern numbers. This

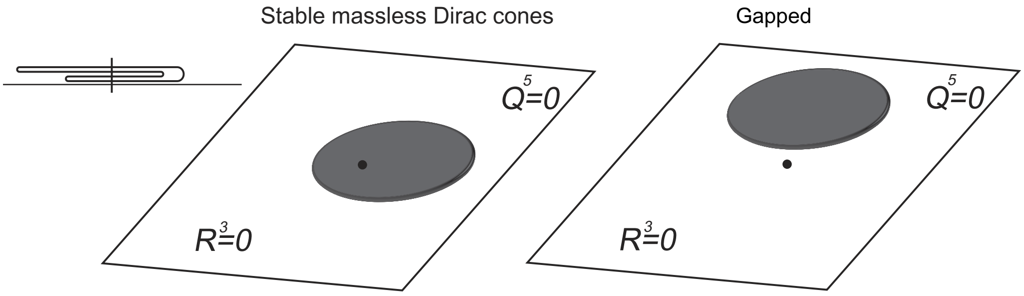

Figure 2. Collapsed images of maps into hyperplanes $M_2 \to \boldsymbol{R} \subset \mathbb{R}^2 : (R_3 = 0)$ and $M_4 \to \boldsymbol{Q} \subset \mathbb{R}^4 : (R_3 = 0)$ with chiral symmetric minimum models.

is topological stability and these topological numbers are given by the covering degrees of the maps as [52]

$$C_1 = -\deg \boldsymbol{R}(M_2) : M_2 \to S^2, \quad C_2 = -\deg \boldsymbol{Q}(M_4) : M_4 \to S^4.$$

To have well-defined Chern numbers, the gap has to be always open. However, in some situations, the gap may collapse. Generically speaking, this is accidental (accidental degeneracy). In other words, one may need to fine-tune physical parameters that occur at a quantum critical point. By imposing some restriction by symmetry, the situation may change and the gap closing has topological stability. Let us here impose 'chiral symmetry' and restrict the parameter space. The chiral operator in the minimum model is given by $\Gamma = \sigma_3$, $\Gamma^2 = 1$. The Hamiltonians of the minimum models satisfy $\{H_{\mathbb{C}}, \Gamma\} = 2R_3$, $\{H_{\mathbb{H}}, \Gamma\} = 2Q_5$. That is, the equators (S^1 and S^3, respectively) are characterized as chiral symmetrical spaces

$$\{H_{\mathbb{C}}(\boldsymbol{R}), \Gamma\} = 0 \; (\boldsymbol{R} \in S^1), \quad \{H_{\mathbb{H}}(\boldsymbol{Q}), \Gamma\} = 0 \; (\boldsymbol{Q} \in S^3).$$

When the Hamiltonians do have chiral symmetry, the parameter spaces $\boldsymbol{R}(M_2)$ (for $H_{\mathbb{C}}$) and $\boldsymbol{Q}(M_4)$ (for $H_{\mathbb{H}}$) are collapsed into the hyperplane $\mathbb{R}^2(R_3 = 0)$ and $\mathbb{R}^3(Q_5 = 0)$. Then we have two situations for images $\boldsymbol{R}(M_2)/\boldsymbol{Q}(M_4)$ (see figure 2): in one case $\boldsymbol{R}(M_2)/\boldsymbol{Q}(M_4)$ includes the origin, and in the other case it does not. When the image includes the origin, the energy gap collapses and the gap linearly vanishes as a function of parameter x generically. This results in Dirac-cone like energy dispersion. The doubling is also topologically clear (see the inset of figure 2). These Dirac cones are generically topologically stable, that is, stable against small but finite perturbation, since the images $\boldsymbol{R}(M_2) \subset \mathbb{R}^2$ and $\boldsymbol{Q}(M_4) \subset \mathbb{R}^4$. The topological stability of Dirac cones in two/four dimensions is discussed in relation to graphene and the Nielsen–Ninomiya theorem [53]–[55].

Here we comment on our quaternionic description of the Yang monopole to SU(2) gauge theory. The gauge structure of the TR-invariant system is symplectic and the gauge group of the simplest situation is Sp(1), which is mathematically equivalent to SU(2). Therefore, the results of the Sp(1) gauge structure we have described are directly related to SU(2) gauge theory. Our description of the Yang monopole is closely related to the instanton of the SU(2) gauge theory [30], [47]–[49], [51]. By the mathematical equivalence Sp(1) = SU(2), the quaternionic description of the Yang monopole here can be understood as a re-description of a known

SU(2) gauge structure. However, our parallel discussion of the U(1) and Sp(1) gauge structures without/with KR degeneracy simplifies the physical understanding of the SU(2) gauge structure, especially with our explicit gauge fixing and treatment of the gauge singularities of the Berry connections. Finally, note that the SU(2) gauge structure originating from the Sp(1) gauge structure of the TR-invariant system is not related to the conservation of spins. The spin is not a conserved quantity in most of the TR-invariant system such as the QSH systems with spin–orbit interaction. The multi-component structure by the spin is necessary to have the nontrivial Sp(1) gauge structure, but the spin itself is not a conserved quantity.

6. Symmetry-protected $\mathbb{Z}_2$-quantization

As discussed, Chern numbers are gauge invariant and intrinsically integer and apparently have topological stability. This implies that the quantization is stable for small but finite perturbation for the Hamiltonian. This topological stability does play a crucial role, for example, in the theory of quantized Hall effects. Note that the dimension of parameter space to define Chern numbers is necessarily even. The winding number W_{S^1} and the Pontrjagin index W_{S^3} are also topological and defined for spaces with odd dimensions. In odd dimensions, one may also define quantized quantities if one imposes additional symmetry requirements. They are generalizations of the Berry phase and generically gauge dependent as a phase of the wavefunction [8, 13]. This implies that these quantities are essentially quantum mechanical and do not have any classical correspondents. They also have a fundamental advantage in the identification of topological ordered states [12, 13]. An example is a $\mathbb{Z}_2$-quantization of the Berry phase for the TR-invariant system without KR degeneracy $\Theta^2 = 1$ [13]–[16]. The focus of this section is to extend the idea and supply a generic condition for the $\mathbb{Z}_2$-quantization.

Now let us start by defining generic Berry phases $\gamma_1(A)$ and $\gamma_3(a)$ as

$$\gamma_1(A) = \frac{\mathrm{i}}{2\pi}\int_{S^1}\omega_1(A), \qquad \gamma_3(a) = -\frac{1}{8\pi^2}\int_{S^3}\omega_3(a),$$

where $\gamma_1(A)$ is for a generic system (without degeneracy $M = 1$) and $\gamma_3(a)$ is for a system with KR degeneracy using quaternionic notation. Note here that the same topological quantity by the integral of the Chern–Simons form is discussed in several papers [28, 37, 56]. They are not invariant for the gauge transformation $A_g = g^{-1}Ag + g^{-1}\mathrm{d}g$ $(g \in U(1))$ and $a_g = g^{-1}ag + g^{-1}\mathrm{d}g$ $(g \in \mathrm{Sp}(1))$. Therefore, they are not well defined (as they are) but are gauge independent and well defined in modulo 1 as [13]

$$\gamma_1(A_g) = \gamma_1(A) + W_{S^1}(g) \equiv \gamma_1(A), \qquad \gamma_3(a_g) = \gamma_3(a) + W_{S^3}(g) \equiv \gamma_3(a),$$

since the gauge dependence is due to a nontrivial large gauge transformation. These contributions are topological and integers as $W_{S^1}(g) \in \mathbb{Z}$ and $W_{S^1}(g) \in \mathbb{Z}$ [13] as far as the gauge transformations are regular over S^1 and S^3. A phase factor of the Berry phase $e^{\mathrm{i}2\gamma}$ $(\gamma = 2\pi\gamma_1)$ is gauge independent and is a well-defined quantity (observed as a geometrical phase), but the phase γ itself is gauge dependent [8, 13].

Generically speaking, these generic Berry phases γ_1 and γ_3 may take any real values even in modulo 1. However they can be quantized when the system obeys some symmetry requirement, which we discuss below.

6.1. $\mathbb{Z}_2$-quantization of a TR-invariant system without KR degeneracy

Let us first consider a TR-invariant system without KR degeneracy [13]–[16]. This is realized for quantum systems with an even number of quantum spins. Since the Hamiltonian $\mathcal{H}$ does commute with the TR operator Θ, which is anti-unitary, $[\mathcal{H}, \Theta] = 0$,

$$\mathcal{H}(x)\psi(x) = \epsilon(x)\psi(x), \quad \mathcal{H}(x)\psi^\Theta(x) = \epsilon(x)\psi^\Theta(x), \quad \psi^\Theta \equiv \Theta\psi.$$

Owing to the uniqueness of the state, ψ and ψ^Θ are only different in phase, that is, the corresponding Berry connections $A = \psi^\dagger d\psi$ and $A^\Theta = (\psi^\Theta)^\dagger d\psi^\Theta$ are transformed into each other by some gauge transformation g, $A = g^{-1}A^\theta g + g^{-1}dg$, as $\gamma_1(A) \equiv \gamma_1(A^\Theta) \bmod 1$, since the gauge transformation is, generically, well defined on the parameter space $x \in S^1$. Also the TR operation for the many-spin state ψ is written as $\Theta = U\mathcal{K}$ with some parameter-independent unitary transformation U. Then the Berry connection is written as

$$A^\Theta = (\psi^\Theta)^\dagger d\psi^\Theta = \mathcal{K}A = -A$$

since the normalization $\psi^\dagger\psi = 1$ implies that $0 = (d\psi^\dagger)\psi + \psi^\dagger d\psi = \widetilde{d\psi^\dagger\psi} + A = \widetilde{\psi} d\psi^* + A = A^* + A$. Now we have two conditions for the Berry phases

$$\gamma_1(A) \equiv \gamma_1(A^\Theta) = -\gamma_1(A) \mod 1.$$

Therefore, allowed values of the Berry phase are restricted to two as $\gamma_1(A) = 0, \frac{1}{2}$. This is the $\mathbb{Z}_2$-quantization of the Berry phase for the unique TR-invariant state.

In most of the application [13]–[16], we have used a $U(1)$ twist $e^{i\theta}$, $\theta : 0 \to 2\pi$ as a parameter. In this case, the condition of the $\mathbb{Z}_2$-quantization is reformulated from a more generic point of view (see below).

6.2. $\mathbb{Z}_2$-quantization by inversion/reflection equivalence

Similar quantizations protected by symmetry occur for the generic Berry phases γ_1 and γ_3 when the system (with parameter) satisfies the following *inversion/reflection equivalence*. Inversion/reflection equivalence implies the existence of the unitary operator $U_\mathcal{I}$ or $U_\mathcal{R}$,

$$H(x_\mathcal{I}) = U_\mathcal{I}^\dagger H(x) U_\mathcal{I} \quad \text{or} \quad H(x_\mathcal{R}) = U_\mathcal{R}^\dagger H(x) U_\mathcal{R},$$

where $H(x)$ is a complex or a quaternionic Hamiltonian for $x \in S^1$ or $x \in S^3$, respectively. Inversion in parameter space is defined as $x_\mathcal{I} = -x$ and reflection is one of the following three: $x_\mathcal{R} = (-x_1, x_2, x_3)$, $x_\mathcal{R} = (x_1, -x_2, x_3)$ or $x_\mathcal{R} = (x_1, x_2, -x_3)$. As for the $x \in S^1$ case, reflection is the same as the inversion. This is a *sufficient* condition for $\mathbb{Z}_2$-quantization.

Although we use the quaternion notation with the reflection below (with KR degeneracy), it is also true for the inversion and the complex cases. The isolated KR multiplet, denoted as $\psi(x)$ with energy $E(x)$, satisfies $H(x_\mathcal{R})\psi(x_\mathcal{R}) = U_\mathcal{R}^\dagger H(x) U_\mathcal{R}\psi(x_\mathcal{R}) = E(x_\mathcal{R})\psi(x_\mathcal{R})$ due to reflection equivalence. It implies

$$H(x)\psi_\mathcal{R}(x) = E(x_\mathcal{R})\psi_\mathcal{R}(x),$$

where $\psi_{\mathcal{R}}(x) = U_{\mathcal{R}}\psi(x_{\mathcal{R}})$. Since the unitary equivalence between $H(x)$ and $H(x_{\mathcal{R}})$ implies that all of the eigenvalues are equal to each other, we may generically assume $E(x_{\mathcal{R}}) = E(x)$ supplementing a unitary transformation of reshuffling the KR degenerated eigenspaces. Now, as for the isolated eigenspace of the KR multiplet, $\psi(x)$ and $\psi_{\mathcal{R}}(x)$ are different just in Sp(1) phase, which implies that the corresponding Berry connections are gauge equivalent, $\psi_{\mathcal{R}}(x) = \psi(x)g, {}^{\exists}g \in \mathrm{Sp}(1)$,

$$a_{\mathcal{R}}(x) = \psi_{\mathcal{R}}^{\dagger}(x)\mathrm{d}\psi_{\mathcal{R}}(x) = \psi^{\dagger}(x_{\mathcal{R}})\mathrm{d}\psi(x_{\mathcal{R}}) = a(x_{\mathcal{R}}) = g^{-1}a(x)g + g^{-1}\mathrm{d}g.$$

Then the generic Berry phases satisfy $\gamma_1(A_{\mathcal{R}}) \equiv \gamma_1(A)$ and $\gamma_3(a_{\mathcal{R}}) \equiv \gamma_3(a)$ in modulo 1. Here note that γ_1 and γ_3 are defined by the integral over the odd dimensional spaces S^1 and S^3. Therefore, the generic Berry phases γ_1 and γ_3 are *odd by the inversion/reflection of parameter spaces* S^2 *and* S^3, $x \to x_{\mathcal{I}}$ *or* $x \to x_{\mathcal{R}}$, as $\gamma_1(A_{\mathcal{I}}) = \gamma_1(A_{\mathcal{R}}) = -\gamma_1(A)$ and $\gamma_3(a_{\mathcal{I}}) = \gamma_3(a_{\mathcal{R}}) = -\gamma_3(a)$. Therefore, we have a $\mathbb{Z}_2$-quantization of the Berry phases as

$$\gamma_1(A_{\mathcal{I}}) \equiv \gamma_1(A_{\mathcal{R}}) \equiv \gamma_1(A) = 0,\ 1/2 \quad (\mathrm{mod}\ 1),$$

$$\gamma_3(a_{\mathcal{I}}) \equiv \gamma_3(a_{\mathcal{R}}) \equiv \gamma_3(a) = 0,\ 1/2 \quad (\mathrm{mod}\ 1).$$

6.3. Chiral symmetry for minimum models

The chiral symmetry of the minimum models discussed before is a typical example of systems with inversion equivalence because the anti-commutators between the unitary operator $\Gamma = \Gamma^{\dagger}$ and $H_{\mathbb{C}}\,/H_{\mathbb{H}}$ are rewritten as

$$\Gamma^{\dagger}H_{\mathbb{C}}(\boldsymbol{R})\Gamma = -H_{\mathbb{C}}(\boldsymbol{R}) = H_{\mathbb{C}}(-\boldsymbol{R}) = H_{\mathbb{C}}(\boldsymbol{R}_{\mathcal{I}}),$$

$$\Gamma^{\dagger}H_{\mathbb{H}}(\boldsymbol{Q})\Gamma = -H_{\mathbb{H}}(\boldsymbol{Q}) = H_{\mathbb{H}}(-\boldsymbol{Q}) = H_{\mathbb{H}}(\boldsymbol{R}_{\mathcal{I}}),$$

where the models are defined on the equators as $\boldsymbol{R} \in S^1$ and $\boldsymbol{Q} \in S^3$. This is what we need for the $\mathbb{Z}_2$-quantization of γ_1 and γ_3. We explicitly confirm it by direct calculations below.

Let us first consider a generic case without KR degeneracy. In the north pole gauge, the multiplet at the equator $R_3 = 0$, $|z| = 1$ is given as

$$\Psi_N = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ \bar{z} \end{bmatrix}.$$

Then we have $A_N = \frac{1}{2}z\mathrm{d}\bar{z} = \frac{1}{2}g_{\mathbb{C}}^{-1}\mathrm{d}g_{\mathbb{C}}$ $(g_{\mathbb{C}} = \bar{z} \in S^1)$, which implies $\gamma_1(A_N) = \frac{1}{2}W_{S^1}(g_{\mathbb{C}}) = -1/2$. If we take the south pole gauge, we have

$$\Psi_S = \frac{1}{\sqrt{2}}\begin{bmatrix} z \\ 1 \end{bmatrix}, \qquad A_S = \tfrac{1}{2}\bar{z}\mathrm{d}z = -\tfrac{1}{2}z\mathrm{d}\bar{z} = -A_N \qquad (\bar{z}z = 1).$$

This implies $\gamma_1(A_S) = +\frac{1}{2} \equiv \gamma_1(A_N)$ (mod 1), which is consistent with the general consideration and $\mathbb{Z}_2$-quantization.

With KR degeneracy, the connection is obtained just by replacing z with q. Then we have the Berry connections in the two gauges as $a_N = \frac{1}{2}q\mathrm{d}\bar{q}$ and $a_S = \frac{1}{2}\bar{q}\mathrm{d}q$. Note here that

$a_S \neq -a_N$, which is different from the case without KR degeneracy. Then using $\mathrm{d}q = -q\mathrm{d}\bar{q}q$ ($\bar{q}q = 1$, $\mathrm{d}\bar{q}q = -\bar{q}\mathrm{d}q$) and $da_N = \frac{1}{2}\mathrm{d}q\mathrm{d}\bar{q} = -\frac{1}{2}q\mathrm{d}\bar{q}q \cdot \mathrm{d}\bar{q} = -\frac{1}{2}(q\mathrm{d}\bar{q})^2$, we have

$$\omega_3(a_N) = T(a_N da_N + \tfrac{2}{3}a_N^3) = T(-\tfrac{1}{4}(qd\bar{q})^3 + \tfrac{1}{12}(qd\bar{q})^3) = -\tfrac{1}{6}T(qd\bar{q})^3$$
$$\gamma_3(a_N) = \frac{1}{48\pi^2}\int_{S^3} T(g_{\mathbb{H}}^{-1}dg_{\mathbb{H}})^3 = \frac{1}{2}W_{S^3}(g_{\mathbb{H}}) = -\frac{1}{2}, \quad g_{\mathbb{H}} \in Sp(1).$$

Similarly, we have $a_S = \frac{1}{2}\bar{q}\mathrm{d}q = -\frac{1}{2}\bar{q}\cdot q\mathrm{d}\bar{q}q = -\frac{1}{2}\mathrm{d}\bar{q}q$, $\mathrm{d}a_S = \frac{1}{2}\mathrm{d}\bar{q}\mathrm{d}q = -\frac{1}{2}\mathrm{d}\bar{q}\cdot q\mathrm{d}\bar{q}q = -\frac{1}{2}(\mathrm{d}\bar{q}q)^2$ and

$$\omega_3(a_S) = T\left(a_S\mathrm{d}a_S + \tfrac{2}{3}a_S^3\right) = T\left(\tfrac{1}{4}(\mathrm{d}\bar{q}q)^3 - \tfrac{1}{12}(\mathrm{d}\bar{q}q)^3\right) = \tfrac{1}{6}T(\mathrm{d}\bar{q}q)^3 = \tfrac{1}{6}T(q\mathrm{d}\bar{q})^3,$$
$$\gamma_3(a_S) = -\gamma_3(a_N) = \tfrac{1}{2} \equiv \gamma_3(a_N) \mod 1.$$

This again confirms the $\mathbb{Z}_2$-quantization of the quaternionic minimum model with chiral symmetry.

6.4. Reflection and TR invariance without KR degeneracy

The quantization of the $\mathbb{Z}_2$ Berry phase discussed in section 6.1 [13] can be considered as the quantization due to the reflection equivalence discussed in section 6.2 when the parameter introduced is the $U(1)$ twist $\mathrm{e}^{\mathrm{i}x}$ and the other parameters are all real. It is simply due to the following observation of TR invariance:

$$\Theta^{-1}H(\mathrm{e}^{\mathrm{i}x})\Theta = U^\dagger H(\mathrm{e}^{-\mathrm{i}x})U = H(\mathrm{e}^{\mathrm{i}x}),$$

where U is a unitary operator to change $c_{i\sigma} \to (-)^{(1-\sigma)/2}c_{i-\sigma}$ for the fermions and the spins $\boldsymbol{S}_i = \frac{1}{2}\boldsymbol{c}_i^\dagger\boldsymbol{\sigma}\boldsymbol{c}_i$, $\boldsymbol{c}_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$. This is just the inversion or reflection equivalence as discussed in section 6.2.

7. Topological charge and nonlinear σ-models

Finally in this section, let us calculate topological charges of the nonlinear σ-model [30, 49], [57]–[60] as applications of the gauge-invariant forms of Chern numbers C_1 and C_2 in section 4.

7.1. Topological charge without KR degeneracy [57, 58, 61]

Let us start by considering an x-dependent two-component normalized state

$$\Psi(x) = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}, \; \Psi^\dagger\Psi = 1 = |\mathrm{Re}\, z_1|^2 + |\mathrm{Im}\, z_1|^2 + |\mathrm{Re}\, z_2|^2 + |\mathrm{Im}\, z_2|^2,$$

which defines S^3. Then the following three real quantities, n_1, n_2 and n_3, are defined as a CP^1 representation of n_i (i = 1, 2, 3):

$$\boldsymbol{n}(x) = \begin{bmatrix} n^1 \\ n^2 \\ n^3 \end{bmatrix} = \Psi^\dagger \begin{bmatrix} \sigma^1 \\ \sigma^2 \\ \sigma^3 \end{bmatrix} \Psi = \begin{bmatrix} \Psi^\dagger\sigma^1\Psi \\ \Psi^\dagger\sigma^2\Psi \\ \Psi^\dagger\sigma^3\Psi \end{bmatrix} = \begin{bmatrix} \mathrm{Tr}_2\, \sigma^1 P \\ \mathrm{Tr}_2\, \sigma^2 P \\ \mathrm{Tr}_2\, \sigma^3 P \end{bmatrix},$$

where $\sigma_a = \sigma^a$ and the projection, $P(x) = \Psi\Psi^\dagger$, into the subspace spanned by $\Psi(x)$ is introduced.

Since $\mathrm{Tr} P = \Psi^\dagger\Psi = 1$, the projection is expanded as $P = \frac{1}{2}E_2 + P_i\sigma^i$. The coefficients are given as $P_i = \mathrm{Tr}\ P\frac{1}{2}\sigma^i = \frac{1}{2}n^i$. Now we have rewritten $P = \frac{1}{2}(E_2 + n_i\sigma^i) = \frac{1}{2}(E_2 + H_{\mathbb{C}}(\boldsymbol{n}))$ and $H_{\mathbb{C}} = \boldsymbol{n}\cdot\boldsymbol{\sigma} = 2P - E_2$. Then $H_{\mathbb{C}}^2 = 4P - 4P + E_2 = E_2 = n_i\sigma_i n_j\sigma_j = n_i n_i + \sum_{i<j} n_i n_j\{\sigma_i, \sigma_j\} = |\boldsymbol{n}|^2 E_2$. This implies $|\boldsymbol{n}|^2 = 1$. Therefore, the state Ψ can be considered as a positive energy eigenstate of $H_{\mathbb{C}}$ by identifying $\boldsymbol{n} = \boldsymbol{R}$. It makes a CP^1 representation of the SO(3) nonlinear σ-model.

Using this decomposition of the three vectors $\boldsymbol{n}$, let us discuss the topological charge of the current

$$J^\mu = \frac{1}{8\pi}\epsilon^{\mu\nu\lambda}\epsilon_{abc}n^a\partial_\nu n^b\partial_\lambda n^c$$

The topological charge is evaluated as

$$\begin{aligned}
Q_{\mathbb{C}} &= \int \mathrm{d}x^1\mathrm{d}x^2 J^3 = \frac{1}{8\pi}\int \mathrm{d}x^1\mathrm{d}x^2\epsilon^{3\nu\lambda}\epsilon_{abc}n^a\partial_\nu n^b\partial_\lambda n^c \\
&= \frac{1}{8\pi}\int \mathrm{d}x^1\mathrm{d}x^2\epsilon_{abc}(n^a\partial_1 n^b\partial_2 n^c - n^a\partial_2 n^b\partial_1 n^c) \\
&= \frac{1}{8\pi}\int \epsilon_{abc}n^a\mathrm{d}n^b\mathrm{d}n^c = \frac{1}{8\pi}\int \epsilon_{abc}(\mathrm{Tr}\,\sigma^a P)(\mathrm{Tr}\,\sigma^b\mathrm{d}P)(\mathrm{Tr}\,\sigma^c\mathrm{d}P)
\end{aligned}$$

Now writing $\mathrm{d}P = \mathrm{d}P_a\sigma^a$, we have

$$Q_{\mathbb{C}} = \frac{1}{8\pi}\int \epsilon_{abc}2^3 P_a\mathrm{d}P_b\mathrm{d}P_c = \frac{1}{\pi}\int \epsilon_{abc}P_a\mathrm{d}P_b\mathrm{d}P_c$$

Also note that $\mathrm{Tr}P\mathrm{d}P\mathrm{d}P = P_a\mathrm{d}P_b\mathrm{d}P_c\mathrm{Tr}\sigma^a\sigma^b\sigma^c = P_a\mathrm{d}P_b\mathrm{d}P_c\mathrm{i}\epsilon^{abd}\,\mathrm{Tr}\sigma_d\sigma^c = 2\mathrm{i}\epsilon^{abc}P_a\mathrm{d}P_b\mathrm{d}P_c$. Therefore, we finally have

$$C_1 = \frac{\mathrm{i}}{2\pi}\int \mathrm{d}\omega_1 = \frac{\mathrm{i}}{2\pi}\int \mathrm{Tr}(P\mathrm{d}P\mathrm{d}P) = \frac{\mathrm{i}}{2\pi}\int (2\mathrm{i})\epsilon_{abc}P_a\mathrm{d}P_b\mathrm{d}P_c = -Q_{\mathbb{C}}$$

This gives a direct relation between the first Chern number and the topological charge of the SO(3) nonlinear σ-model.

7.2. Topological charge with KR degeneracy [30, 49], [57]–[60]

Similarly to KR degeneracy, let us consider an x-dependent four-component normalized KR pair, which is described by the two-component quaternionic vector

$$\psi(x) = \begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} \in \mathbb{H}^2,\ \psi^\dagger\psi = 1 = (\psi_1^0)^2 + (\psi_1^1)^2 + (\psi_1^2)^2 + (\psi_1^3)^2 + (\psi_2^0)^2 + (\psi_2^1)^2 + (\psi_2^2)^2 + (\psi_2^3)^2,$$

which defines S^7 where $\mathbb{H} \ni \psi_i = \psi_i^0 + \psi_i^1 i_{\mathbb{H}} + \psi_i^2 j_{\mathbb{H}} + \psi_i^3 k_{\mathbb{H}}$, $\psi_i^a \in \mathbb{R}$ $(a = 0, 1, 2, 3, i = 1, 2)$. Then the following five real quantities, n_1, n_2, n_3, n_4, n_5, are defined by HP^1 representation as

$$\boldsymbol{n}(x) = \begin{pmatrix} n^1 \\ n^2 \\ n^3 \\ n^4 \\ n^5 \end{pmatrix} = \frac{1}{2} T\psi^\dagger \begin{pmatrix} \Sigma^1 \\ \Sigma^2 \\ \Sigma^3 \\ \Sigma^2 \\ \Sigma^5 \end{pmatrix} \psi = \frac{1}{2} \begin{pmatrix} T\psi^\dagger \Sigma^1 \psi \\ T\psi^\dagger \Sigma^2 \psi \\ T\psi^\dagger \Sigma^3 \psi \\ T\psi^\dagger \Sigma^4 \psi \\ T\psi^\dagger \Sigma^5 \psi \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \mathrm{Tr}\, T\ \Sigma^1 p \\ \mathrm{Tr}\, T\ \Sigma^2 p \\ \mathrm{Tr}\, T\ \Sigma^3 p \\ \mathrm{Tr}\, T\ \Sigma^4 p \\ \mathrm{Tr}\, T\ \Sigma^5 p \end{pmatrix},$$

$$\Sigma^1 = \begin{bmatrix} 0 & i_{\mathbb{H}} \\ \bar{i}_{\mathbb{H}} & 0 \end{bmatrix}, \quad \Sigma^2 = \begin{bmatrix} 0 & j_{\mathbb{H}} \\ \bar{j}_{\mathbb{H}} & 0 \end{bmatrix}, \quad \Sigma^3 = \begin{bmatrix} 0 & k_{\mathbb{H}} \\ \bar{k}_{\mathbb{H}} & 0 \end{bmatrix}, \quad \Sigma^4 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \Sigma^5 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

where $\Sigma^a = \Sigma_a = (\Sigma^a)^\dagger$, $(\Sigma^a)^2 = E_2$, $\{\Sigma_a, \Sigma_b\} = 0$, $\Sigma^a \Sigma^b \Sigma^c \Sigma^d = \epsilon^{abcde} \Sigma_e$ (when a, b, c, d, e are all different) and $p(x) = \psi\psi^\dagger$ is a projection, into the subspace spanned by the KR pair $\psi(x)$.

Since $\mathrm{Tr}Tp = T\psi^\dagger\psi = 2$, the projection is expanded as $p = \frac{1}{2}E_2 + p_a\Sigma^a$. The coefficients are given as $p_a = \mathrm{Tr}\, T\ (\Sigma^a p)/4 = n^a/2$. Now we have rewritten $p = \frac{1}{2}(E_2 + n_a\Sigma^a) = \frac{1}{2}(E_2 + H_{\mathbb{H}}(\boldsymbol{n}))$ and $H_{\mathbb{H}} = \boldsymbol{n} \cdot \boldsymbol{\Sigma} = 2p - E_2$. Then $H_{\mathbb{H}}^2 = 4p - 4p + E_2 = E_2 = n_i \Sigma_i n_j \Sigma_j = n_i n_i E_2 + \sum_{i<j} n_i n_j \{\Sigma_i, \Sigma_j\} = |\boldsymbol{n}|^2 E_2$. This implies $|\boldsymbol{n}|^2 = 1$. Therefore, the state ψ can be considered as a positive energy KR multiplet of $H_{\mathbb{H}}$ by identifying $\boldsymbol{n} = \boldsymbol{Q}$. This establishes the relation for the HP^1 representation of the SO(5) nonlinear σ-model.

Again using this decomposition of the five vectors $\boldsymbol{n}$, let us discuss the topological charge $Q_{\mathbb{H}}$ following [30, 59, 60]:

$$\begin{aligned} J^{\sigma\tau\omega} &= N^{-1}\epsilon^{\mu\nu\lambda\kappa\rho\sigma\tau\omega}\epsilon_{abcde} n^a \partial_\mu n^b \partial_\nu n^c \partial_\lambda n^d \partial_\rho n^e, \\ Q_{\mathbb{H}} &= \int \mathrm{d}x^1 \mathrm{d}x^2 \mathrm{d}x^3 \mathrm{d}x^4\ J^{567} = N^{-1} \int \mathrm{d}x^1 \mathrm{d}x^2 \mathrm{d}x^3 \mathrm{d}x^4\ \epsilon^{\mu\nu\lambda\rho 567} \epsilon_{abcde} n^a \partial_\mu n^b \partial_\nu n^c \partial_\lambda n^d \partial_\rho n^e \\ &= N^{-1} \int \epsilon_{abcde} n^a \mathrm{d}n^b \mathrm{d}n^c \mathrm{d}n^d \mathrm{d}n^e \\ &= N^{-1} 2^{-5} \int \epsilon_{abcde} (\mathrm{Tr}\, T\ \Sigma^a p)(\mathrm{Tr}\, T\ \Sigma^b \mathrm{d}p)(\mathrm{Tr}\, T\ \Sigma^c \mathrm{d}p)(\mathrm{Tr}\, T\ \Sigma^d \mathrm{d}p)(\mathrm{Tr}\, T\ \Sigma^e \mathrm{d}p), \end{aligned}$$

where N is a normalization constant.

Writing $\mathrm{d}p = \mathrm{d}p^a \Sigma_a$, we have $Q_{\mathbb{H}} = 2^5 N^{-1} \int \epsilon_{abcde} p^a \mathrm{d}p^b \mathrm{d}p^c \mathrm{d}p^d \mathrm{d}p^e$. Also we can show that $\mathrm{Tr}T\ (p\mathrm{d}p\mathrm{d}p)^2 = 4\epsilon_{abcde} p^a \mathrm{d}p^b \mathrm{d}p^c \mathrm{d}p^d \mathrm{d}p^e$. Therefore, we have

$$C_2 = -\frac{1}{8\pi^2} \int \mathrm{Tr}\, T\ (p\mathrm{d}p\mathrm{d}p)^2 = -\frac{1}{2\pi^2} \int \epsilon_{abcde} p^a \mathrm{d}p^b \mathrm{d}p^c \mathrm{d}p^d \mathrm{d}p^e \propto Q_{\mathbb{H}}.$$

This is again the direct relation between the second Chern number of the HP^1 model and the topological charge of the SO(5) nonlinear σ-model.

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