A memo on the construction of the $\pi_n[R_{2-n}] = \mathbb{Z}_2$ invariant

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Let the classifying spaces R_n be as follows:

$$\begin{array}{c|c} n & R_n \\ \hline 0 & O(N+M)/O(N)\times O(M) \\ 1 & O(N) \\ 2 & O(2N)/U(N) \\ 3 & U(2N)/Sp(N) \\ 4 & Sp(N+M)/Sp(N)\times Sp(M) \\ 5 & Sp(N) \\ 6 & Sp(N)/U(N) \\ 7 & U(N)/O(N) \end{array} \tag{1}$$

The limits and unions over N are omitted. We call n the symmetry class. The purpose of this note is to give a numerical implementation of an invariant that detects

$$\pi_n[R_{2-n}] = \mathbb{Z}_2. \tag{2}$$

In the following, the Hamiltonian $H_{\boldsymbol{k}}$ is always assumed to satisfy the Hermiticity condition

$$H_{\boldsymbol{k}}^\dagger = H_{\boldsymbol{k}}. \tag{3}$$

We also assume the flattening condition $H_{\boldsymbol{k}}^2 = 1$. The space on which the Hamiltonian is defined is taken to be the sphere S^n.

Moreover, whenever we write q_k, it denotes a unitary matrix $q_k \in U(N)$.

1 Formulation as part of a geometric quantity valued in $\mathbb{R}/2\mathbb{Z}$

Notice that the symmetry class $(2-n)$ can be regarded as the symmetry class $(3-n)$ with an additional chiral symmetry Γ. Therefore, a Hamiltonian in symmetry class $(2-n)$ may be regarded as a Hamiltonian in symmetry class $(3-n)$ by forgetting the chiral symmetry Γ. Since

$$\pi_n[R_{3-n}] = 0 \tag{4}$$

in this situation, a Hamiltonian $H_{\boldsymbol{k}}$ on the n-sphere S^n can be extended to the $(n+1)$-dimensional ball D^{n+1}, whose boundary is S^n. Fix one such extension $\tilde{H}_{\boldsymbol{k}}$, and define the geometric quantity

$$\Theta[H_{\boldsymbol{k}}] = \int_{D^{n+1}} f(\tilde{H}_{\boldsymbol{k}}) \in \mathbb{R} \tag{5}$$

using the integrand $f(\tilde{H}_{\boldsymbol{k}})$ of the Chern number or winding number that characterizes $\pi_{n+1}[R_{3-n}] = 2\mathbb{Z}$. Changing the extension produces an ambiguity in $2\mathbb{Z}$, and hence

$$\Theta[H_{\boldsymbol{k}}] \in \mathbb{R}/2\mathbb{Z} \tag{6}$$

is well-defined in this sense. The chiral symmetry Γ imposes the constraint $\Theta[H_{\boldsymbol{k}}] = -\Theta[H_{\boldsymbol{k}}]$, and therefore

$$\Theta[H_{\boldsymbol{k}}] \in \{0, 1\} \tag{7}$$

holds. This is precisely the $\mathbb{Z}_2$ invariant.

For a numerical implementation of this construction, the following issue arises:

- The ordinary Chern–Simons term and WZ term take values in $\mathbb{R}/\mathbb{Z}$. How should one numerically implement Chern–Simons and WZ terms that take values in $\mathbb{R}/2\mathbb{Z}$?

1.1 $(2-n) \to (3-n)$

The change of symmetry class is implemented as follows:

- When chiral symmetry is absent, forget the Hermiticity condition.
- When chiral symmetry is present, forget the chiral symmetry.

Indeed, when chiral symmetry is absent, either TRS or PHS is present, and the symmetries for a Hermitian Hamiltonian H_k are written as

$$\mathrm{AI}: \quad H_k^* = H_k, \tag{8}$$
$$\mathrm{D}: \quad H_k^\top = -H_k, \tag{9}$$
$$\mathrm{AII}: \quad \sigma_y H_k^* \sigma_y = H_k, \tag{10}$$
$$\mathrm{C}: \quad \sigma_y H_k^\top \sigma_y = -H_k. \tag{11}$$

If we forget the Hermiticity condition on H_k, these symmetries are precisely the symmetries of the off-diagonal block of a Hermitian Hamiltonian H_k in classes BDI, DIII, CII, and CI, respectively.

When chiral symmetry is present, it is enough to keep imposing Hermiticity and forget the chiral symmetry.

1.2 Example: $n = 0$. Class D

Consider a class-D Hamiltonian

$$H_k^\top = -H_k, \quad k \in \{0, 1\}. \tag{12}$$

The $\mathbb{Z}_2$ invariant

$$\mathrm{Pf}\,[H_0]/\mathrm{Pf}\,[H_1] \in \pm 1 \tag{13}$$

is defined. Let us reformulate this $\mathbb{Z}_2$ invariant using the strategy above.

The symmetry shift is realized by forgetting the Hermiticity condition, but here we also record the formulation obtained by adding chiral symmetry. To regard class D as class DIII with an additional chiral symmetry, it is enough to double the Hamiltonian and add chiral symmetry. If

$$H'_k = \begin{pmatrix} & H_k \\ H_k^\dagger & \end{pmatrix}, \tag{14}$$

then H'_k satisfies the class-DIII symmetries

$$\sigma_z H'_k \sigma_z = -H'_k, \quad \sigma_y H_k'^* \sigma_y = H'_k. \tag{15}$$

Furthermore, the Hermiticity of H_k is equivalent to adding the further symmetry

$$\sigma_y H'_k \sigma_y = -H'_k. \tag{16}$$

The procedure above is equivalent simply to forgetting the Hermiticity of H_k, without needing to double H_k. Choose one homotopy $\widetilde{H}_{k\in[0,1]}$ connecting the non-Hermitian class-D Hamiltonians H_0 and H_1. Here $\tilde{H}_k$ is defined so as to satisfy the symmetry

$$\tilde{H}_k^\top = -\tilde{H}_k. \tag{17}$$

The $\mathbb{R}/2\mathbb{Z}$ quantity is defined by

$$\frac{1}{2\pi i} \int_0^1 d \log \det \tilde{H}_k \in \mathbb{R}/2\mathbb{Z}. \tag{18}$$

The ambiguity is $2\mathbb{Z}$ because the Pfaffian is defined under the condition $\tilde{H}_k^\top = -\tilde{H}_k$, and

$$\frac{1}{2\pi i} \oint d \log \det \tilde{H}_k = \frac{1}{\pi i} \oint d \log \mathrm{Pf}\, \tilde{H}_k \in 2\mathbb{Z}. \tag{19}$$

1.3 Example: $n = 1$. Class BDI

Consider a class-BDI Hamiltonian, or more precisely its off-diagonal part,

$$q_k^* = q_k, \quad k \in S^1. \tag{20}$$

That is, $q_k \in O(N)$. The $\mathbb{Z}_2$ invariant is computed by lifting to $Spin(N)$, but let us formulate it using the strategy above.

To regard it as a class-D Hamiltonian, it is enough to form a Hamiltonian by placing q_k in the off-diagonal blocks:

$$H_k = \begin{pmatrix} & q_k \\ q_k^\dagger & \end{pmatrix}, \quad \sigma_z H_k^\top \sigma_z = -H_k. \tag{21}$$

Choose one extension $\tilde{H}_{k \in D^2}$ to D^2. The extension $\tilde{H}_k$ is chosen to satisfy the class-D symmetry. Define the $\mathbb{R}/2\mathbb{Z}$ quantity by

$$\Theta[H_k] = \frac{i}{2\pi} \int_{D^2} \mathrm{tr}\,[F] \in \mathbb{R}/2\mathbb{Z}. \tag{22}$$

The chiral symmetry implies $\Theta[H_k] = -\Theta[H_k]$, and $\Theta[H_k] \in \{0, 1\}$ is the $\mathbb{Z}_2$ invariant.

1.4 Example: $n = 2$. Class AI

Consider a class-AI Hamiltonian

$$H_k^* = H_k, \quad k \in S^2. \tag{23}$$

The $\mathbb{Z}_2$ invariant is known as the second Stiefel–Whitney class, but here we try to formulate it as an $\mathbb{R}/4\pi\mathbb{Z}$ quantity.

As in the case $n = 0$, if we regard H_k as a non-Hermitian Hamiltonian, then $H_k \in O(n)$, namely it takes values in the classifying space R_1. Choose one extension $\tilde{H}_{k \in D^3}$ to the three-dimensional ball D^3, and define the WZ term

$$\Theta[H_k] = \frac{1}{24\pi^2} \int_{D^3} \mathrm{tr}\,[\tilde{H}_k^\top d\tilde{H}_k] \in \mathbb{R}/2\mathbb{Z}. \tag{24}$$

Hermiticity implies $\Theta[H_k] = -\Theta[H_k]$, and $\Theta[H_k] \in \{0, 1\}$ is the $\mathbb{Z}_2$ invariant.

1.5 Example: $n = 3$. Class CI

Consider a class-CI Hamiltonian, or more precisely its off-diagonal part,

$$q_k^\top = q_k, \quad k \in S^3. \tag{25}$$

To regard it as a class-AI Hamiltonian, it is enough to form a Hamiltonian by placing q_k in the off-diagonal blocks:

$$H_k = \begin{pmatrix} & q_k \\ q_k^\dagger & \end{pmatrix}, \quad \sigma_x H_k^* \sigma_x = H_k. \tag{26}$$

Choose one extension $\tilde{H}_{k \in D^4}$ to D^4. The extension $\tilde{H}_k$ is chosen to satisfy the class-AI symmetry. Define the $\mathbb{R}/4\pi\mathbb{Z}$ quantity by

$$\Theta[H_k] = \frac{-1}{8\pi^2} \int_{D^4} \mathrm{tr}\,[F^2] \in \mathbb{R}/2\mathbb{Z}. \tag{27}$$

The chiral symmetry implies $\Theta[H_k] = -\Theta[H_k]$, and $\Theta[H_k] \in \{0, 1\}$ is the $\mathbb{Z}_2$ invariant.

Comments:

- In the end, the issue is how to numerically implement a geometric quantity valued in $\mathbb{R}/2\mathbb{Z}$, and how to guarantee that the ambiguity is $2\mathbb{Z}$ rather than $\mathbb{Z}$.
- The extension obtained after dropping the Hermiticity condition may perhaps be performed canonically, for example by adding $+i\omega$; this is separate from whether such a construction is useful numerically.

Leaving aside whether the construction can be implemented numerically, one can see as follows that a $\mathbb{Z}_2$ invariant is defined when the base space is S^3. Consider the long exact sequence of homotopy groups

$$\to \pi_3[O] \xrightarrow{2} \pi_3[U] \to \pi_3[U/O] \to \pi_2[O] = 0. \tag{28}$$

Decompose S^3 into the northern hemisphere U_N and the southern hemisphere U_S, and take continuous gauges on them:

$$q = Q_N Q_N^\top, \quad \boldsymbol{k} \in U_N, \tag{29}$$

$$q = Q_S Q_S^\top, \quad \boldsymbol{k} \in U_S. \tag{30}$$

The transition function on the equator S^2 is

$$S_{NS} = Q_N^\dagger Q_S \in O(N), \tag{31}$$

but since $\pi_2[O] = 0$, there is no obstruction. Thus we may assume the existence of a global gauge on S^3,

$$q = QQ^\top. \tag{32}$$

Then the winding number

$$W_3[Q] \in \mathbb{Z} \tag{33}$$

is defined. Under a gauge transformation that does not destroy the global nature of Q,

$$Q \mapsto QS, \quad S : S^3 \to O(N), \tag{34}$$

the winding number changes as

$$W_3[Q] \mapsto W_3[QS] = W_3[Q] + W_3[S], \quad W_3[S] \in 2\mathbb{Z}. \tag{35}$$

Therefore

$$W_3[Q] \mod 2 \tag{36}$$

is a $\mathbb{Z}_2$ invariant.

- This construction follows immediately from the long exact sequence of homotopy groups, but I believe it was written somewhere in a paper, so this should be checked.