Visualizasion for $\pi_1(SO(3)/D_2)$ and rotation of eigenvectors

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Abstract

In [1] we've known $\pi_1(SO(3)/D_2) \simeq Q$. In this article we will visualize $SO(3)/D_2$ and $\pi_1(SO(3)/D_2)$ to obtain a nice picture describing rotation of eigenframes.

Contents

1 Background:relationship between 3-band Hermitian Hamiltonian and $SO(3)/D_2$

In this article we only consider hermitian Hamiltonian without band degeneracy. You can find more detail in [1].

Definition 1.1. space of Hamiltonians $\mathcal{H} = \{H = u_1^T u_1 + 2u_2^T u_2 + 3u_3^T u_3 | [u_1, u_2, u_3] \in SO(3)/D_2\}$

Remark 1.2. $[u_1, u_2, u_3] \in SO(3)$, the following four elements determine the same H in $\mathcal{H}$, that's why we quotient D_2.:

$[u_1, u_2, u_3] \sim [-u_1, -u_2, u_3] \sim [-u_1, u_2, -u_3] \sim [u_1, -u_2, -u_3]$

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2 Visualizasion of $SO(3)/D_2$

We've known $SO(3) = \{M \in GL(3,\mathbb{R}) | M^T M = I, det M = 1\}$, a group of "hand-preserving" rotations. The following we focus on another way to describe $SO(3)$.

Any rotation can be described by a pair $(\hat{r}, \theta)$ which means rotate along $\hat{r}$ by θ.

Definition 2.1. Denote $\phi(\hat{r}, \theta)$ the rotation along axis $\hat{r}$ by angle θ, where $\hat{r} \in S^2$ and $\theta \in [0, 2\pi]$.

So $SO(3) = \{\phi(\hat{r}, \theta) | \hat{r} \in S^2, \theta \in [0, 2\pi]\}$

Then we want to make parametrize space of $SO(3)$ smaller and visualize $SO(3)$.

Fact 2.2. There are two properties easily check:

(1)$\phi(\hat{r}, \theta) = \phi(-\hat{r}, 2\pi - \theta)$

(2)In particular, $\phi(\hat{r}, \pi) = \phi(-\hat{r}, \pi)$

The first fact means we can always make the second parameter θ lies in $[0, \pi]$. For example, $\phi(\hat{x}, 3\pi/2) = \phi(\hat{x}, 2\pi - 3\pi/2) = \phi(\hat{x}, \pi/2)$.

We can view $SO(3)$ as a solid sphere(ball) with radium π. Any point $\vec{t}$ in this ball represnts the rotation $\phi(\vec{t}/\left\|\vec{t}\right\|, \left\|\vec{t}\right\|)$. For example, the bold point in Fig1 is $\phi(\hat{y}, \pi/2)$, the rotation along $\hat{y}$ by $\pi/2$.

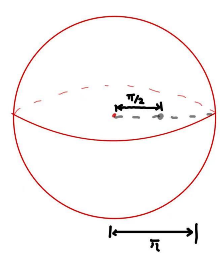

Figure 1: Parametrization of $SO(3)$

The second of fact shows that we should glue the antipodal points of the boundary of this ball, see Fig2.

Conclution 2.3. $SO(3)$ is a ball with radium π with identifying antipodal points, i.e., $SO(3) \simeq B^3(\pi)/\sim$, where $x \sim y \Leftrightarrow x, y \in \partial B^3(\pi)$ and $x = -y$

Next, we want to visualize $SO(3)/D_2$.

Fact 2.4. $D_2 = \{\phi(\hat{x}, \pi), \phi(\hat{y}, \pi), \phi(\hat{z}, \pi), id\}$

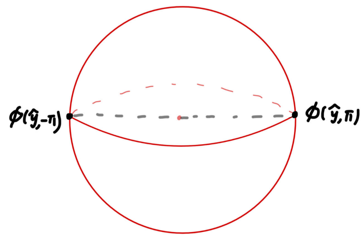

Figure 2: Antipodal points are the same in $SO(3)$

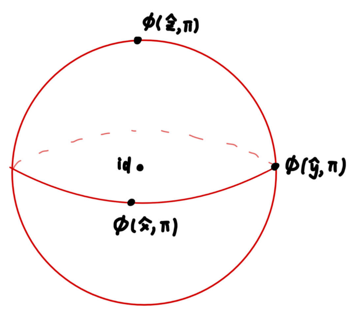

Figure 3: D_2 in $SO(3)$

We can view D_2 as the following four points in Fig3

Conclution 2.5. $SO(3)/D_2$ is a ball with radium π after the following two procedure:

(1)glue antipodal points

(2)glue four points in Fig3 to a point

3 The fundamental group of $SO(3)/D_2$

Fact 3.1. $\pi_1(SO(3)/D_2) \simeq Q = \{\pm 1, \pm i, \pm j, \pm k\}$

Property 3.2. We have the following bijections:

$SO(3)/D_2 \leftrightarrow$ space of Hamiltonians $\leftrightarrow$ space of eigenframes

where space of Hamiltonians is the space in Definition 1.1.

Proof. $SO(3)/D_2 \leftrightarrow$ {space of Hamiltonians} $\leftrightarrow$ {spaces of eigenframes}

$\phi(\hat{r}, \theta) \mapsto H = u_1^T u_1 + 2u_2^T u_2 + 3u_3^T u_3 \mapsto [u_1, u_2, u_3]$

where $[u_1, u_2, u_3] = \phi(\hat{r}, \theta)[e_1, e_2, e_3]$ and $[e_1, e_2, e_3]$ is the standard frame in $\mathbb{R}^3$.

□

By Property 3.2, we have

Conclution 3.3. Any loop in $SO(3)/D_2$ is an evolution of the eigenframe, i.e., any element in $\pi_1(SO(3)/D_2)$ is an evolution of the eigenframe.

Example 3.4. Consider loop L_1, L_5, L_6 in Fig4 in which $\hat{x}$, $\hat{y}$, $\hat{z}$ corresponding to the first, second and third eigenvectors.

Evolution of eigenframe on loop L_1: the first eigenvector ($\hat{x}$) fixed, the second ($\hat{y}$) and third ($\hat{z}$) eigenvectors rotate by π.

Evolution of eigenframe on loop L_6: the second eigenvector ($\hat{y}$) fixed, the first ($\hat{x}$) and third ($\hat{z}$) eigenvectors rotate by π.

Evolution of eigenframe on loop L_5: the third eigenvector ($\hat{z}$) fixed, the first ($\hat{x}$) and second ($\hat{y}$) eigenvectors rotate by π.

The following example is a more detailed computation.

Example 3.5. Evolution on Loop L_1. Parametrization shown in Fig5.

By [2],The rotation matrix of rotating along $[a_1, a_2, a_3]$ by angle ψ is:

$$\begin{bmatrix} \cos\psi + (1-\cos\psi)\, {a_1}^2 & (1-\cos\psi)\, a_1 a_2 - \sin\psi a_3 & (1-\cos\psi)\, a_1 a_3 + \sin\psi a_2 \\ (1-\cos\psi)\, a_1 a_2 + \sin\psi a_3 & \cos\psi + (1-\cos\psi)\, {a_2}^2 & (1-\cos\psi)\, a_2 a_3 - \sin\psi a_1 \\ (1-\cos\psi)\, a_1 a_3 - \sin\psi a_2 & (1-\cos\psi)\, a_2 a_3 + \sin\psi a_1 & \cos\psi + (1-\cos\psi)\, {a_3}^2 \end{bmatrix}$$

In this case, $a_1 = 0, a_2 = cos\theta, a_3 = sin\theta, \psi = \pi$. Then the rotation matrix, i.e., eigenframes are:

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & \cos 2\theta & \sin 2\theta \\ 0 & \sin 2\theta & -\cos 2\theta \end{bmatrix}$$

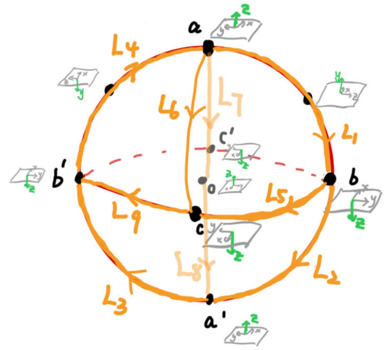

Figure 4: loops in $SO(3)/D_2$

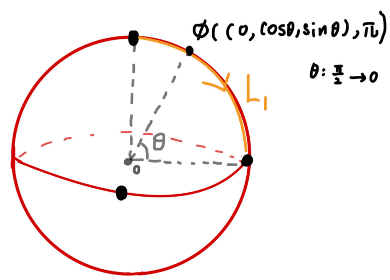

Figure 5: loop L_1

which is parametrized by θ.

So evolution of eigenframe on loop L_1 is: the first eigenvector ($\hat{x}$) fixed, the second ($\hat{y}$) and third ($\hat{z}$) eigenvectors rotate by π.

8 points in Fig6 is one point. Besides, loops should be start and end at same point. Hence we only need to consider loops in Fig6.

Conclution 3.6. All nontrivial loops can be represented by loops(yellow lines) in Fig6 (We omit arrows)

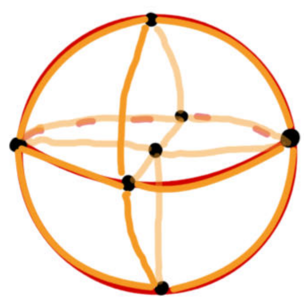

Figure 6: “Base loops” in $SO(3)/D_2$

To illustrate $\pi_1(SO(3)/D_2)$, we have the following obvious properties:

- $L_1 = L_4$. Indeed, in L_1, $\hat{y}$ and $\hat{z}$ rotate clockwise, while in L_4^{-1}, $\hat{y}$ and $\hat{z}$ rotate counterclockwise. Hence, $L_1 = (L_4^{-1})^{-1} = L_4$

  Corollary 3.7. $L_1 = L_2 = L_3 = L_4$

  Proof. By step(2) of Conclusion 2.5, we have $L_3 = L_1$ and $L_2 = L_4$. By Corollary 3.6, $L_2 = L_1$. □

  Corollary 3.8. The order $|L_1| = 4$

  Proof. $L_1^4 = L_1L_2L_3L_4$ =trivial loop and obviously $L_1^2, L_1^3 \neq$ trivial loop. □

  Corollary 3.9. $L_1^2 = -1$

  Proof. $L_1^4 = 1$ so $L_1^2 = -1$ □

- Similarly, $L_7 = L_8$ and $|L_7| = 4$. Hence, we can only focus on the 1/8 ball. We've known $\pi_1(SO(3)/D_2) \simeq Q$, so the visualizing of $\pi_1(SO(3)/D_2)$ is as in Fig7:

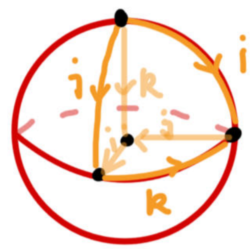

Figure 7: $\pi_1(SO(3)/D_2)$

Remark 3.10. Note that I only choose a special element to illustrate prperties. For example, if I prove $L_1 = L_2$, we also have $L_5 = L_9$ in Fig4.

Reasonable Guess: When two eigenvectors rotate π, there is a degeneracy of these two bands. Besides, we should consider orientations. For example, on L_1 (resp. L_2), $\hat{y}$ and $\hat{z}$ rotate π, so L_1 (resp. L_2) (loop of charge i) encloses a degeneracy formed by the second and third band with orientation $+$. In contrast, L_1^{-1} encloses a degeneracy formed by the second and third bands with orientation $-$. (Reference [1] thinks it is right, but I do not know why.)

Remark 3.11. For loop -1, evolution of eigenframe end at the initial state, one may think it's a trivial loop, which is wrong. It is like a spin in physics, which should rotate 4π to return to the initial. Rotate 2π is just $-1 \neq 1$.

Relationship between [1,Fig.3A to C] "Two NLs of the same orientation between the same pair of bands are described by $\{-1\}$[1]". With the guess, the loop L_1L_2 encloses two degeneracies with the same orientation formed by **second and third band**. So L_1L_2 is the charge of -1. A similar analysis shows that L_7L_8 is the loop encloses two degeneracies with the same orientation formed by **first and second bands**. The transformation in [1,Fig.3A to C] is the deformation from L_7L_8 to L_1L_2 on our ball, i.e., from $k^2 = -1$ to $i^2 = -1$ (see Fig**??**(b)).

4 Further discussion

This visualization is useful because **the $SO(3)/D_2$ ball combines the rotation behaviors of frames to the loop which plays same role as bundle**. I think it's a nice picture.

For nonHermitian case, if we can find a group, whose loop contain both information of evolution of hermitian and evolution of eigenframes, then same trick can be played. However, it seems difficult to find such a group.

References

[1] QuanSheng Wu, Alexey A. Soluyanov, and Tomáš Bzdušek. Non-Abelian band topology in noninteracting metals. Science, 365:1273–1277, 2019

[2] [Online] Available at: `https://zhuanlan.zhihu.com/p/462935097?utm_medium=social&utm_psn=1793394524518756352&utm_source=wechat_session`.