A Discrete Formulation of Three Dimensional Winding Number

Ken Shiozaki

YITP, Kyoto University

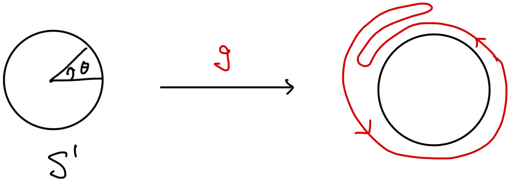
May 31, 2024, @NYU ABU DHABI

Based on K.S., arXiv:2403.05291.

1D Winding number

- Consider a continuous map from S^1 to $U(1)$:

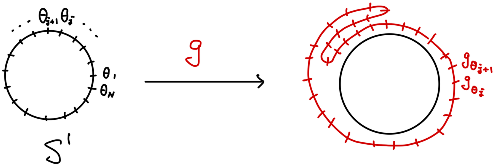
$$g : S^1 \to U(1), \quad \theta \mapsto g_\theta \in U(1).$$



- Winding number is defined as How many times this map winds over $U(1)$.
- If g is smooth, the winding number is written as an integral form

$$W_1[g] = \frac{1}{2\pi} \oint d\theta \frac{\partial}{\partial\theta} \log g_\theta \in \mathbb{Z}.$$

1D Winding number (cont.)



- The winding number W_1 can also be written as the discrete sum of small angles:
- Approximate S^1 with a set of vertices $0 = \theta_1 < \theta_2 < \cdots < \theta_N < \theta_{N+1} = 2\pi$, then,

$$W_1^{\text{dis}}\left[\{g_{\theta_j}\}_{j=1}^N\right] = \frac{1}{2\pi i}\sum_{j=1}^N \log(g_{\theta_{j+1}}/g_{\theta_j}) \in \mathbb{Z}.$$

- Nice points:
  - The small angle $\log(g_{\theta_{j+1}}/g_{\theta_j})$ has no $2\pi i$ ambiguity, if g_{θ_j} and $g_{\theta_{j+1}}$ is close enough.
  - The quantization is manifest. Since

$$e^{2\pi i W_1^{\text{dis}}\left[\{g_{\theta_j}\}_{j=1}^N\right]} = \prod_{j=1}^N (g_{\theta_{j+1}}/g_{\theta_j}) \equiv 1.$$

Winding number in general

- The winding number is generalized to continuous and oriented maps from any odd-dimensional close manifold X_{2n+1} to $U(N)$

$$g : X_{2n+1} \to U(N).$$

- $\pi_{2n+1}[U(N \to \infty)] = \mathbb{Z}$.
- For smooth maps, the winding number is given by

$$W_{2n+1}[g] = \frac{n!}{(2n+1)!(2\pi i)^{n+1}} \int_{X_{2n+1}} \mathrm{tr}\left[(g^\dagger dg)^{2n+1}\right] \in \mathbb{Z}.$$

- Question: Is there a discrete formula for the winding number $W_{2n+1}[g]$?
- My definition of a discrete formula:

> (i) Based on a lattice approximation Λ of the manifold X_{2n+1}.
> (ii) The computational cost is $O(|\Lambda|)$, the number of vertices of lattice Λ.
> (iii) manifestly quantized.

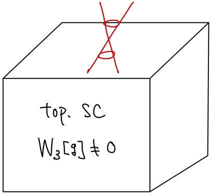
- We found a discrete formula of this sense for $W_3[g]$, the 3D winding number.

Why 3D winding number? Ex. topological band theory

- 3D time-reversal invariant topological superconductors are classified by $\mathbb{Z}$ and characterized by $W_3[g]$ with

$$g : T^3 \to \mathrm{GL}_N(\mathbb{C}), \quad g_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} + i\delta_{\boldsymbol{k}}.$$

  Here, $\boldsymbol{k} \in T^3$ lives in 3D Brillouin zone torus, $\varepsilon_{\boldsymbol{k}}$ is the normal part of the electron (Bloch Hamiltonian), and $\delta_{\boldsymbol{k}}$ comes from the superconducting gap function.
- $W_3[g]$ gapless Majorana Weyl fermions appear on the sample boundary.



Why 3D winding number? Ex. topological band theory (cont.)

- For example, the He-B phase is known to have $W_3[g] = 1$, where $g_{\boldsymbol{k}}$ is given from

$$\varepsilon_{\boldsymbol{k}} = \frac{\boldsymbol{k}^2}{2m} - \mu, \quad \delta_{\boldsymbol{k}} = \frac{\Delta}{v_F}\boldsymbol{k} \cdot \boldsymbol{\sigma}.$$

- But in numerical calculations such as first-principle calculation, the Bloch Hamiltonian $\varepsilon_{\boldsymbol{k}}$ is not written as a function over the Brillouin zone torus, but just a data of matrices over a discretized Brillouin zone torus.
- So, a discrete calculation formula of $W_3[g]$ is desirable.

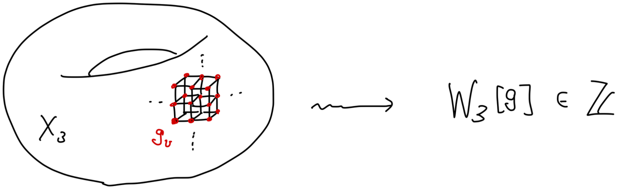
What we want to do

Input data:

- Λ: a lattice approximation of 3D oriented and closed manifold X_3.
- $\{g_v\}_{v\in\Lambda}$, a set of $U(N)$ matrices over Λ.
- For any adjacent vertices v, v', unitary matrices g_v and $g_{v'}$ are close to each other. For example, $||I_N - g_v^\dagger g_{v'}|| < \delta$ with some small constant δ [1].

Output:

- 3D Winding winding number $W_3[g] \in \mathbb{Z}$.



[1] I have not established yet the upper limit of δ (Admissibility condition) so that our discrete formula works.

Strategy

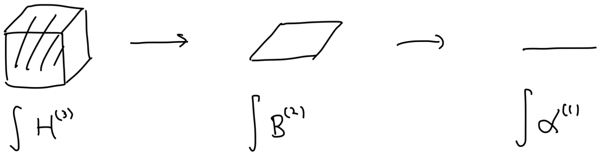
Volume integral over cube

$\Rightarrow$ Surface integral over plaquette

$\Rightarrow$ Loop integral over the boundary of plaquette (Berry phase)

$\Rightarrow$ Discrete approximation of Berry phase

$\Rightarrow$ Discrete formula of $W_3[g]$



Basic bundle gerbe

- Our derivation is a straightforward application of the *basic bundle gerbe* [2] over $SU(N)$ [Gawędzki=Reis, hep-th/0205233].

WZW BRANES AND GERBES

KRZYSZTOF GAWĘDZKI and NUNO REIS

Laboratoire de Physique, ENS-Lyon,
46, Allée d'Italie, F-69364 Lyon, France

Received 30 July 2002

- There is a canonical gerbe connection over $SU(N)$ whose 3-form curvature is $\frac{1}{24\pi^2}\mathrm{tr}\left[(g^\dagger dg)^3\right]$ representing $H^3(SU(N),\mathbb{Z}) = \mathbb{Z}$.
- Pulling back it to X_3, we have a gerbe connection over X_3.
- Cf. The usual 1-form Berry connection is given by pull back of a canonical connection over $\mathbb{C}P^\infty$.

[2] A gerbe is a "2-form $U(1)$ connection" in hep-th context.

Global 3-form → local 2-form over patch

- We begin with the integral formula of $W_3[g]$,

$$W_3[g] = \frac{1}{2\pi}\int_{X_3} H(g), \quad H(g) = \frac{1}{12\pi}\mathrm{tr}\,[(g^\dagger dg)^3].$$

- Because H is closed as $dH = 0$, there *locally* exists a 2-form B such that $H = dB$.
- Diagonilizing g,

$$g = \gamma\Lambda\gamma^\dagger, \quad \gamma \in U(N), \quad \Lambda = \mathrm{diag}(e^{i\phi_1}, \dots, e^{i\phi_N}),$$

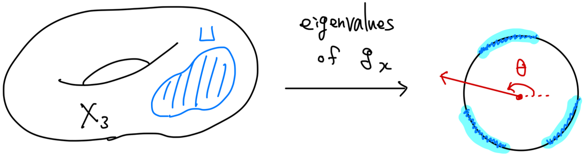
we get the 2-from B explicitly as in [Gawędzki=Reis, hep-th/0205233]

$$B = \frac{1}{4\pi}\mathrm{tr}\,[\gamma^\dagger d\gamma\Lambda\gamma^\dagger d\gamma\Lambda^{-1}] + \frac{1}{2\pi}\mathrm{tr}\,\left[(\log\Lambda)(\gamma^\dagger d\gamma)^2\right].$$

- Here, $\log\Lambda$ is ill-defined, since $\log e^{i\phi} \sim i\phi$ has the $2\pi i$ ambiguity.
- We have to fix a branch of $\log$, which is why B can not be a global 2-form.

θ-gap

- To fix a branch of $\log$, we introduce a gap condition for unitary matrices $g \in U(N)$.
- For a $\theta \in [0, 2\pi)$, we say that g_x has the θ-gap over $U \subset X_3$ if none of eigenvalues of g_x for $x \in U$ are $e^{i\theta}$ [Carpentier=Delplace=Fruchart=Gawędzki=Tauber, 1503.04157].



- If U is small enough, at least one θ-gap should be found.
- Thus, X_3 has a covering $\{U_j\}_j$ so that g_x has the θ_j-gap over U_j.

Explicit form of B and its gauge invariance

- Over a patch U_j, the 2-form is explicitly given by

$$B_{\theta_j} = \frac{1}{4\pi}\mathrm{tr}\,[\gamma^\dagger d\gamma\Lambda\gamma^\dagger d\gamma\Lambda^{-1}] + \frac{1}{2\pi}\mathrm{tr}\,[(\log_{\theta_j}\Lambda)(\gamma^\dagger d\gamma)^2], \quad x \in U_j.$$

- Here, $\log_\theta$ specifies the branch of $\log$ so that

$$\log_\theta e^{i\phi} = i\phi, \quad \theta \le \phi < \theta + 2\pi.$$

- The 1st term of B_θ is a global 2-form as it does not depend on θ.
- Remark The diagonalization unitary matrix γ is not unique as it $g = \gamma\Lambda\gamma^\dagger$ is unchanged under "gauge transformations"

$$\gamma \mapsto \gamma W, \quad W\Lambda = \Lambda W, \quad W \in U(N).$$

The 2-form B_θ is gauge-invariant.

Local 2-form over patch $\to$ Local 1-form over patch intersection

- The key property of Gawędzki-Reis's construction is that the difference of B_θ between two different θ-gaps is a total derivative.
- This occurs because the change in the branch of $\log$ is a constant:

$$\log_{\theta_1} e^{i\phi} - \log_{\theta_2} e^{i\phi} = \begin{cases} 2\pi i \times \mathrm{sgn}(\theta_1 - \theta_2) & (\min(\theta_1, \theta_2) < \phi < \max(\theta_1, \theta_2)), \\ 0 & (\text{otherwise}). \end{cases}$$

Local 2-form over patch $\to$ Local 1-form over patch intersection (cont.)

- Thus,

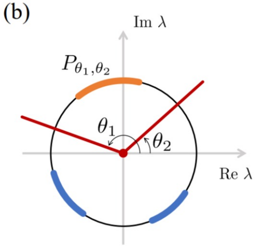
$$\log_{\theta_1} \Lambda - \log_{\theta_2} \Lambda = 2\pi i \times \operatorname{sgn}(\theta_1 - \theta_2) \times P_{\theta_1,\theta_2}.$$

  Here, P_{θ_1,θ_2} is the orthogonal projector onto the eigenspace of g_x between θ_1 and θ_2 [Carpentier=Delplace=Fruchart=Gawędzki=Tauber, 1503.04157].

- Explicitly, writing the eigenstates of g as

$$g \left|u_n\right\rangle = e^{i\phi_n} \left|u_n\right\rangle ,$$

$$P_{\theta_1,\theta_2} = \sum_{n:\min(\theta_1,\theta_2)<\phi_n<\max(\theta_1,\theta_2)} \left|u_n\right\rangle \left\langle u_n\right|$$



Local 2-form over patch $\to$ Local 1-form over patch intersection (cont.)

- Over a two patch intersection $x \in U_1 \cap U_2$, we get

$$\begin{aligned}
B_{\theta_1} - B_{\theta_2} &= \frac{1}{2\pi} \mathrm{tr}\left[(\log_{\theta_1} \Lambda - \log_{\theta_2} \Lambda)(\gamma^\dagger d\gamma)^2\right] \\
&= \frac{1}{2\pi} \mathrm{tr}\left[2\pi i \times \mathrm{sgn}(\theta_1 - \theta_2) \times P_{\theta_1,\theta_2} \times (\gamma^\dagger d\gamma)^2\right] \\
&= i \times \mathrm{sgn}(\theta_1 - \theta_2) \sum_{n:\min(\theta_1,\theta_2)<\phi_n<\max(\theta_1,\theta_2)} \sum_{m=1}^{N} \langle u_n | du_m \rangle \langle u_m | du_n \rangle \\
&= -i \times \mathrm{sgn}(\theta_1 - \theta_2) \sum_{n:\min(\theta_1,\theta_2)<\phi_n<\max(\theta_1,\theta_2)} d \langle u_n | du_n \rangle \\
&= d \left[-i \times \mathrm{sgn}(\theta_1 - \theta_2) \sum_{n:\min(\theta_1,\theta_2)<\phi_n<\max(\theta_1,\theta_2)} \langle u_n | du_n \rangle \right] \\
&=: d\alpha_{\theta_1,\theta_2}, \quad x \in U_1 \cap U_2.
\end{aligned}$$

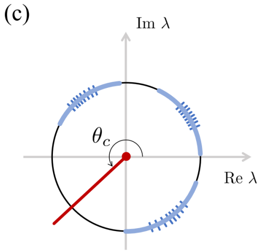
- The 1-form $\alpha_{\theta_1,\theta_2}$ is the Berry connection between θ_1 and θ_2!

Discrete formula

- Now we are ready to construct the discrete formula of $W_3[g]$.
- Give a cubic lattice approximation Λ of X_3. (Any cell decomposition works as well.)
- 3D winding number $W_3[g]$ is the sum of integrals over cubes.

$$W_3[g] = \frac{1}{2\pi} \sum_{c \in \{\text{cubes}\}} \int_c H(g).$$

- On each cube c, we pick a θ-gap parameter $\theta_c \in [0, 2\pi)$ by smearing eigenvalues over eight vertices of the corner of the cube c.



Discrete formula (cont.)

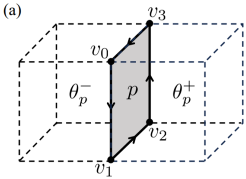
- Then, each integral can be written as a surface integral.

$$W_3[g] = \frac{1}{2\pi} \sum_{c \in \{\text{cubes}\}} \int_c dB_{\theta_c} = \frac{1}{2\pi} \sum_{c \in \{\text{cubes}\}} \int_{\partial c} B_{\theta_c}.$$

- This is further simplified to the sum of surface integrals over all plaquette.

$$W_3[g] = \frac{1}{2\pi} \sum_{p \in \{\text{plaquettes}\}} \int_p (B_{\theta_p^-} - B_{\theta_p^+}).$$

Here, θ_p^+ and θ_p^- correspond to the gap parameters of cubes adjacent to plaquette p, in directions parallel and antiparallel to p's normal vector, respectively:



Discrete formula (cont.)

- Therefore, $W_3[g]$ can be written as the sum of Berry phases of all over plaquettes.

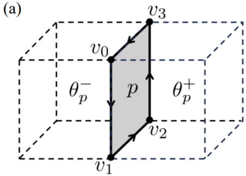
$$W_3[g] = \frac{1}{2\pi} \sum_{p \in \{\text{plaquettes}\}} \int_p d\alpha_{\theta_p^-, \theta_p^+} = \frac{1}{2\pi} \sum_{p \in \{\text{plaquettes}\}} \oint_{\partial p} \alpha_{\theta_p^-, \theta_p^+}$$

- Final step. The Berry phase over a small plaquette is approximated by the product of inner products. For example, if $\alpha_{\theta_p^-, \theta_p^+}$ is composed of a single band $|u_{n_0}\rangle$,

$$\oint_{\partial p} \alpha_{\theta_p^-, \theta_p^+} \cong \mathrm{sgn}(\theta_p^+ - \theta_p^-) \times \mathrm{Arg}\left[\prod_{j=0,1,2,3} \langle u_{n_0}(v_{j+1}) \,|\, u_{n_0}(v_j) \rangle \right] =: \Phi_p.$$

(Φ_p is defined for general cases as well.)

- The Berry flux Φ_p is small enough so that Φ_p can be considered as an $\mathbb{R}$-valued quantity, not $\mathbb{R}/2\pi\mathbb{Z}$-valued.



Discrete formula (cont.)

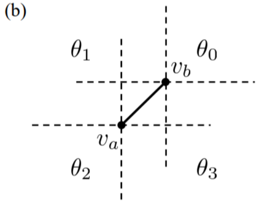
- We got the discrete formula

$$W_3^{\mathrm{dis}}[\{g\}_{v\in\Lambda}] = \frac{1}{2\pi} \sum_{p\in\{\mathrm{plaquettes}\}} \Phi_p \in \mathbb{Z}.$$

- This formula can be evaluated only by diagonalizing the matrix g over the vertices $v \in \Lambda$ approximating X_3. $\rightarrow$ the computational cost is $O(|\Lambda|)$.
- Moreover, the quantization of $W_3^{\mathrm{dis}}[\{g\}_{v\in\Lambda}]$ is manifest: We can show that

$$e^{2\pi i W_3^{\mathrm{dis}}[\{g\}_{v\in\Lambda}]} = \prod_{p\in\{\mathrm{plaquettes}\}} e^{i\Phi_p} \equiv 1,$$

using the cocycle condition around the edges. □



Sanity check

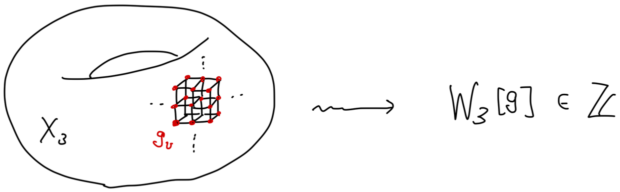
- We have checked that the discrete formula $W_3^{\rm dis}[g]$ does works only for a simple 2×2 model

$$g_{\boldsymbol{k}} = \sum_{\mu=x,y,z} \sin k_\mu \sigma_\mu - i(m + \sum_{\mu=x,y,z} \cos k_\mu) \mathbf{1}_2$$
$$+ (\text{small random } \boldsymbol{k}\text{-dependent perturbation}).$$

Without perturbation, $W_3[g] = -2$ for $|m| < 1$, $W_3[g] = 1$ for $1 < |m| < 3$, and $W_3[g] = 0$ else.

Summary and Outlook

- We proposed a discrete formula for the 3D winding number $W_3[g]$, a generalization of the Fukui-Hatsugai-Suzuki formula for the 1st Chern number ch_1.
- The numerical cost is $O(|\Lambda|)$, where $|\Lambda|$ is the number of mesh vertices.



- It is interesting to generalize the discrete formula for the 2nd Chern number ch_2. Can ch_2 be written only with the set of points of the Grassmann manifold over mesh vertices of a 4-manifold X_4? Does the 2-gerbe structure of the Chern-Simons 3-form help us in this regard?