Note: On Lattice Approximation Formulae for Topological Invariants

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May 31, 2026

Abstract

We summarize formulations of topological invariants, of the kind discussed in band theory, that are suitable for numerical computation.

1 The Case $S^1 \to U(N)$

Write a coordinate on S^1 as $k \in [0, 2\pi]$, identifying $k = 2\pi$ with $k = 0$. Consider a continuous map

$$g : S^1 \to U(N), \quad k \mapsto g_k, \tag{1}$$

The degree of g, or the "one-dimensional winding number" $W_1[g]$, is defined by how many times the $U(1)$ phase $\det g_k$ winds. If g is smooth, it is given by

$$W_1[g] = \frac{1}{2\pi i} \oint_0^{2\pi} d \log \det g_k = \frac{1}{2\pi i} \oint_0^{2\pi} \mathrm{tr}\, [g_k^\dagger f g_k] \in \mathbb{Z} \tag{2}$$

In numerical calculations in band theory and related settings, one often does not have an explicit expression for the $U(N)$-valued function g_k; instead, it is given only on a set of lattice points Λ approximating S^1. For example, take

$$\Lambda = \{k = \frac{2\pi n}{L} \in [0, 2\pi] | n = 0, \dots, L-1\} \tag{3}$$

and consider data consisting of L matrices in $U(N)$,

$$\{g_k\}_{k \in \Lambda} \tag{4}$$

in a situation where neighboring $U(N)$ values g_k and g_{k+1} are sufficiently "close." More precisely, "close" means that the two points g_k, g_{k+1} satisfy a condition under which the continuous interpolation between them is unique. For instance, if

$$g_{k+1} g_k^\dagger = \gamma \mathrm{diag}(e^{i\theta_1}, \dots, e^{i\theta_N}) \gamma^\dagger \tag{5}$$

is a diagonalization and the arguments θ_n of all eigenvalues $e^{i\theta_n}$, $n = 1, \dots, N$, satisfy $-\pi + \theta_{\mathrm{gap}} < \theta_n < \pi - \theta_{\mathrm{gap}}$ for some finite constant $\theta_{\mathrm{gap}} > 0$, then g_k and g_{k+1} can be interpolated uniquely:

$$g_{k+t} = \gamma \mathrm{diag}(e^{it\theta_1}, \dots, e^{it\theta_N}) \gamma^\dagger g_k, \quad t \in [0, 1]. \tag{6}$$

A finite θ_{gap} also guarantees numerical stability. If a continuous function g_k, $k \in S^1$, is uniquely interpolated from the set of $U(N)$ values $\{g_k\}_{k \in \Lambda}$ on lattice points, then the degree $W_1[g]$ is defined even when g_k itself is specified only on the lattice.

The problem is the following.

Let $|\Lambda|$ be the number of points in the lattice Λ. Give an algorithm which computes the degree $W_1[g]$ from the lattice data $\{g_k\}_\Lambda$, is quantized, and has computational cost $O(|\Lambda|)$.[a] Here "quantized" means that the result is always an integer.

[a]It was pointed out that, if polynomial time in $|\Lambda|$ were allowed, one could couple to Wilson–Dirac fermions and look at spectral flow, or construct overlap fermions and compute the index. I therefore changed the requirement to $O(|\Lambda|)$.

We call an algorithm, or a formula for an invariant, satisfying the above requirements simply a lattice approximation formula.

For $W_1[g]$ there is a simple method. Divide the integral into intervals and rewrite it as a sum over pieces. Write the lattice approximation formula for the topological invariant $W_1[g]$ as $W_1^{\rm lat}[g]$.

$$W_1^{\rm lat}[g] = \frac{1}{2\pi}\sum_{k=0}^{L-1} \mathrm{Arg}(\det g_{k+1}/\det g_k) \tag{7}$$

is sufficient. Here $-\pi \leq \mathrm{Arg}\ z < \pi$. Quantization is guaranteed because

$$e^{2\pi i W_1^{\rm lat}[g]} = \prod_{k=0}^{L-1} \det g_{k+1}/\det g_k = 1 \tag{8}$$

2 $X_2 \to \mathrm{Gr}_N(\mathbb{C}^{N+M})$

As a nontrivial example, consider the degree of a map to a Grassmannian. Let X_2 be an oriented closed two-dimensional manifold, and let $\mathrm{Gr}_N(\mathbb{C}^{N+M}) = U(N+M)/(U(N)\times U(M))$ be the complex Grassmannian. Consider a smooth map

$$P : X_2 \to \mathrm{Gr}_N(\mathbb{C}^{N+M}), \quad X_2 \ni k \mapsto P_k, \tag{9}$$

As a concrete representation of P_k, take it to be an orthogonal projection of rank N in the space of $(N+M)\times(N+M)$ matrices:

$$P_k \in \mathrm{Mat}_{(N+M)\times(N+M)}(\mathbb{C}), \quad \mathrm{rank}[P_k] = N, \quad P_k^2 = P_k, \quad P_k^\dagger = P_k. \tag{10}$$

Here $P_k^\dagger$ denotes the Hermitian conjugate of the matrix P_k. The degree of P, namely the first Chern character, is given by

$$ch_1[P] = \frac{i}{2\pi}\int_{X_2} \mathrm{Tr}[PdPdP] \in \mathbb{Z}. \tag{11}$$

In band theory, the lattice approximation formula for $ch_1[P]$ is known as the Fukui–Hatsugai–Suzuki formula [1]. We recall the construction. Approximate X_2 by a triangulation, and denote the set of vertices by Λ. An arbitrary polygonal decomposition would also be fine. Each triangle of the lattice Λ is assumed to be sufficiently "small" to satisfy the condition stated below. For each triangle Δ^2, choose a "local trivialization" $\Phi_{\Delta^2,k}$ of P_k, $k \in \Delta^2$:

$$P_k = \Phi_{\Delta^2,k}\Phi_{\Delta^2,k}^\dagger, \quad k \in \Delta^2. \tag{12}$$

Here $\Phi_{\Delta^2,k}$ is an orthonormal frame satisfying $\Phi_{\Delta^2,k}^\dagger\Phi_{\Delta^2,k} = 1_N$. A direct calculation gives

$$\mathrm{Tr}[PdPdP] = d\ \mathrm{tr}\,[\Phi_{\Delta^2}^\dagger d\Phi_{\Delta^2}], \quad k \in \Delta^2, \tag{13}$$

where tr is the trace over $N\times N$ matrices. This gives the expression

$$ch_1[P] = \frac{i}{2\pi}\sum_{\Delta^2}\int_{\Delta^2} d\ \mathrm{tr}\,[\Phi_{\Delta^2}^\dagger d\Phi_{\Delta^2}] \tag{14}$$

$$= \frac{i}{2\pi}\sum_{\Delta^2}\oint_{\partial\Delta^2} \mathrm{tr}\,[\Phi_{\Delta^2}^\dagger d\Phi_{\Delta^2}] \tag{15}$$

Note that the second equality is valid only when $\Phi_{\Delta^2,k}$ is defined continuously also in the interior of the triangle Δ^2. If $\Phi_{\Delta^2,k}$ is defined continuously only on the boundary $k \in \partial\Delta^2$ of the triangle, the line integral has an ambiguity by 2π:

$$\oint_{\partial\Delta^2} i\mathrm{tr}\,[\Phi^\dagger_{\Delta^2} d\Phi_{\Delta^2}] \sim \oint_{\partial\Delta^2} i\mathrm{tr}\,[\Phi^\dagger_{\Delta^2} d\Phi_{\Delta^2}] + 2\pi. \tag{16}$$

In other words, the $U(1)$ phase

$$z_{\Delta^2} := \exp\left[-\oint_{\partial\Delta^2} \mathrm{tr}\,[\Phi^\dagger_{\Delta^2} d\Phi_{\Delta^2}]\right] \in U(1) \tag{17}$$

is well-defined even when the local trivialization $\Phi_{\Delta^2,k}$ is given only on the boundary $\partial\Delta^2$.

Write the vertices of a triangle as $\Delta^2 = (v_0v_1v_2)$. The $U(1)$ phase z_{Δ^2} can be approximated using only the local trivializations $\Phi_{v_0}, \Phi_{v_1}, \Phi_{v_2}$ at the vertices v_0, v_1, v_2:

$$\begin{aligned} z_{\Delta^2} \cong z^{\mathrm{lat}}_{\Delta^2} &:= \exp\left[i \arg\det[\Phi^\dagger_{v_0}\Phi_{v_2}\Phi^\dagger_{v_2}\Phi_{v_1}\Phi^\dagger_{v_1}\Phi_{v_0}]\right] && (18)\\ &= \exp\left[i \arg\det[\Phi^\dagger_{v_0}\Phi_{v_2}]\det[\Phi^\dagger_{v_2}\Phi_{v_1}]\det[\Phi^\dagger_{v_1}\Phi_{v_0}]\right]. && (19)\end{aligned}$$

The $U(1)$ phase $z^{\mathrm{lat}}_{\Delta^2}$ can also be obtained without introducing the local trivializations Φ_v, using only the orthogonal projections P_v at the vertices:

$$z^{\mathrm{lat}}_{\Delta^2} = Z[P_{v_2}P_{v_1}P_{v_0}] \tag{20}$$

Here, for a diagonalizable square matrix A, $Z[A]$ is defined as the product of the nonzero eigenvalues of A, namely

$$Z[A] := \prod_{\lambda\in\mathrm{Spec}(A),\lambda\neq 0} \lambda. \tag{21}$$

We write $\mathrm{Spec}(A)$ for the set of eigenvalues of A, counted with multiplicity. Assume that the lattice Λ is sufficiently "fine" to satisfy the following condition: there exists a finite $\theta_{\mathrm{gap}} > 0$ such that

$$|\mathrm{Arg}\ z^{\mathrm{lat}}_{\Delta^2}| < \pi - \theta_{\mathrm{gap}}. \tag{22}$$

Under this condition, the argument is defined as a numerically stable real number. Thus the lattice approximation formula for $ch_1[P]$ is obtained as

$$ch^{\mathrm{lat}}_1[P] := \frac{1}{2\pi}\sum_{\Delta^2} \mathrm{Arg}\ z^{\mathrm{lat}}_{\Delta^2}. \tag{23}$$

The quantization $ch^{\mathrm{lat}}_1[P] \in \mathbb{Z}$ follows from

$$e^{2\pi i ch^{\mathrm{lat}}_1[P]} = \prod_{\Delta^2} z^{\mathrm{lat}}_{\Delta^2} = \prod_{\Delta^2}\prod_{v_0v_1\in\mathrm{edges\ in}\ \partial\Delta^2} \exp i \arg\det[\Phi^\dagger_{v_1}\Phi_{v_0}] \tag{24}$$

because the contributions associated with each edge v_0v_1 cancel between the two adjacent triangles, giving $e^{2\pi i ch^{\mathrm{lat}}_1[P]} = 1$.

3 $X_3 \to U(N)$

Let X_3 be an oriented closed three-dimensional manifold. Consider a smooth map

$$g : X_3 \to U(N), \quad X_3 \ni k \mapsto g_k, \tag{25}$$

The degree, or the "three-dimensional winding number," is

$$W_3[g] = \frac{1}{24\pi^2}\int_{X_3} \mathrm{tr}\,[(g^\dagger dg)^3] \in \mathbb{Z} \tag{26}$$

The 3-form $\frac{1}{24\pi^2}\mathrm{tr}\,[(g^\dagger dg)^3]$ represents the generator of the de Rham cohomology $H_{\mathrm{dR}}[U(N)]$ corresponding to the generator of $H^3[U(N),\mathbb{Z}] = \mathbb{Z}$.

The lattice approximation formula for $W_3[g]$ is given in [2].

4 $X_4 \to \mathrm{Gr}_N(\mathbb{C}^{N+M})$: An Example of an Open Problem

Let X_4 be an oriented closed four-dimensional manifold, and let $\mathrm{Gr}_N(\mathbb{C}^{N+M}) = U(N+M)/(U(N) \times U(M))$ be the complex Grassmannian. Consider a smooth map

$$P : X_4 \to \mathrm{Gr}_N(\mathbb{C}^{N+M}), \quad X_4 \ni k \mapsto P_k, \tag{27}$$

$$P_k \in \mathrm{Mat}_{(N+M)\times(N+M)}(\mathbb{C}), \quad \mathrm{rank}[P_k] = N, \quad P_k^2 = P_k, \quad P_k^\dagger = P_k, \tag{28}$$

The degree of P, namely the second Chern character, is given by

$$ch_2[P] = \frac{1}{2}(\frac{i}{2\pi})^2 \int_{X_4} \mathrm{Tr}[P(dPdP)^2]. \tag{29}$$

The quantized value depends on the global structure of X_4. For example, when $X_4 = S^4$ or T^4, one has $ch_2[P] \in \mathbb{Z}$. A lattice approximation formula for $ch_2[P]$ is an open problem.

5 A More General Problem Setting

For the ten classifying spaces of K-theory and KO-theory, and for a manifold X of general dimension, lattice approximation formulae for topological invariants are mostly open problems. The ten spaces are given as follows:

C_0	$\cup_M \lim_{N\to\infty} U(2N)/U(2N-M) \times U(2N+M)$
C_1	$\lim_{N\to\infty} U(N)$
R_0	$\cup_M \lim_{N\to\infty} O(2N)/O(2N-M) \times O(2N+M)$
R_1	$\lim_{N\to\infty} O(N)$
R_2	$\lim_{N\to\infty} O(2N)/U(N)$
R_3	$\lim_{N\to\infty} U(2N)/Sp(N)$
R_4	$\cup_M \lim_{N\to\infty} Sp(2N)/Sp(2N-M) \times Sp(2N+M)$
R_5	$\lim_{N\to\infty} Sp(N)$
R_6	$\lim_{N\to\infty} Sp(N)/U(N)$
R_7	$\lim_{N\to\infty} U(N)/O(N)$

Here

$$Sp(N) = \{g \in U(2N) | i\sigma_y g^* (i\sigma_y)^\dagger = g\}, \quad i\sigma_y = \begin{pmatrix} & 1_N \\ -1_N & \end{pmatrix}, \tag{30}$$

is the symplectic group. For a matrix A, we write A^* for its complex conjugate. The spaces C_n are the classifying spaces of K-theory, and the spaces R_n are the classifying spaces of KO-theory.

$$K^{-n}(X) = [X, C_n], \tag{31}$$

$$KO^{-n}(X) = [X, R_n]. \tag{32}$$

In particular, the classification over spheres is given by

$$\tilde{K}^{-n}(S^p) = K^{-n}(X, pt) = \pi_p[C_n] = \pi_0[C_{n+p}], \tag{33}$$

$$\tilde{KO}^{-n}(S^p) = KO^{-n}(X, pt) = \pi_p[R_n] = \pi_0[R_{n+p}], \tag{34}$$

n mod 2	0	1
$\pi_0[C_n]$	$\mathbb{Z}$	0

n mod 8	0	1	2	3	4	5	6	7
$\pi_0[R_n]$	$\mathbb{Z}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	$2\mathbb{Z}$	0	0	0

Points of the ten spaces are realized either by Hermitian matrices $h^\dagger = h$ satisfying $h^2 = 1$ (that is, matrices with eigenvalues ± 1), or by $U(N)$-valued matrices $q \in U(N)$, with additional constraints imposed when necessary. The conditions are summarized as follows:

C_0	h, no constraint
C_1	q, no constraint
R_0	$h, h^* = h$
R_1	$q, q^* = q$
R_2	$h, h^* = -h$
R_3	$q, q^\top = -q$
R_4	$h, (i\sigma_y)h^*(i\sigma_y)^\dagger = h$
R_5	$q, (i\sigma_y)q^*(i\sigma_y)^\dagger = q$
R_6	$h, (i\sigma_y)h^*(i\sigma_y)^\dagger = -h$
R_7	$q, q^\top = q$

The problem is:

For given h, q, give lattice approximation formulae for the topological invariants that characterize the K- and KO-groups.

References

[1] Takahiro Fukui, Yasuhiro Hatsugai, Hiroshi Suzuki, *Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances*, arXiv:cond-mat/0503172.

[2] KS, *A discrete formulation for three-dimensional winding number*, arXiv:2403.05291.