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Symmetric Fermi projections and Kitaev's table: topological phases of matter in low dimensions

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We review Kitaev's celebrated "periodic table" for topological phases of condensed matter, which identifies ground states (Fermi projections) of gapped periodic quantum systems up to continuous deformations. We study families of projections which depend on a periodic crystal momentum and respect the symmetries that characterize the various classes of topological insulators. Our aim is to classify such families in a systematic, explicit, and constructive way: we identify numerical indices for all symmetry classes and provide algorithms to deform families of projections whose indices agree. Aiming at simplicity, we illustrate the method for 0- and 1-dimensional systems, and recover the (weak and strong) topological invariants proposed by Kitaev and others.

I. INTRODUCTION

The goal of the present article is to re-derive the classification of topological phases of quantum matter proposed by Kitaev in his "periodic table" [27] by means of basic tools from the topology (in particular homotopy theory) of classical groups, and standard factorization results in linear algebra. Kitaev's table classifies ground states of free-fermion systems according to their symmetries and the dimension of the configuration space. We reformulate the classification scheme in terms of homotopy theory, and proceed to investigate the latter issue in dimension $d \in \{0, 1\}$. We restrict ourselves to low dimensions in order to illustrate our approach, and to provide constructive proofs for all the classes, using explicit factorization of the matrices that appear. Our intent is thus similar to previous works by Zirnbauer and collaborators [19, 24, 25], which however formulate the notion of free-fermion ground state in a different way, amenable to the investigation of many-body systems.

The Kitaev classification can be obtained in various ways, using different mathematical tools. Let us mention for instance derivations coming from index theory [17], K-theory [31, 34] and KK-theory [4]. In addition to this (non-exhaustive) list, one should add the numerous works focusing on one particular case of the table. Our goal here is to provide a short and synthetic derivation of this table, using simple linear algebra.

A. Setting

Let \mathcal{H} be a complex Hilbert space of finite dimension dim $\mathcal{H} = N$. For $0 \le n \le N$, *n*-dimensional subspaces of \mathcal{H} are in one-to-one correspondence with elements of the *Grassmannian*

$$\mathcal{G}_n(\mathcal{H}) := \left\{ P \in \mathcal{B}(\mathcal{H}) : P^2 = P = P^*, \operatorname{Tr}(P) = n \right\}$$

which is comprised of rank-*n* orthogonal projections in the algebra $\mathcal{B}(\mathcal{H})$ of linear operators on \mathcal{H} . In this paper we are interested in orthogonal-projection-valued continuous functions $P : \mathbb{T}^d \to \mathcal{G}_n(\mathcal{H})$ which satisfy certain symmetry conditions (to be listed below), and in classifying homotopy classes of such maps. Here $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$ is a *d*-dimensional torus, which we often identify with $[-\frac{1}{2}, \frac{1}{2}]^d$ with periodic boundary conditions. We write $k \ni \mathbb{T}^d \mapsto P(k) \in \mathcal{G}_n(\mathcal{H})$ for such maps, or $\{P(k)\}_{k \in \mathbb{T}^d}$.



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The discrete symmetries that one may want to impose on a family of projections come from those of the underlying quantum-mechanical system. We set the following definitions. Recall that a map $T : \mathcal{H} \to \mathcal{H}$ is anti-unitary if it is anti-linear $(T(\lambda x) = \overline{\lambda}T(x))$ and

$$\forall x, y \in \mathcal{H}, \quad \langle Tx, Ty \rangle_{\mathcal{H}} = \langle y, x \rangle_{\mathcal{H}} \qquad (= \overline{\langle x, y \rangle_{\mathcal{H}}}).$$

Definition I.1 (Time-reversal symmetry). Let $T : \mathcal{H} \to \mathcal{H}$ be an anti-unitary operator such that $T^2 = \varepsilon_T \mathbb{I}_{\mathcal{H}}$ with $\varepsilon_T \in \{-1, 1\}$. We say that a continuous map $P : \mathbb{T}^d \to \mathcal{G}_n(\mathcal{H})$ satisfies **time-reversal symmetry**, or in short T-symmetry, if

$$T^{-1}P(k)T = P(-k),$$
 (*T*-symmetry).

If $\varepsilon_T = 1$, this T-symmetry is said to even, and if $\varepsilon_T = -1$ it is odd.

Definition I.2 (Charge-conjugation/particle-hole symmetry). Let $C : \mathcal{H} \to \mathcal{H}$ be an anti-unitary operator such that $C^2 = \varepsilon_C \mathbb{I}_{\mathcal{H}}$ with $\varepsilon_C \in \{-1, 1\}$. We say that a continuous map $P : \mathbb{T}^d \to \mathcal{G}_n(\mathcal{H})$ satisfies charge-conjugation symmetry (also called particle-hole symmetry), or in short C-symmetry, if

$$C^{-1}P(k)C = \mathbb{I}_{\mathcal{H}} - P(-k), \quad (C\text{-symmetry}).$$

If $\varepsilon_C = 1$, this C-symmetry is said to even, and if $\varepsilon_C = -1$ it is odd.

Definition I.3 (Chiral symmetry). Let $S : \mathcal{H} \to \mathcal{H}$ be a unitary operator such that $S^2 = \mathbb{I}_{\mathcal{H}}$. We say that $P : \mathbb{T}^d \to \mathcal{G}_n(\mathcal{H})$ satisfies chiral or sublattice symmetry, or in short S-symmetry, if

$$S^{-1}P(k)S = \mathbb{I}_{\mathcal{H}} - P(k), \quad (S\text{-symmetry}).$$

The simultaneous presence of two symmetries implies the presence of the third. In fact, the following assumption is often postulated [32]:

Assumption I.4. Whenever T- and C- symmetries are both present, we assume that their product S := TC is an S-symmetry, that is, S is unitary and $S^2 = \mathbb{I}_{\mathcal{H}}$.

We are not aware of a model in which this assumption is not satisfied, *i.e.* in which the S symmetry is unrelated to the T- and C- ones.

Remark I.5. This assumption is tantamount to require that the operators T and C commute or anti-commute among each other, depending on their even/odd nature. Indeed, the product of two anti-unitary operators is unitary, and the requirement that S := TC satisfies $S^2 = \mathbb{I}_{\mathcal{H}}$ reads

$$TCTC = \mathbb{I}_{\mathcal{H}} \iff TC = C^{-1}T^{-1} = \varepsilon_T \varepsilon_C CT.$$

The same sign determines whether S commutes or anti-commutes with T and C. Indeed, we have

$$SC = TC^2 = \varepsilon_C T, \quad CS = CTC = T^{-1}C^{-1}C = \varepsilon_T T \quad so \quad SC = \varepsilon_T \varepsilon_C CS,$$

and similarly $ST = \varepsilon_T \varepsilon_C TS$.

Taking into account all possible types of symmetries leads to 10 symmetry classes for maps $P: \mathbb{T}^d \to \mathcal{G}_n(\mathcal{H})$, the famous *tenfold way of topological insulators* [32]. The names of these classes are given in Table I, and are taken from the original works of E. Cartan [5, 6] for the classification of symmetric spaces, which were originally mutuated in [1, 19] in the context of random-matrix-valued σ -models. For a dimension $d \in \mathbb{N} \cup \{0\}$ and a rank $n \in \mathbb{N}$, and for a Cartan label X of one of these 10 symmetry classes, we denote by X(d, n, N) the set of continuous maps $P: \mathbb{T}^d \to \mathcal{G}_n(\mathcal{H})$, with dim $(\mathcal{H}) = N$, and respecting the symmetry requirements of class X.

Given two continuous maps $P_0, P_1 \in X(d, n, N)$, we ask the following questions:



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- Can we find explicit Index \equiv Index^X_d maps, which are numerical functions (integer- or integer-mod-2-valued) so that Index(P_0) = Index(P_1) iff P_0 and P_1 are path-connected in X(d, n, N)?
- If so, how to compute this Index?
- In the case where $\operatorname{Index}(P_0) = \operatorname{Index}(P_1)$, how to construct explicitly a path P_s , $s \in [0, 1]$ connecting P_0 and P_1 in X(d, n, N)?

In this paper, we answer these questions for all the 10 symmetry classes, and for $d \in \{0, 1\}$. We analyze the classes one by one, often choosing a basis for \mathcal{H} in which the different symmetry operators T, C and S have a specific normal form. In doing so, we recover Cartan's symmetric spaces as X(d = 0, n, N) – see the boxed equations in the body of the paper. The topological indices that we find are summarized in Table I (we make no claim on the group-homomorphism nature of the Index maps we provide). Our findings agree with the previously mentioned "periodic tables" from the physics literature [27, 32] if one also takes into account the weak \mathbb{Z}_2 invariants (see Remark III.8). We note that the d = 0 column is not part of the original table. It is related (but not equal) to the d = 8 column by Bott periodicity [3]. For our purpose, it is useful to have it explicitly in order to derive the d = 1 column.

Symmetry				Constraints		Indices	
Cartan label	T	C	S	n	N	d = 0	d = 1
Α	0	0	0			0	0
AIII	0	0	1		N = 2n	0	\mathbb{Z}
AI	1	0	0			0	0
BDI	1	1	1		N = 2n	\mathbb{Z}_2	$\mathbb{Z}_2 \times \mathbb{Z}$
D	0	1	0		N = 2n	\mathbb{Z}_2	$\mathbb{Z}_2 \times \mathbb{Z}_2$
DIII	-1	1	1	$n=2m\in 2\mathbb{N}$	N=2n=4m	0	\mathbb{Z}_2
AII	-1	0	0	$n=2m\in 2\mathbb{N}$	$N=2M\in 2\mathbb{N}$	0	0
CII	-1	-1	1	$n=2m\in 2\mathbb{N}$	N=2n=4m	0	\mathbb{Z}
С	0	-1	0		N = 2n	0	0
CI	1	-1	1		N = 2n	0	0

Table I: A summary of our main results on the topological "Indices" of the various symmetry classes of Fermi projections. In the "Symmetry" column, we list the sign characterizing the symmetry as even or odd; an entry "0" means that the symmetry is absent. Some "Constraints" may be needed for the symmetry class X(d, n, N) to be non-empty.

B. Notation

For $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, we denote by $\mathcal{M}_N(\mathbb{K})$ the set of $N \times N$ \mathbb{K} -valued matrices. We denote by $K \equiv K_N : \mathbb{C}^N \to \mathbb{C}^N$ the usual complex conjugation operator. For a complex matrix $A \in \mathcal{M}_N(\mathbb{C})$, we set $\overline{A} := KAK$ and $A^T := \overline{A^*}$, where A^* is the adjoint matrix of A for the standard scalar product on \mathbb{C}^N .

We then denote by $\mathcal{S}_N(\mathbb{K})$ the set of hermitian matrices $(A = A^*)$, and by $\mathcal{A}_N(\mathbb{K})$ the one of skew-hermitian matrices $(A = -A^*)$. When $\mathbb{K} = \mathbb{C}$, we sometimes drop the notation \mathbb{C} . Also, we denote by $\mathcal{S}_N^{\mathbb{R}}(\mathbb{C})$ and $\mathcal{A}_N^{\mathbb{R}}(\mathbb{C})$ the set of symmetric $(A^T = A)$ and antisymmetric matrices $(A^T = -A)$. We denote by U(N) the subset of unitary matrices, by SU(N) the set of unitaries with determinant 1, by O(N) the subset of orthogonal matrices, and by SO(N) the subset of orthogonal matrices with determinant 1.

We denote by $\mathbb{I} \equiv \mathbb{I}_N$ the identity matrix of \mathbb{C}^N . When N = 2M is even, we also introduce the symplectic matrix

$$J \equiv J_{2M} := \begin{pmatrix} 0 & \mathbb{I}_M \\ -\mathbb{I}_M & 0 \end{pmatrix}.$$

The symplectic group $\operatorname{Sp}(2M; \mathbb{K})$ is defined by

$$\operatorname{Sp}(2M;\mathbb{K}) := \left\{ A \in \mathcal{M}_{2M}(\mathbb{K}) : A^T J_{2M} A = J_{2M} \right\}.$$
(I.1)

The *compact* symplectic group Sp(M) is

$$Sp(M) := Sp(2M; \mathbb{C}) \cap U(2M) = \{ U \in U(2M) : U^T J_{2M} U = J_{2M} \}.$$

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C. Structure of the paper

We study the classes one by one. We begin with the *complex classes* A and AIII in Section II, where no anti-unitary operator is present. We then study non-chiral *real* classes (without S-symmetry) in Section III, and chiral classes in Section IV. In Appendix A, we review some factorizations of matrices, which allow us to prove our results.

II. COMPLEX CLASSES: A AND AIII

The symmetry classes A and AIII are often dubbed as *complex*, since they do not involve any antiunitary symmetry operator, and thus any "real structure" induced by the complex conjugation. By contrast, the other 8 symmetry classes are called *real*. Complex classes where studied, for example, in [10, 31].

A. Class A

In class A, no discrete symmetry is imposed. We have in this case

Theorem II.1 (Class A). The sets A(0, n, N) and A(1, n, N) are path-connected.

Proof. Since no symmetry is imposed and $\mathbb{T}^0 = \{0\}$ consists of a single point, we have $A(0, n, N) = \mathcal{G}_n(\mathcal{H})$. It is known [22, Ch. 8, Thm. 2.2] that the complex Grassmannian is connected, hence so is A(0, n, N). This property follows from the fact that the map $U(N) \to \mathcal{G}_n(\mathcal{H})$ which to any $N \times N$ unitary matrix associates the linear span of its first *n* columns (say in the canonical basis for $\mathcal{H} \simeq \mathbb{C}^N$), viewed as orthonormal vectors in \mathcal{H} , induces a bijection

$$A(0, n, N) \simeq \mathcal{G}_n(\mathcal{H}) \simeq U(N)/U(n) \times U(N-n).$$
(II.1)

Since U(N) is connected, so is A(0, n, N).

To realize this explicitly, we fix a basis of $\mathcal{H} \simeq \mathbb{C}^N$. Let $P_0, P_1 \in A(0, n, N)$. For $j \in \{0, 1\}$, we choose a unitary $U_j \in U(N)$ such that its *n* first column vectors span the range of P_j . We then choose a self-adjoint matrix $A_j \in \mathcal{S}_N$ so that $U_j = e^{iA_j}$. We now set, for $s \in (0, 1)$,

$$U_s := e^{iA_s}, \quad A_s := (1-s)A_0 + sA_1$$

The map $s \mapsto U_s$ is continuous, takes values in U(n), and connects U_0 and U_1 . The projection P_s on the first n column vectors of U_s then connects P_0 and P_1 , as wanted.

We now prove our statement concerning A(1, n, N). Let $P_0, P_1: \mathbb{T}^1 \to \mathcal{G}_n(\mathcal{H})$ be two periodic families of projections. Recall that we identify $\mathbb{T}^1 \simeq [-1/2, 1/2]$. Consider the two projections $P_0(-\frac{1}{2}) = P_0(\frac{1}{2})$ and $P_1(-\frac{1}{2}) = P_1(\frac{1}{2})$, and connect them by some continuous path $P_s(-\frac{1}{2}) = P_s(\frac{1}{2})$ as previously. The families $P_0(k)$ and $P_1(k)$, together with the maps $P_s(-\frac{1}{2})$ and $P_s(\frac{1}{2})$, define a continuous family of projectors on the boundary $\partial\Omega$ of the square

$$\Omega := \left[-\frac{1}{2}, \frac{1}{2}\right] \times [0, 1] \ni (k, s). \tag{II.2}$$

It is a standard result (see for instance [15, Lemma 3.2] for a constructive proof) that such families can be extended continuously to the whole set Ω . This gives an homotopy $P_s(k) = P(k, s)$ between P_0 and P_1 .

B. Class AIII

In class AIII, only the S-symmetry is present. It is convenient to choose a basis in which S is diagonal. This is possible thanks to the following Lemma, which we will use several times in classes where the S-symmetry is present.

Lemma II.2. Assume AIII(d = 0, n, N) is non-empty. Then N = 2n, and there is a basis of \mathcal{H} in which S has the block-matrix form

$$S = \begin{pmatrix} \mathbb{I}_n & 0\\ 0 & -\mathbb{I}_n \end{pmatrix}.$$
 (II.3)



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In this basis, a projection P satisfies $S^{-1}PS = \mathbb{I}_{\mathcal{H}} - P$ iff it has the matrix form

$$P = \frac{1}{2} \begin{pmatrix} \mathbb{I}_n & Q \\ Q^* & \mathbb{I}_n \end{pmatrix} \quad with \quad Q \in \mathcal{U}(n).$$
(II.4)

Proof. Let $P_0 \in AIII(0, n, N)$. Since $S^{-1}P_0S = \mathbb{I}_{\mathcal{H}} - P_0$, P_0 is unitarily equivalent to $\mathbb{I}_{\mathcal{H}} - P_0$, hence $\mathcal{H} = \text{Ran } P_0 \oplus \text{Ran } (\mathbb{I}_{\mathcal{H}} - P_0)$ is of dimension N = 2n.

Let $(\psi_1, \psi_2, \cdots, \psi_n)$ be an orthonormal basis for Ran P_0 . We set

$$\forall i \in \{1, \cdots, n\}, \quad \phi_i := \frac{1}{\sqrt{2}}(\psi_i + S\psi_i), \quad \phi_{n+i} = \frac{1}{\sqrt{2}}(\psi_i - S\psi_i).$$

The family $(\phi_1, \dots, \phi_{2n})$ is an orthonormal basis of \mathcal{H} , and in this basis, S has the matrix form (II.3).

For the second point, let $P \in AIII(0, n, 2n)$, and decompose P in blocks:

$$P = \frac{1}{2} \begin{pmatrix} P_{11} & P_{12} \\ P_{12}^* & P_{22} \end{pmatrix}$$

The equation $S^{-1}PS = \mathbb{I}_{\mathcal{H}} - P$ implies that $P_{11} = P_{22} = \mathbb{I}_n$. Then, the equation $P^2 = P$ shows that $P_{12} =: Q$ is unitary, and (II.4) follows.

The previous Lemma establishes a bijection $P \longleftrightarrow Q$, that is

$$\mathrm{AIII}(0,n,2n)\simeq \mathrm{U}(n).$$

For $P \in AIII(d, n, 2n)$, we denote by $Q : \mathbb{T}^d \to U(n)$ the corresponding periodic family of unitaries.

For a curve \mathcal{C} homeomorphic to \mathbb{S}^1 , and for $Q : \mathcal{C} \to U(n)$, we denote by Winding (\mathcal{C}, Q) the usual winding number of the determinant of Q along \mathcal{C} .

Theorem II.3 (Class AIII). The set AIII(d, n, N) is non-empty iff N = 2n.

- The set AIII(0, n, 2n) is path-connected.
- Define the index map $\operatorname{Index}_{1}^{\operatorname{AIII}}$: $\operatorname{AIII}(1, n, 2n) \to \mathbb{Z}$ by

 $\forall P \in \operatorname{AIII}(1, n, 2n), \quad \operatorname{Index}_{1}^{\operatorname{AIII}}(P) := \operatorname{Winding}(\mathbb{T}^{1}, Q).$

Then P_0 is homotopic to P_1 in AIII(1, n, 2n) iff $\operatorname{Index}_1^{\operatorname{AIII}}(P_0) = \operatorname{Index}_1^{\operatorname{AIII}}(P_1)$.

Proof. We already proved that N = 2n. Since U(n) is connected, so is AIII(0, n, 2n). A constructive path can be constructed as in the previous section using exponential maps.

We now focus on AIII(d = 1, n, 2n). Analogously, the question of whether two maps in AIII(1, n, 2n) are continuously connected by a path can be translated in whether two unitary-valued maps $Q_0, Q_1 \colon \mathbb{T}^1 \to U(n)$ are homotopic to each other. As in the previous proof, consider the unitaries $Q_0(-\frac{1}{2}) = Q_0(\frac{1}{2}) \in U(n)$ and $Q_1(-\frac{1}{2}) = Q_1(\frac{1}{2}) \in U(n)$. Connect them by some $Q_s(-\frac{1}{2}) = Q_s(\frac{1}{2})$ in U(n). This defines a U(n)-valued map on $\partial\Omega$, where the square Ω is defined in (II.2).

It is well known that one can extend such a family of unitaries to the whole Ω iff Winding $(\partial\Omega, Q) = 0$ (see [15, Section IV.B] for a proof, together with a constructive proof of the extension in the case where the winding vanishes). In our case, due to the orientation of the boundary of Ω and of the periodicity of $Q_0(k), Q_1(k)$, we have

Winding $(\partial \Omega, Q) =$ Winding $(\mathbb{T}^1, Q_1) -$ Winding $(\mathbb{T}^1, Q_0),$

which is independent of the previously constructed path $Q_s(\frac{1}{2})$. The conclusion follows.

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Next we consider those symmetry classes which are characterized by the presence of a *single* anti-unitary symmetry: a *T*-symmetry (which even in class AI and odd in class AII) or a *C*-symmetry (which is even in class D and odd in class C). In particular, these classes involve anti-unitarily intertwining P(k) and P(-k). For these symmetry classes, the analysis of their path-connected components in dimension d = 1 is reduced to that of dimension d = 0, thanks to the following Lemma.

Lemma III.1 (Real non-chiral classes in d = 1). Let $X \in \{AI, AII, C, D\}$. Then P_0 and P_1 are in the same connected component of X(1, n, N) iff

- $P_0(0)$ and $P_1(0)$ are in the same connected component in X(0, n, N), and
- $P_0(\frac{1}{2})$ and $P_1(\frac{1}{2})$ are in the same connected component in X(0, n, N).

Proof. We give the argument for the class X = D, but the proof is similar for the other classes. First, we note that if $P_s(k)$ connects P_0 and P_1 in D(1, n, N), then for $k_0 \in \{0, \frac{1}{2}\}$ one must have $C^{-1}P_s(k_0)C = \mathbb{I}_{\mathcal{H}} - P_s(k_0)$, so $P_s(k_0)$ connects $P_0(k_0)$ and $P_1(k_0)$ in D(d = 0, n, N).

Let us prove the converse. Assume that P_0 and P_1 are two projection-valued maps in D(1, n, N) so that there exist paths $P_s(k_0)$ connecting $P_0(k_0)$ and $P_1(k_0)$ in D(0, n, N), for the high symmetry points $k_0 \in \{0, \frac{1}{2}\}$. Denote by Ω_0 the half-square

$$\Omega_0 := [0, \frac{1}{2}] \times [0, 1] \quad \ni (k, s), \tag{III.1}$$

(compare with (II.2)). The families

$$\{P_0(k)\}_{k\in[0,1/2]}, \{P_1(k)\}_{k\in[0,1/2]}, \{P_s(0)\}_{s\in[0,1]} \text{ and } \{P_s(\frac{1}{2})\}_{s\in[0,1]}$$

together define a continuous family of projectors on the boundary $\partial \Omega_0$. As was already mentioned in Section II A, this family can be extended continuously on the whole set Ω_0 .

This gives a continuous family $\{P_s(k)\}_{k \in [0,1/2], s \in [0,1]}$ which connects continuously the restrictions of P_0 and P_1 to the half-torus $k \in [0, \frac{1}{2}]$. We can then extend the family of projections to $k \in [-\frac{1}{2}, 0]$ by setting

$$\forall k \in [-\frac{1}{2}, 0], \ \forall s \in [0, 1], \quad P_s(k) := C [\mathbb{I}_{\mathcal{H}} - P_s(-k)] C^{-1}.$$

By construction, for all $s \in [0, 1]$, the map P_s is in D(1, n, N). In addition, since at $k_0 \in \{0, \frac{1}{2}\}$ we have $P_s(k_0) \in D(0, n, N)$, the above extension is indeed continuous as a function of k on the whole torus \mathbb{T}^1 . This concludes the proof.

A. Class AI

In class AI, the relevant symmetry is an anti-unitary operator T with $T^2 = \mathbb{I}_{\mathcal{H}}$. This case was studied for instance in [9, 13, 30].

Lemma III.2. If T is an anti-unitary operator on \mathcal{H} such that $T^2 = \mathbb{I}_{\mathcal{H}}$, then there is a basis of \mathcal{H} in which T has the matrix form $T = K_N$.

Proof. We construct the basis by induction. Let $\psi_1 \in \mathcal{H}$ be a normalized vector. if $T\psi_1 = \psi_1$, we set $\phi_1 = \psi_1$, otherwise we set

$$\phi_1 := i \frac{\psi_1 - T\psi_1}{\|\psi_1 - T\psi_1\|}.$$

In both cases, we have $T\phi_1 = \phi_1$ and $\|\phi_1\| = 1$, which gives our first vector of the basis. Now take ψ_2 orthogonal to ϕ_1 . We define ϕ_2 as before. If $\phi_2 = \psi_2$, then ϕ_2 is automatically orthogonal to ϕ_1 . This also holds in the second case, since

$$\langle \psi_2 - T\psi_2, \phi_1 \rangle = -\langle T\psi_2, \phi_1 \rangle = -\langle T\phi_1, T^2\psi_2 \rangle = -\langle \phi_1, \psi_2 \rangle = 0,$$

where we used twice that $\langle \psi_2, \phi_1 \rangle = 0$. We go on, and construct the vectors ϕ_k inductively for $1 \le k \le N$. This gives an orthonormal basis in which T = K.

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Proof. In a basis in which $T = K_N$, we have the identification

$$AI(0, n, N) = \left\{ P \in \mathcal{G}_n(\mathbb{C}^N) : \overline{P} = P \right\}$$

In other words, AI(0, n, N) consists of *real* subspaces of \mathcal{H} , *i.e.* those that are fixed by the complex conjugation T = K. One can therefore span such subspaces (as well as their orthogonal complement) by orthonormal *real* vectors. This realizes a bijection similar to (II.1), but where unitary matrices are replaced by orthogonal ones: more precisely

$$\operatorname{AI}(0, n, N) \simeq \operatorname{O}(N) / \operatorname{O}(n) \times \operatorname{O}(N - n).$$

We adapt the argument in the proof of Theorem II.1 to show that the latter space is path-connected. Let $P_0, P_1 \in AI(0, n, N)$. We choose two *real* bases of \mathcal{H} , which we identify with columns of orthogonal matrices $U_0, U_1 \in O(N)$, so that the first *n* vectors of U_j span the range of P_j , for $j \in \{0, 1\}$. In addition, by flipping the first vector, we may assume $U_0, U_1 \in SO(N)$. Then there is $A_0, A_1 \in \mathcal{A}_N(\mathbb{R})$ so that $U_j = e^{A_j}$ for $j \in \{0, 1\}$. We then set $U_s := e^{A_s}$ with $A_s = (1 - s)A_0 + sA_1$. The projection P_s on the first *n* column vectors of U_s then interpolates between P_0 and P_1 , as required. In view of Lemma III.1, the path-connectedness of AI(0, n, N) implies the one of AI(1, n, N).

B. Class AII

In class AII we have $T^2 = -\mathbb{I}_{\mathcal{H}}$. This case was studied for instance in [7, 11, 14, 16, 29].

Lemma III.4. There is an anti-unitary map $T : \mathcal{H} \to \mathcal{H}$ with $T^2 = -\mathbb{I}_{\mathcal{H}}$ iff dim $\mathcal{H} = N = 2M$ is even. In this case, there is a basis of \mathcal{H} in which T has the matrix form

$$T = \begin{pmatrix} 0 & K_M \\ -K_M & 0 \end{pmatrix} = J_{2M} K_{2M}.$$
 (III.2)

Proof. First, we note that $T\psi$ is always orthogonal to ψ . Indeed, we have

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$$\langle \psi, T\psi \rangle = \langle T^2\psi, T\psi \rangle = -\langle \psi, T\psi \rangle, \text{ hence } \langle \psi, T\psi \rangle = 0.$$
 (III.3)

We follow the strategy employed *e.g.* in [16] and [7, Chapter 4.1], and construct the basis by induction. Let $\psi_1 \in \mathcal{H}$ be any normalized vector, and set $\psi_2 := T\psi_1$. The family $\{\psi_1, \psi_2\}$ is orthonormal by (III.3). If $\mathcal{H} \neq \text{Span}\{\psi_1, \psi_2\}$, then there is $\psi_3 \in \mathcal{H}$ orthonormal to this family. We then set $\psi_4 = T\psi_3$, and claim that ψ_4 is orthonormal to the family $\{\psi_1, \psi_2, \psi_3\}$. First, by (III.3), we have $\langle \psi_3, \psi_4 \rangle = 0$. In addition, we have

$$\langle \psi_4, \psi_1 \rangle = \langle T\psi_3, \psi_1 \rangle = \langle T\psi_1, T^2\psi_3 \rangle = -\langle \psi_2, \psi_3 \rangle = 0,$$

and, similarly,

$$\langle \psi_4, \psi_2 \rangle = \langle T\psi_3, T\psi_1 \rangle = \langle T^2\psi_1, T^2\psi_3 \rangle = \langle \psi_1, \psi_3 \rangle = 0.$$

We proceed by induction. We first obtain that the dimension of \mathcal{H} is even, N = 2M, and we construct an explicit basis $\{\psi_1, \dots, \psi_{2M}\}$ for \mathcal{H} . In the orthonormal basis $\{\psi_1, \psi_3, \psi_5, \dots, \psi_{2M-1}, \psi_2, \psi_4, \dots, \psi_{2M}\}$, the operator T has the matrix form (III.2).

Theorem III.5 (Class AII). The sets AII(0, n, N) and AII(1, n, N) are non-empty iff $n = 2m \in 2\mathbb{N}$ and $N = 2M \in 2\mathbb{N}$. Both are path-connected.

Proof. The proof follows the same lines as that of Theorems II.1 and III.3. The condition $T^{-1}PT = P$ for $P \in AII(0, n, N)$ means that the range of the projection P is stable under the action of T. This time, the operator T endows the Hilbert space \mathcal{H} with a *quaternionic* structure, namely the matrices $\{iI_{\mathcal{H}}, T, iT\}$ satisfy the same algebraic relations as the basic quaternions $\{i, j, k\}$: they square to $-I_{\mathcal{H}}$, they pairwise anticommute and the product of two successive ones cyclically gives the third. This allows to realize the class AII(0, 2m, 2M) as

$$\operatorname{AII}(0, 2m, 2M) \simeq \operatorname{Sp}(M) / \operatorname{Sp}(m) \times \operatorname{Sp}(M - m).$$

Matrices in Sp(M) are exponentials of Hamiltonian matrices, that is, matrices A such that $J_{2M}A$ is symmetric [18, Prop. 3.5 and Coroll. 11.10]. Such matrices form a (Lie) algebra, and therefore the same argument as in the proof of Theorem III.3 applies, yielding path-connectedness of AII(0, 2m, 2M). This in turn implies, in combination with Lemma III.1, that AII(1, 2m, 2M) is path-connected as well.

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We now come to classes where the C-symmetry is present. We first focus on the even case, $C^2 = +\mathbb{I}_{\mathcal{H}}$, characterizing class D. One of the most famous models in this class is the 1-dimensional Kitaev chain [26]. We choose to work in the basis of \mathcal{H} in which C has the form $C = K_N$ (see Lemma III.2). This is different from the "energy basis", of common use in the physics literature, in which C is block-off-diagonal, mapping "particles" to "holes" and vice-versa. We find this other basis more convenient for our purpose.

C. Class D

Lemma III.6. The set D(0, n, N) is non-empty iff N = 2n. In this case, and in a basis where $C = K_N$, a projection P is in D(0, n, 2n) iff it has the matrix form

$$P = \frac{1}{2}(\mathbb{I}_N + iA), \quad with \quad A \in \mathcal{O}(2n) \cap \mathcal{A}_{2n}(\mathbb{R}).$$

Proof. A computation shows that

$$\begin{cases} P^* = P \\ P^2 = P \\ C^{-1}PC = \mathbb{I} - P \end{cases} \iff \begin{cases} A^* = -A \\ A^2 = -\mathbb{I}_N \\ \overline{A} = A \end{cases} \iff \begin{cases} A^*A = \mathbb{I}_N \\ A = \overline{A} = -A^T. \end{cases}$$

This proves that $P \in D(0, n, N)$ iff $A \in O(N) \cap \mathcal{A}_N(\mathbb{R})$. In particular, we have $\det(A) = (-1)^N \det(-A) = (-1)^N \det(A^T) = (-1)^N \det(A)$, so N = 2m is even. Finally, since the diagonal of A is null, we have $n = \operatorname{Tr}(P) = \frac{1}{2}\operatorname{Tr}(\mathbb{I}_N) = m$.

In Corollary A.4 below, we prove that a matrix A is in $O(2n) \cap A_{2n}(\mathbb{R})$ iff it is of the form

$$A = W^T J_{2n} W$$
, with $W \in O(2n)$.

In addition, we have $W_0^T J_{2n} W_0 = W_1^T J_{2n} W_1$ with $W_0, W_1 \in O(2n)$ iff $W_0 W_1^* \in Sp(n) \cap O(2n)$. Finally, in Proposition A.5, we show that $Sp(n) \cap O(2n) \simeq U(n)$. Altogether, this shows that

$$D(0, n, 2n) \simeq O(2n) \cap \mathcal{A}_{2n}(\mathbb{R}) \simeq O(2n)/U(n).$$

To identify the connected components of this class, recall that for an anti-symmetric matrix $A \in \mathcal{A}_{2n}^{\mathbb{R}}(\mathbb{C})$, we can define its *Pfaffian*

$$Pf(A) := \frac{1}{2^n n!} \sum_{\sigma} \operatorname{sgn}(\sigma) \prod_{i=1}^n a_{\sigma(2i-1),\sigma(2i)},$$
(III.4)

where the above sum runs over all permutations over 2n labels and $sgn(\sigma)$ is the sign of the permutation σ . The Pfaffian satisfies

$$\operatorname{Pf}(A)^2 = \det(A).$$

On the other hand, if $A \in O(2n)$, then $det(A) \in \{\pm 1\}$, so if $A \in O(2n) \cap \mathcal{A}_{2n}(\mathbb{R})$, we must have det(A) = 1 and $Pf(A) \in \{\pm 1\}$.

Theorem III.7 (Class D). The set D(d, n, N) is non-empty iff N = 2n.

• The set D(0, n, 2n) has two connected components. Define the index map $\operatorname{Index}_0^D \colon D(0, n, 2n) \to \mathbb{Z}_2 \simeq \{\pm 1\}$ by

$$\forall P \in D(0, n, 2n), \quad \text{Index}_0^D(P) := Pf(A).$$

Then P_0 is homotopic to P_1 in D(0, n, 2n) iff $Index_0^D(P_0) = Index_0^D(P_1)$.

• The set D(1, n, 2n) has four connected components. Define the index map $\operatorname{Index}_1^D \colon D(1, n, 2n) \to \mathbb{Z}_2 \times \mathbb{Z}_2$ by

$$\forall P \in \mathcal{D}(1, n, 2n), \quad \operatorname{Index}_{1}^{\mathcal{D}}(P) := \left(\operatorname{Pf}(A(0)), \operatorname{Pf}(A(\frac{1}{2}))\right).$$

Then P_0 is homotopic to P_1 in D(1, n, 2n) iff $\operatorname{Index}_1^D(P_0) = \operatorname{Index}_1^D(P_1)$.

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Proof. We start with D(0, n, N = 2n). Let $P_0, P_1 \in D(0, n, 2n)$. It is clear that if $Pf(A_0) \neq Pf(A_1)$, then P_0 and P_1 are in two different connected components (recall that $Pf(\cdot)$ is a continuous map, with values in $\{\pm 1\}$ in our case).

It remains to construct an explicit homotopy in the case where $Pf(A_0) = Pf(A_1)$. In Corollary A.4 below, we recall that a matrix A is in $O(2n) \cap \mathcal{A}_{2n}(\mathbb{R})$ iff there is $V \in SO(2n)$ so that

$$A = V^T D V$$
, with $D = (1, 1, \cdots, 1, \operatorname{Pf}(A)) \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

So, if $A_0, A_1 \in O(2n) \cap \mathcal{A}_{2n}(\mathbb{R})$ have the same Pfaffian, it is enough to connect the corresponding V_0 and V_1 in SO(2n). The proof follows since SO(2n) is path-connected (compare with the proof of Theorem III.3). The case for D(d = 1, n, 2n) is now a consequence of Lemma III.1.

Remark III.8. For 1-dimensional translation-invariant systems, one can distinguish between a weak (i.e., lowerdimensional, depending solely on P(k) at k = 0) index

$$\operatorname{Index}_{0}^{D}(P(0)) = \operatorname{Pf}(A(0)) \in \mathbb{Z}_{2}$$

and a strong (i.e., "truly" 1-dimensional) index

$$\widetilde{\mathrm{Index}_0^{\mathrm{D}}}(P) := \mathrm{Pf}(A(0)) \cdot \mathrm{Pf}(A(\frac{1}{2})) \in \mathbb{Z}_2.$$

Only the latter \mathbb{Z}_2 -index appears in the periodic tables for free ground states [27]. Our proposed index

$$\operatorname{Index}_{1}^{D}(P) = \left(\operatorname{Pf}(A(0)), \operatorname{Pf}(A(\frac{1}{2}))\right) \in \mathbb{Z}_{2} \times \mathbb{Z}_{2}$$

clearly contains the same topological information of both the weak and strong indices. A similar situation will appear in class BDI (see Section IVA).

D. Class C

We now focus on the odd C-symmetry class, where $C^2 = -\mathbb{I}_{\mathcal{H}}$. Thanks to Lemma III.4, N = 2M is even, and we can choose a basis of \mathcal{H} in which C has the matrix form

$$C = \begin{pmatrix} 0 & K_M \\ -K_M & 0 \end{pmatrix} = J_{2M} K_{2M}$$

Recall that $\operatorname{Sp}(n) := \operatorname{Sp}(2n; \mathbb{C}) \cap \operatorname{U}(2n)$.

Lemma III.9. The set C(0, n, N) is non-empty iff N = 2n (hence n = M). A projection P is in C(0, n, 2n) iff it has the matrix form

$$P = \frac{1}{2} \left(\mathbb{I}_{2n} + iJ_{2n}A \right), \quad with \quad A \in \operatorname{Sp}(n) \cap \mathcal{S}_{2n}^{\mathbb{R}}(\mathbb{C}).$$

Proof. With this change of variable, we obtain that

$$\begin{cases} P = P^* \\ P^2 = P \\ C^{-1}PC = \mathbb{I}_{2n} - P \end{cases} \iff \begin{cases} A^* J_{2n} = J_{2n}A \\ J_{2n}AJ_{2n}A = -\mathbb{I}_{2n} \\ \overline{A}J_{2n} = J_{2n}A. \end{cases}$$

With the two first equations, we obtain $AA^* = \mathbb{I}_{2n}$, so $A \in U(2n)$. With the first and third equations, we get $A^T = A$, so $A \in S_{2n}^{\mathbb{R}}(\mathbb{C})$, and with the two last equations, $A^T J_{2n} A = J_{2n}$, so $A \in \mathrm{Sp}(2n; \mathbb{C})$. The result follows.

In Corollary A.2 below, we prove that a matrix A is in $\operatorname{Sp}(n) \cap \mathcal{S}_{2n}^{\mathbb{R}}(\mathbb{C})$ iff it is of the form

 $A = V^T V$, for some $V \in \operatorname{Sp}(n)$.

In addition, $A = V_0^T V_0 = V_1^T V_1$ with $V_0, V_1 \in \operatorname{Sp}(n)$ iff $V_1 V_0^* \in \operatorname{Sp}(n) \cap \operatorname{O}(2n) \simeq \operatorname{U}(n)$ (see the already mentioned Proposition A.5 for the last bijection). This proves that

$$C(0, n, N) \simeq Sp(n) \cap \mathcal{S}_{2n}^{\mathbb{R}}(\mathbb{C}) \simeq Sp(n)/U(n).$$

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Proof. For C(d = 0, n, 2N), it is enough to prove that $Sp(n) \cap \mathcal{S}_{2n}^{\mathbb{R}}(\mathbb{C})$ is path-connected. To connect A_0 and A_1 in $Sp(n) \cap \mathcal{S}_{2n}(\mathbb{C})$ it suffices to connect the corresponding V_0 and V_1 in Sp(2n). This can be done as we already saw in the proof of Theorem III.5. Invoking Lemma III.1 allows to conclude that C(1, n, 2n) is path-connected as well.

IV. REAL CHIRAL CLASSES: BDI, DIII, CII AND CI

We now focus on the chiral real classes; by Assumption I.4, the chiral symmetry operator S will come from the combination of a T-symmetry with a C-symmetry. In what follows, we will always find a basis for \mathcal{H} in which S := TC has the form (II.3). In particular, Lemma II.2 applies, and any $P \in X(d, n, 2n)$ for $X \in \{BDI, DIII, CII, CI\}$ will be of the form

$$P(k) = \frac{1}{2} \begin{pmatrix} \mathbb{I}_n & Q(k) \\ Q(k)^* & \mathbb{I}_n \end{pmatrix} \quad \text{with} \quad Q(k) \in \mathcal{U}(n).$$
(IV.1)

The T-symmetry (or equivalently the C-symmetry) of P(k) translates into a condition for Q(k), of the form

$$F_T(Q(k)) = Q(-k). \tag{IV.2}$$

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With these remarks, we are able to formulate the analogue of Lemma III.1 for real chiral classes.

Lemma IV.1 (Real chiral classes in d = 1). Let $X \in \{BDI, DIII, CII, CI\}$. Then P_0 and P_1 are in the same connected component in X(1, n, 2n) iff

- $P_0(0)$ and $P_1(0)$ are in the same connected component in X(0, n, 2n),
- $P_0(\frac{1}{2})$ and $P_1(\frac{1}{2})$ are in the same connected component in X(0, n, 2n), and
- there exists a choice of the above interpolations $P_s(0)$, $P_s(\frac{1}{2})$, $s \in [0,1]$, and therefore of the corresponding unitaries $Q_s(0)$, $Q_s(\frac{1}{2})$ as in (IV.1), such that

Winding
$$(\partial \Omega_0, Q) = 0$$
,

where Ω_0 is the half-square defined in (III.1), and where Q is the continuous family of unitaries defined on $\partial \Omega_0$ via the families

$$\left[Q_0(k)\right]_{k\in[0,1/2]}, \quad \left\{Q_1(k)\right\}_{k\in[0,1/2]}, \quad \left\{Q_s(0)\right\}_{s\in[0,1]}, \quad and \quad \left\{Q_s(\frac{1}{2})\right\}_{s\in[0,1]}$$

Proof. As was already mentioned, the vanishing of the winding in the statement is equivalent to the existence of a continuous extension of the map $Q(k, s) \equiv Q_s(k)$ to $(k, s) \in \Omega_0$. For $k \in [-\frac{1}{2}, 0]$ and $s \in [0, 1]$, we define

$$Q_s(k) := F_T(Q_s(-k)),$$

where F_T is the functional relation in (IV.2). Using (IV.1), we can infer the existence of a family of projections $\{P_s(k)\}_{k\in\mathbb{T}^1}$ which depends continuously on $s\in[0,1]$, is in X(1,n,2n) for all $s\in[0,1]$, and restricts to P_0 and P_1 at s=0 and s=1, respectively. This family thus provides the required homotopy.

A. Class BDI

We start from class BDI, characterized by even T- and C-symmetries.

Lemma IV.2. Assume BDI(0, n, N) is non empty. Then N = 2n, and there is a basis of \mathcal{H} in which

$$T = \begin{pmatrix} K_n & 0 \\ 0 & K_n \end{pmatrix}, \quad C = \begin{pmatrix} K_n & 0 \\ 0 & -K_n \end{pmatrix}, \quad so \ that \quad S = TC = \begin{pmatrix} \mathbb{I}_n & 0 \\ 0 & -\mathbb{I}_n \end{pmatrix}.$$

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Proof. Let $P_0 \in BDI(0, n, 2n)$, and let $\{\phi_1, \dots, \phi_n\}$ be an orthonormal basis for Ran P_0 such that $T\phi_j = \phi_j$ for all $1 \leq j \leq n$ (see Lemma III.2). We set

$$\forall 1 \le j \le n, \quad \phi_{n+j} = C\phi_j.$$

Since C is anti-unitary, and maps $\operatorname{Ran} P_0$ into $\operatorname{Ran} (\mathbb{I} - P_0)$, the family $\{\phi_1, \dots, \phi_{2n}\}$ is an orthonormal basis for \mathcal{H} . Since T and C commute, we have for all $1 \leq j \leq n$,

$$T\phi_{n+j} = TC\phi_j = CT\phi_j = C\phi_j = \phi_{n+j}, \quad \text{and} \quad C\phi_{n+j} = C^2\phi_j = \phi_j.$$
(IV.3)

Therefore in this basis the operators T and C take the form

$$T = \begin{pmatrix} K_n & 0\\ 0 & K_n \end{pmatrix}, \quad C = \begin{pmatrix} 0 & K_n\\ K_n & 0 \end{pmatrix} \text{ and } S = \begin{pmatrix} 0 & \mathbb{I}_n\\ \mathbb{I}_n & 0 \end{pmatrix}.$$

We now change basis via the matrix $U := \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I}_n & \mathbb{I}_n \\ \mathbb{I}_n & -\mathbb{I}_n \end{pmatrix}$ to obtain the result.

Using Lemma IV.2, one can describe a projection P(k) with its corresponding unitary Q(k). The condition $T^{-1}P(k)T = P(-k)$ reads

$$\overline{Q}(-k) = Q(k).$$

So a projection P is in BDI(0, n, 2n) iff the corresponding matrix $Q \in U(n)$ satisfies $\overline{Q} = Q$, that is $Q \in O(n)$. This proves that

 $BDI(0, n, 2n) \simeq O(n).$

Recall that O(n) has two connected components, namely det⁻¹{±1}.

Theorem IV.3 (Class BDI). The set BDI(d, n, N) is non-empty iff N = 2n.

• Let $\operatorname{Index}_{0}^{\operatorname{BDI}}$: $\operatorname{BDI}(0, n, 2n) \to \mathbb{Z}_{2}$ be the index map defined by

 $\forall P \in BDI(0, n, 2n), \quad Index_0^{BDI}(P) = det(Q).$

Then P_0 is homotopic to P_1 in BDI(0, n, 2n) iff $Index_0^{BDI}(P_0) = Index_0^{BDI}(P_1)$.

• There is an index map $\operatorname{Index}_{1}^{\operatorname{BDI}}$: $\operatorname{BDI}(1, n, 2n) \to \mathbb{Z}_{2} \times \mathbb{Z}$ such that P_{0} is homotopic to P_{1} in $\operatorname{BDI}(1, n, 2n)$ iff $\operatorname{Index}_{1}^{\operatorname{BDI}}(P_{0}) = \operatorname{Index}_{1}^{\operatorname{BDI}}(P_{1})$.

Proof. Recall that SO(n) is path-connected, see the proof of Theorem III.3. The complement $O(n) \setminus SO(n)$ is in bijection with SO(n), by multiplying each orthogonal matrix with determinant -1 by the matrix diag(1, 1, ..., 1, -1). This proves the first part.

We now focus on dimension d = 1. Let P(k) be in BDI(1, n, 2n), and let Q(k) be the corresponding unitary. Let $\alpha(k) : [0, \frac{1}{2}] \to \mathbb{R}$ be a continuous map so that

$$\forall k \in [0, \frac{1}{2}], \quad \det Q(k) = e^{i\alpha(k)}.$$

Since Q(0) and $Q(\frac{1}{2})$ are in O(n), we have det $Q(0) \in \{\pm 1\}$ and det $Q(\frac{1}{2}) \in \{\pm 1\}$. We define

$$\mathcal{W}^{1/2}(P) := \mathcal{W}^{1/2}(Q) := \frac{1}{\pi} \left(\alpha(\frac{1}{2}) - \alpha(0) \right) \quad \in \mathbb{Z}$$

The number $\mathcal{W}^{1/2}(Q) \in \mathbb{Z}$ counts the number of *half turns* that the determinant is winding as k goes from 0 to $\frac{1}{2}$. We call this map the *semi-winding*. We finally define the index map $\mathrm{Index}_1^{\mathrm{BDI}} : \mathrm{BDI}(1, n, 2n) \to \mathbb{Z}_2 \times \mathbb{Z}$ by

 $\forall P \in BDI(1, n, 2n), \quad Index_1^{BDI}(P) := \left(\det Q(0), \ \mathcal{W}^{1/2}(P)\right) \in \mathbb{Z}_2 \times \mathbb{Z}.$

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Let P_0, P_1 be in BDI(1, n, 2n) such that $\operatorname{Index}_1^{\operatorname{BDI}}(P_0) = \operatorname{Index}_1^{\operatorname{BDI}}(P_1)$, and let us construct an homotopy between P_0 and P_1 . First, we have det $Q_0(0) = \det Q_1(0)$, and, since $\mathcal{W}^{1/2}(P_0) = \mathcal{W}^{1/2}(P_1)$, we also have $\det Q_0(\frac{1}{2}) = \det Q_1(\frac{1}{2})$.

Let $Q_s(0)$ be a path in O(n) connecting $Q_0(0)$ and $Q_1(0)$, and let $Q_s(\frac{1}{2})$ be a path connecting $Q_0(\frac{1}{2})$ and $Q_1(\frac{1}{2})$. This defines a continuous family of unitaries on the boundary of the half-square $\Omega_0 := [0, \frac{1}{2}] \times [0, 1]$. Since $Q_s(0)$ and $Q_s(\frac{1}{2})$ are in O(n) for all s, their determinants are constant, equal to $\{\pm 1\}$, and they do not contribute to the winding of the determinant of this unitary-valued map. So the winding along the boundary equals

Winding
$$(\partial \Omega_0, Q) = \mathcal{W}^{1/2}(P_0) - \mathcal{W}^{1/2}(P_1) = 0.$$

Lemma IV.1 allows then to conclude the proof.

B. Class CI

In class CI, the *T*-symmetry is even $(T^2 = \mathbb{I}_{\mathcal{H}})$ while the *C*-symmetry is odd $(C^2 = -\mathbb{I}_{\mathcal{H}})$. Lemma IV.4. Assume CI(0, n, N) is non empty. Then N = 2n, and there is a basis of \mathcal{H} in which

$$T = \begin{pmatrix} 0 & K_n \\ K_n & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & -K_n \\ K_n & 0 \end{pmatrix} \quad so \ that \quad S = TC = \begin{pmatrix} \mathbb{I}_n & 0 \\ 0 & -\mathbb{I}_n \end{pmatrix}.$$
 (IV.4)

Proof. The proof is similar to the one of Lemma IV.2. This time, since $C^2 = -\mathbb{I}$ and TC = -CT, we have, instead of (IV.3),

$$T\phi_{n+j} = TC\phi_j = -CT\phi_j = -C\phi_j = -\phi_{n+j}, \quad \text{and} \quad C\phi_{n+j} = C^2\phi_j = -\phi_j.$$

Using again Lemma IV.2, we describe a projection P(k) with its corresponding unitary Q(k). The condition $T^{-1}P(k)T = P(-k)$ gives

 $Q(-k)^T = Q(k).$

In particular, if $P \in CI(0, n, 2n)$, the corresponding Q satisfies $Q^T = Q$. In Corollary A.2 below, we prove that a matrix Q is in $U(n) \cap S_n^{\mathbb{R}}(\mathbb{C})$ iff it is of the form

$$Q = V^T V$$
, for some $V \in U(n)$.

In addition, we have $Q = V_0^T V_0 = V_1^T V_1$ with $V_0, V_1 \in U(n)$ iff $V_0 V_1^* \in O(n)$. This proves that

 $\boxed{\mathrm{CI}(0,n,2n)\simeq \mathrm{U}(n)\cap \mathcal{S}_n^{\mathbb{R}}(\mathbb{C})\simeq \mathrm{U}(n)/\mathrm{O}(n).}$

Theorem IV.5 (Class CI). The set CI(d, n, N) is non-empty iff N = 2n. It is path-connected both for d = 0 and for d = 1.

Proof. Given two matrices Q_0 , Q_1 in $U(n) \cap \mathcal{S}_n^{\mathbb{R}}(\mathbb{C})$, we can connect them in $U(n) \cap \mathcal{S}_n^{\mathbb{R}}(\mathbb{C})$ by connecting the corresponding V_0 and V_1 in U(n). This proves that CI(0, n, 2n) is connected.

We now focus on the case d = 1. Let $P_0(k)$ and $P_1(k)$ be two families in CI(1, n), with corresponding unitaries Q_0 and Q_1 . Let $V_0(0), V_1(0) \in U(n)$ so that

$$Q_0(0) = V_0(0)^T V_0(0)$$
, and $Q_1(0) = V_1(0)^T V_1(0)$.

Let $V_s(0)$ be a homotopy between $V_0(0)$ and $V_1(0)$ in U(n), and set

$$Q_s(0) := V_s(0)^T V_s(0).$$

Then, $Q_s(0)$ is a homotopy between $Q_0(0)$ and $Q_1(0)$ in CI(0, n, 2n). We construct similarly an homotopy between $Q_0(\frac{1}{2})$ and $Q_1(\frac{1}{2})$ in CI(0, n, 2n). This gives a path of unitaries on the boundary of the half-square Ω_0 . We can extend this family inside Ω_0 iff the winding of the determinant along the boundary loop vanishes.

Let $W \in \mathbb{Z}$ be this winding. There is no reason a priori to have W = 0. However, if $W \neq 0$, we claim that we can cure the winding by modifying the path $V_s(0)$ connecting $V_0(0)$ and $V_1(0)$. Indeed, setting

$$\widetilde{V}_s(0) = \operatorname{diag}(\mathrm{e}^{\mathrm{i}W\pi s/2}, 1, 1, \cdots, 1)V_s(0), \quad \text{and} \quad \widetilde{Q}_s(0) := \widetilde{V}_s(0)^T \widetilde{V}_s(0),$$

we can check that the family $Q_s(0)$ also connects $Q_0(0)$ and $Q_1(0)$ in CI(0, n, 2n), and satisfies

$$\det Q_s(0) = e^{iW\pi s} \det Q_s(0).$$

This cures the winding, and Lemma IV.1 allows to conclude that the class CI(1, n, 2n) is path-connected.

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The class DIII mirrors CI, since here the *T*-symmetry is odd $(T^2 = -\mathbb{I}_{\mathcal{H}})$ while the *C*-symmetry is even $(C^2 = \mathbb{I}_{\mathcal{H}})$. This class has been studied *e.g.* in [12].

Lemma IV.6. Assume DIII(0, n, N) is non empty. Then n = 2m is even, and N = 2n = 4m is a multiple of 4. There is a basis of \mathcal{H} in which

$$T = \begin{pmatrix} 0 & K_n J_n \\ K_n J_n & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & K_n J_n \\ -K_n J_n & 0 \end{pmatrix}, \quad and \quad S = \begin{pmatrix} \mathbb{I}_n & 0 \\ 0 & -\mathbb{I}_n \end{pmatrix}$$

Proof. Let $P_0 \in \text{DIII}(0, n, 2n)$. Since T is anti-unitary, leaves $\text{Ran } P_0$ invariant, and satisfies $T^2 = -\mathbb{I}_{\text{Ran } P_0}$ there, one can apply Lemma III.4 to the restriction of T on $\text{Ran } P_0$. We first deduce that n = 2m is even, and that there is a basis for $\text{Ran } P_0$ of the form $\{\psi_1, \ldots, \psi_{2m}\}$, with $\psi_{m+j} = T\psi_j$. Once again we set $\psi_{2m+j} := C\psi_j$. This time, we have TC = -CT, so, in the basis $\{\psi_1, \ldots, \psi_{4m}\}$, we have

$$T = \begin{pmatrix} KJ_n & 0\\ 0 & -KJ_n \end{pmatrix}, \quad C = \begin{pmatrix} 0 & K\\ K & 0 \end{pmatrix} \quad \text{hence} \quad S = TC = \begin{pmatrix} 0 & J_n\\ -J_n & 0 \end{pmatrix}$$

A computation reveals that

$$U^* \begin{pmatrix} 0 & J_n \\ -J_n & 0 \end{pmatrix} U = \begin{pmatrix} \mathbb{I}_n & 0 \\ 0 & -\mathbb{I}_n \end{pmatrix}, \quad \text{with} \quad U := \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I}_m & 0 & -\mathbb{I}_m & 0 \\ 0 & -\mathbb{I}_m & 0 & \mathbb{I}_m \\ 0 & \mathbb{I}_m & 0 & \mathbb{I}_m \\ \mathbb{I}_m & 0 & \mathbb{I}_m & 0 \end{pmatrix},$$

and that U is unitary. With this change of basis, we obtain the result.

In this basis, we have that $T^{-1}P(k)T = P(-k)$ iff the corresponding Q satisfies

$$J_n Q^T(-k) J_n = -Q(k).$$

In dimension d = 0, the condition becomes $J_n Q^T J_n = -Q$, which can be equivalently rewritten as

$$A^T = -A$$
, with $A := QJ_n$.

The matrix A is unitary and skew-symmetric, $A \in U(n) \cap \mathcal{A}_n^{\mathbb{R}}(\mathbb{C})$. In particular, the Pfaffian of A is well-defined. In Corollary A.4 below, we recall that a matrix A is in $U(n) \cap \mathcal{A}_n^{\mathbb{R}}(\mathbb{C})$ iff it is of the form

$$A = V^T J_n V$$
, with $V \in U(n)$.

In addition, we have $A = V_0^T J_n V_0 = V_1^T J_n V_1$ with $V_0, V_1 \in U(n)$ iff $V_0 V_1^* \in Sp(m)$. Therefore

DIII
$$(0, 2m, 4m) \simeq \mathrm{U}(2m) \cap \mathcal{A}_{2m}^{\mathbb{R}}(\mathbb{C}) \simeq \mathrm{U}(2m)/\mathrm{Sp}(m).$$

Theorem IV.7 (Class DIII). The set DIII(d, n, N) is non-empty iff $n = 2m \in 2\mathbb{N}$ and N = 2n = 4m.

- The set DIII(0, 2m, 4m) is path-connected.
- There is a map $\operatorname{Index}_{1}^{\operatorname{DIII}}$: $\operatorname{DIII}(1, 2m, 4m) \to \mathbb{Z}_{2}$ such that P_{0} is homotopic to P_{1} in $\operatorname{DIII}(1, 2m, 4m)$ iff $\operatorname{Index}_{1}^{\operatorname{DIII}}(P_{0}) = \operatorname{Index}_{1}^{\operatorname{DIII}}(P_{1})$.

The index $Index_1^{DIII}$ is defined below in (IV.5). It matches the usual Teo-Kene formula in [33, Eqn. (4.27)].

Proof. For the first part, it is enough to connect the corresponding matrices V's in U(n), which is path-connected. Let us focus on the case d = 1. Let $P(k) \in \text{DIII}(1, 2m, 4m)$ with corresponding matrices $Q(k) \in \text{U}(2m)$ and $A(k) := J_{2m}^T Q(k) \in \text{U}(2m) \cap \mathcal{A}_{2m}^{\mathbb{R}}(\mathbb{C})$. Let $\alpha(k) : [0, 1/2] \to \mathbb{R}$ be a continuous phase so that

$$\forall k \in [0, \frac{1}{2}], \quad \det A(k) = e^{i\alpha(k)}$$

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Pf
$$A(0) = \sigma_0 e^{i\frac{1}{2}\alpha(0)}$$
, and Pf $A(\frac{1}{2}) = \sigma_{1/2} e^{i\frac{1}{2}\alpha(\frac{1}{2})}$

We define the Index as the product of the two signs $\sigma_0 \cdot \sigma_{1/2}$. Explicitly,

$$Index_1^{DIII}(P) := \frac{e^{i\frac{1}{2}\alpha(0)}}{Pf A(0)} \cdot \frac{e^{i\frac{1}{2}\alpha(\frac{1}{2})}}{Pf A(\frac{1}{2})} \in \{\pm 1\}.$$
 (IV.5)

Note that this index is independent of the choice of the lifting $\alpha(k)$. Actually, this index is 1 if, by following the continuous map $e^{i\frac{1}{2}\alpha(k)}$, that is a continuous representation of $\sqrt{\det(A(k))}$, one goes from Pf A(0) to Pf $A(\frac{1}{2})$, and is -1 if one goes from Pf A(0) to $-Pf A(\frac{1}{2})$.

Let us prove that if $P_0, P_1 \in \text{DIII}(1, 2m, 4m)$, then $\text{Index}_1^{\text{DIII}}(P_0) = \text{Index}_1^{\text{DIII}}(P_1)$ iff there is an homotopy between the two maps. Let $V_0(0), V_1(0) \in U(n)$ be so that

$$A_0(0) = V_0(0)^T J_n V_0(0)$$
, and $A_1(0) = V_1(0)^T J_n V_1(0)$.

Let $V_s(0)$ be a homotopy between $V_0(0)$ and $V_1(0)$ in U(n), and set

$$A_s(0) := V_s(0)^T J_n V_s(0).$$

This gives a homotopy between $A_0(0)$ and $A_1(0)$ in DIII(0, n, 2n). We construct similarly a path $A_s(\frac{1}{2})$ connecting $A_0(\frac{1}{2})$ and $A_1(\frac{1}{2})$ in DIII(0, n, 2n).

Define continuous phase maps $\alpha_0(k)$, $\widetilde{\alpha_s}(\frac{1}{2})$, $\alpha_1(k)$ and $\widetilde{\alpha_s}(0)$ so that

$$k \in [0, \frac{1}{2}], \quad \det A_0(k) = e^{i\alpha_0(k)} \quad \text{and} \quad \det A_1(k) = e^{i\alpha_1(k)},$$

while

$$\forall s \in [0,1], \quad \det A_s(0) = \mathrm{e}^{\mathrm{i}\widetilde{\alpha_s}(0)} \quad \mathrm{and} \quad \det A_s(\frac{1}{2}) = \mathrm{e}^{\mathrm{i}\widetilde{\alpha_s}(\frac{1}{2})},$$

together with the continuity conditions

С

$$\alpha_0(k=\frac{1}{2}) = \widetilde{\alpha_{s=0}}(\frac{1}{2}), \quad \widetilde{\alpha_{s=1}}(\frac{1}{2}) = \alpha_1(k=\frac{1}{2}), \text{ and } \alpha_1(k=0) = \widetilde{\alpha_{s=1}}(0).$$

With such a choice, the winding of det(A) along the loop $\partial \Omega_0$ is

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$$W := \frac{1}{2\pi} \left[\widetilde{\alpha_0}(0) - \alpha_0(0) \right] \in \mathbb{Z}$$

We claim that $W \in 2\mathbb{Z}$ is even iff $\operatorname{Index}_{1}^{\operatorname{DIII}}(P_{0}) = \operatorname{Index}_{1}^{\operatorname{DIII}}(P_{1})$. The idea is to follow a continuation of the phase of $\sqrt{\det A}$ along the boundary. For $j \in \{0, 1\}$, we denote by $\varepsilon_{j} := \operatorname{Index}_{1}^{\operatorname{DIII}}(P_{j})$ the index for the sake of clarity. By definition of the Index, we have

$$\frac{e^{i\frac{1}{2}\alpha_0(\frac{1}{2})}}{\Pr A_0(\frac{1}{2})} = \frac{e^{i\frac{1}{2}\alpha_0(0)}}{\Pr A_0(0)} \varepsilon_0, \quad \text{and, similarly,} \quad \frac{e^{i\frac{1}{2}\alpha_1(\frac{1}{2})}}{\Pr A_1(\frac{1}{2})} = \frac{e^{i\frac{1}{2}\alpha_1(0)}}{\Pr A_1(0)} \varepsilon_1$$

On the segment $(k, s) = \{\frac{1}{2}\} \times [0, 1]$, the map $s \mapsto \operatorname{Pf} A_s(\frac{1}{2})$ is continuous, and is a continuous representation of the square root of the determinant. So

$$\frac{e^{i\frac{1}{2}\widetilde{\alpha_{0}}(\frac{1}{2})}}{\Pr A_{0}(\frac{1}{2})} = \frac{e^{i\frac{1}{2}\widetilde{\alpha_{1}}(\frac{1}{2})}}{\Pr A_{1}(\frac{1}{2})}, \text{ and similarly, } \frac{e^{i\frac{1}{2}\widetilde{\alpha_{0}}(0)}}{\Pr A_{0}(0)} = \frac{e^{i\frac{1}{2}\widetilde{\alpha_{1}}(0)}}{\Pr A_{1}(0)}$$

Gathering all expressions, and recalling the continuity conditions, we obtain

$$\frac{\mathrm{e}^{\mathrm{i}\frac{1}{2}\widetilde{\alpha_0}(0)}}{\mathrm{Pf}\,A_0(0)} = \varepsilon_0\varepsilon_1\frac{\mathrm{e}^{\mathrm{i}\frac{1}{2}\alpha_0(0)}}{\mathrm{Pf}\,A_0(0)}, \quad \mathrm{so} \quad \mathrm{e}^{\mathrm{i}\pi W} = \varepsilon_0\varepsilon_1.$$

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This proves our claim.

If the indices differ, then we have $\varepsilon_0\varepsilon_1 = -1$, hence W is odd. In particular, $W \neq 0$, and one cannot find an homotopy in this case. Assume now that that two indices are equal, so that $\varepsilon_0\varepsilon_1 = 1$ and $W \in 2\mathbb{Z}$ is even. There is no reason a priori to have W = 0, but we can cure the winding. Indeed, we set

$$\widetilde{A}_s(0) := \widetilde{V}_s(0)^T J_n \widetilde{V}_s(0), \quad \text{with} \quad \widetilde{V}_s(0) := \text{diag}(\mathrm{e}^{\mathrm{i}\pi W s}, 1, \cdots, 1) V_s(0).$$

The family $A_s(0)$ is a continuous family connecting $A_0(0)$ and $A_1(0)$ in DIII(0, n, 2n). In addition, we have det $\widetilde{A}_s(0) = e^{2i\pi Ws} \det A_s(0)$, so this new interpolation curves the winding. Invoking Lemma IV.1 concludes the proof.

D. Class CII

Finally, it remains to study the class CII, in which we have both $T^2 = -\mathbb{I}_{\mathcal{H}}$ and $C^2 = -\mathbb{I}_{\mathcal{H}}$.

Lemma IV.8. Assume CII(0, n, N) is non empty. Then n = 2m is even, and N = 2n = 4m is a multiple of 4. There is a basis of \mathcal{H} in which

$$T = \begin{pmatrix} -K_n J_n & 0\\ 0 & -K_n J_n \end{pmatrix}, \quad C = \begin{pmatrix} K_n J_n & 0\\ 0 & -K_n J_n \end{pmatrix}, \quad and \quad S = \begin{pmatrix} \mathbb{I}_n & 0\\ 0 & -\mathbb{I}_n \end{pmatrix}.$$

Proof. The proof is similar to the one of Lemma IV.6. Details are left to the reader.

In this basis, the condition $T^{-1}P(k)T = P(-k)$ reads, in terms of Q,

$$J_n \overline{Q}(k) J_n = -Q(-k)$$
, or equivalently $Q(k)^T J_n Q(-k) = J_n$.

In particular, in dimension d = 0, we have $Q \in U(2m) \cap Sp(2m; C) = Sp(m)$. So

$$\operatorname{CII}(0, 2m, 4m) \simeq \operatorname{Sp}(m).$$

Theorem IV.9 (Class CII). The set CII(d, n, N) is non-empty iff $n = 2m \in 2\mathbb{N}$ and N = 2n = 4m.

- The set CII(0, 2m, 4m) is path-connected.
- Define the map $\operatorname{Index}_{1}^{\operatorname{CII}}$: $\operatorname{CII}(1, 2m, 4m) \to \mathbb{Z}$ by

$$\forall P \in \operatorname{CII}(1, 2m, 4m), \quad \operatorname{Index}_{1}^{\operatorname{CII}}(P) := \operatorname{Winding}(\mathbb{T}^{1}, Q).$$

Then P_0 is homotopic to P_1 in CII(1, 2m, 4m) iff $\operatorname{Index}_1^{\operatorname{CII}}(P_0) = \operatorname{Index}_1^{\operatorname{CII}}(P_1)$.

Proof. We already proved in Theorem III.5 that Sp(m) is connected, which yields the first part.

For the d = 1 case, we first note that if $Q \in \operatorname{Sp}(m)$, we have $Q^T J_n Q = J_n$. Taking Pfaffians, we get $\det(Q) = 1$. As in the proof of Theorem IV.3, we deduce that any path $Q_s(0)$ connecting $Q_0(0)$ and $Q_1(0)$ in $\operatorname{Sp}(m)$ has a determinant constant equal to 1, hence does not contribute to the winding. The proof is then similar to the one of Theorem IV.3.

Appendix A: Matrix factorizations

In this appendix, we show how to factorize certain classes of matrices we encountered in the main body of the paper. The first result has been discovered many times, and is known as the Autonne–Tagaki factorization [2]. The proof we present is found in [20, Cor. 4.4.4] for the complex case, and in [8] for the symplectic case. For the sake of the reader, we give a unified proof which employs also tools from [23] in the symplectic case.

Recall that we denote by $\mathcal{S}_n^{\mathbb{R}}(\mathbb{C})$ the set of $n \times n$ (complex) matrices, symmetric in the sense $A = A^T$, and by $\mathcal{A}_n^{\mathbb{R}}(\mathbb{C})$ the anti-symmetric ones, satisfying $A = -A^T$.

Theorem A.1 (Autonne–Tagaki factorization). Let $A \in S_n^{\mathbb{R}}(\mathbb{C})$, and let Λ be the diagonal matrix composed of the (non-negative) singular values of A. Then there is a unitary $U \in U(n)$ such that $A = U\Lambda U^T$.

If n = 2m and A is also symplectic, i.e. $A^T J_n A = J_n$, then U and Λ can be chosen to be symplectic as well.

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The above factorization is not a spectral decomposition, which involves similarities of the form U^*AU rather than congruences of the form U^TAU .

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Proof. By definition, singular values of A are the (non-negative) square roots of the eigenvalues of the positive Hermitian operator $H := A^*A$. The operator H is hermitian, hence diagonalizable, of the form $H = W\Lambda^2 W^*$ for some $W \in U(n)$. Define

$$L := W^T A W$$

and observe that $L^T = L$. Using the unitarity of W and the symmetry of A, we have

$$L^*L = W^*A^*\overline{W}W^TAW = W^*A^*AW = \Lambda^2,$$

$$LL^* = W^TAWW^*A^*\overline{W} = W^TA\overline{AW} = \overline{W^*A^*AW} = \overline{\Lambda^2} = \Lambda^2,$$

as Λ^2 is real-valued. So $LL^* = L^*L$, *i.e.* the operator L is normal, thus admits a polar decomposition L = VP with $P := (L^*L)^{1/2} = \Lambda$ and $V \in U(n)$ which *commute* among each other. As Λ is diagonal and V commutes with it, we may choose V to be diagonal as well. In particular, it is symmetric, $V = V^T$. If $V = \text{diag}(e^{i\phi_1}, \ldots, e^{i\phi_n})$, denote by $V^{1/2} := \text{diag}(e^{i\phi_1/2}, \ldots, e^{i\phi_n/2})$. This gives

$$W^T A W = L = V \Lambda = V^{1/2} \Lambda V^{1/2}$$
 hence $A = U \Lambda U^T$ with $U := \overline{W} V^{1/2}$.

In the symplectic case, we can prove that each matrix appearing previously can be chosen symplectic as well. For the matrices W and Λ^2 , this follows from [23, Prop. 3]. We directly check that L is symplectic if A is, and its polar decomposition L = VP can be chosen with V and P symplectic [23, Prop. 4].

We deduce the following useful corollary. The fact that $Sp(m) \cap O(2m) \simeq U(m)$ is proved below in Proposition A.5.

Corollary A.2.

• A matrix A is in $U(n) \cap \mathcal{S}_n^{\mathbb{R}}(\mathbb{C})$ iff it is of the form

$$A = V^T V$$
 with $V \in U(n)$

In addition, $A = V_0^T V_0 = V_1^T V_1$ with $V_0, V_1 \in U(n)$ iff $V_0 V_1^* \in O(n)$. In particular, $U(n) \cap \mathcal{S}_n^{\mathbb{R}}(\mathbb{C}) \simeq U(n)/O(n)$. • A matrix A is in $O(n) \cap \mathcal{S}_n^{\mathbb{R}}(\mathbb{C})$ iff there is $0 \le j \le n$ so that A is of the form

$$A = V^T D_j V$$
 with $V \in SO(n)$, and $D_j := \operatorname{diag}(\underbrace{1, \cdots, 1}_{j}, \underbrace{-1, \cdots, -1}_{n-j})$.

The set $O(n) \cap S_n^{\mathbb{R}}(\mathbb{C})$ has n+1 connected components, labeled by the signature.

• Assume n = 2m. A matrix A is in $\operatorname{Sp}(m) \cap \mathcal{S}_{2m}^{\mathbb{R}}(\mathbb{C})$ iff it is of the form

$$A = V^T V$$
 with $V \in \operatorname{Sp}(m)$

In addition, $A = V_0^T V_0 = V_1^T V_1$ with $V_0, V_1 \in \operatorname{Sp}(m)$ iff $V_0 V_1^* \in \operatorname{Sp}(m) \cap \operatorname{O}(2m) \simeq \operatorname{U}(m)$. In particular, $\operatorname{Sp}(m) \cap \mathcal{S}_{2m}^{\mathbb{R}}(\mathbb{C}) \simeq \operatorname{Sp}(m)/\operatorname{U}(m)$.

Proof. If $A \in U(n) \cap S_n^{\mathbb{R}}(\mathbb{C})$, its singular values are all equal to 1, so the Autonne–Tagaki factorization of A is of the form $A = UU^T = V^T V$ with $V = U^T$.

If $A = V_0^T V_0 = V_1^T V_1$ with $V_0, V_1 \in U(n)$, then $Z := V_0 V_1^*$ is unitary, and satisfies $Z = (Z^*)^T = \overline{Z}$, that is Z is real-valued. So $Z \in O(n)$ as wanted.

The proof in the symplectic case is similar.

If $A \in O(n) \cap S_n^{\mathbb{R}}(\mathbb{C})$, then the usual diagonalization of A shows that A is of the form $A = V^T D V$ with $V \in SO(n)$, and D the diagonal matrix with the eigenvalues of A, counting multiplicities, and ranked in decreasing order. Since the eigenvalues of $A \in O(n)$ are ± 1 , we have $D = D_j$ with $j = \dim \operatorname{Ker}(A-1)$. If A_0 and A_1 have different signatures, they are in different connected components of $O(n) \cap S_N^{\mathbb{R}}(\mathbb{C})$, and if they have the same signature, they can be connected by connecting the corresponding V's. This concludes the proof.

The anti-symmetric analogue of the Autonne–Tagaki factorization is known as Hua's decomposition [21, Thm. 7]. We set $J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

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Recall that if n is odd, then $A = -A^T$ is never non-degenerate, since $det(A) = det(A^T) = (-1)^n det(A) = -det(A)$, hence det(A) = 0.

Proof. Consider the positive Hermitian matrix $H := A^*A$. Observe that, in view of the non-degeneracy of A,

$$\det \left(A^*A - \lambda \mathbb{I}_n\right) = \det \left(A^* - \lambda A^{-1}\right) \det(A) = \operatorname{Pf}(A)^2 \left[\operatorname{Pf}\left(A^* - \lambda A^{-1}\right)\right]^2$$

where we used that $A^* - \lambda A^{-1} \in \mathcal{A}_n^{\mathbb{R}}(\mathbb{C})$. Therefore, the characteristic polynomial of H is a perfect square. This implies that its roots (*i.e.* the singular values of A) are of even multiplicity, and in particular their number, which is n, must be even.

Consider now $\Lambda := D \otimes J_2$ as in the statement. If $D = \text{diag}(\lambda_1, \ldots, \lambda_m)$, then

$$\Lambda^*\Lambda = \Lambda^T\Lambda = \operatorname{diag}(\lambda_1^2, \lambda_1^2, \dots, \lambda_m^2, \lambda_m^2)$$

The spectral decomposition of H implies the existence of $W \in U(m)$ such that $H = W\Lambda^*\Lambda W^*$. As in the proof of Theorem A.1, set

$$L := W^T A W.$$

Using that $A^T = -A$, we have $L^T = -L$. We also have $L^*L = \Lambda^*\Lambda$, which can be recast as

$$(L\Lambda^{-1})^{-1} = \Lambda L^{-1} = (\Lambda^*)^{-1}L^* = (L\Lambda^{-1})^*$$

that is, the matrix $L\Lambda^{-1} =: V$ is unitary. The skew-symmetry of L and of Λ also gives

$$V\Lambda = L = -L^T = -\Lambda^T V^T = \Lambda V^T.$$

Diagonalize now the unitary matrix V:

$$V = \Gamma \Delta \Gamma^*$$
 with $\Gamma \in \mathrm{U}(n)$, $\Delta := \mathrm{diag}\left(\mathrm{e}^{\mathrm{i}\phi_1}, \dots, \mathrm{e}^{\mathrm{i}\phi_n}\right)$.

Set also

$$\Delta^{1/2} := \operatorname{diag}\left(\mathrm{e}^{\mathrm{i}\phi_1/2}, \dots, \mathrm{e}^{\mathrm{i}\phi_n/2}\right), \quad V^{1/2} := \Gamma \Delta^{1/2} \Gamma^*.$$

Clearly, $(V^{1/2})^2 = V$ and, by functional calculus, $V^{1/2}\Lambda = \Lambda (V^{1/2})^T$. We obtain

$$W^T A W = L = V \Lambda = V^{1/2} \Lambda (V^{1/2})^T$$

that is

$$A = U (D \otimes J_2) U^T$$
, with $U := (W^T)^* V^{1/2}$

This concludes the proof for the complex case. The real case follows immediately, upon noticing that a real-valued unitary matrix is automatically orthogonal. $\hfill \square$

Corollary A.4.

• A matrix A is in $U(2m) \cap \mathcal{A}_{2m}^{\mathbb{R}}(\mathbb{C})$ iff it is of the form

$$A = V^T J_{2m} V \quad with \quad V \in \mathrm{U}(2m).$$

In addition, $A = V_0^T J_{2m} V_0 = V_1^T J_{2m} V_1$ with $V_0, V_1 \in U(2m)$ iff $V_0 V_1^* \in Sp(m)$. In particular, $U(2m) \cap \mathcal{A}_{2m}^{\mathbb{R}}(\mathbb{C}) \simeq U(2m)/Sp(m)$.

• A matrix A is in $O(2m) \cap \mathcal{A}_{2m}^{\mathbb{R}}(\mathbb{C})$ iff it is of the form

$$A = W^T J_{2m} W \quad with \quad W \in \mathcal{O}(2m). \tag{A.1}$$

and, setting $\Lambda_A := \operatorname{diag}(1, 1, \cdots, 1, \operatorname{Pf}(A)) \otimes J_2$, iff it is also of the form

$$A = V^T \Lambda_A V \quad with \quad V \in \mathrm{SO}(2m). \tag{A.2}$$

If $A = W_0^T J_{2m} W_0 = W_1^T J_{2m} W_1$ with $W_0, W_1 \in O(2m)$, then $W_0 W_1^* \in \operatorname{Sp}(2m; \mathbb{R}) \cap O(2m) \simeq U(m)$. In particular, $O(2m) \cap \mathcal{A}_{2m}^{\mathbb{R}}(\mathbb{C}) \simeq O(2m)/U(m)$.

$$A = U\left(\mathbb{I}_m \otimes J_2\right) U^T. \tag{A.3}$$

Upon reshuffling the columns of $\mathbb{I}_m \otimes J_2$, we can transform $\mathbb{I}_m \otimes J_2$ into J_{2m} . We deduce that there is $V \in U(2m)$ so that $A = V^T J_{2m} V$. If $A = V_0^T J_{2m} V_0 = V_1^T J_{2m} V_1$, with $V_0, V_1 \in U(2m)$, then $Z := V_0 V_1^*$ is in U(2m), and satisfies $Z^T J_{2m} Z = J_{2m}$, that is, Z is symplectic.

The proof for (A.1) is similar. It remains to prove (A.2). Let $A \in O(2m) \cap \mathcal{A}_{2m}^{\mathbb{R}}(\mathbb{C})$. Using (A.3) in the real case, we see that there is $U \in O(2m)$ so that $A = U^T(\mathbb{I}_n \otimes J_2)U$ with $U \in O(2m)$. We have $\det(U) \in \{\pm 1\}$, and

$$Pf(A) = Pf(U^T(\mathbb{I}_n \otimes J_2)U) = \det(U)Pf((\mathbb{I}_n \otimes J_2)) = \det(U).$$

If det(U) = 1, we simply take V := U, otherwise we take

$$V = \operatorname{diag}(1, 1, \cdots, 1, -1)U$$

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We end this Appendix with the following result.

Proposition A.5. The group $\operatorname{Sp}(2m; \mathbb{R}) \cap \operatorname{O}(2m) = \operatorname{Sp}(2m; \mathbb{C}) \cap \operatorname{O}(2m) \subset \operatorname{Sp}(m)$ is isomorphic to $\operatorname{U}(m)$.

Proof. If $U \in \text{Sp}(2m; \mathbb{R}) \cap O(2m)$, then $J_{2m} = U^T J_{2m} U = U^{-1} J_{2m} U$ hence $U J_{2m} = J_{2m} U$. Decomposing U in block form, this condition is equivalent to

$$U = \begin{pmatrix} A & B \\ -B & A \end{pmatrix} = \overline{U} \quad \text{with} \quad A^T A + B^T B = \mathbb{I}_m, \quad A^T B - B^T A = 0.$$

These conditions are equivalent to the fact that the $m \times m$ matrix V := A + iB is unitary. Indeed

$$(A + iB)^*(A + iB) = (A^T - iB^T)(A + iB) = (A^T A + B^T B) + i(A^T B - B^T A) = \mathbb{I}_m.$$

This concludes the proof.

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