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ABSTRACT

We analyze topological invariants, in particular $\mathbb{Z}_2$ invariants, which characterize time reversal invariant topological insulators, in the framework of index theory and K-theory. After giving a careful study of the underlying geometry and K-theory, we formalize topological invariants as elements of *KR* theory. To be precise, the strong topological invariants lie in the higher *KR* groups of spheres; $\widetilde{KR}^{-j-1}(\mathbb{S}^{D+1,d})$. Here j is a *KR*-cycle index, as well as an index counting off the Altland-Zirnbauer classification of Time Reversal Symmetry (TRS) and Particle Hole Symmetry (PHS)—as we show. In this setting, the computation of the invariants can be seen as the evaluation of the natural pairing between *KR*-cycles and *KR*-classes. This fits with topological and analytical index computations as well as with Poincaré Duality and the Baum–Connes isomorphism for free Abelian groups. We provide an introduction starting from the basic objects of real, complex and quaternionic structures which are the mathematical objects corresponding to TRS and PHS. We furthermore detail the relevant bundles and *K*-theories (Real and Quaternionic) that lead to the classification as well as the topological setting for the base spaces.

I. INTRODUCTIONc

The unexpected appearance of a topological $\mathbb{Z}_2$-valued invariant by Kane and Mele[1] has sparked a great effort by many groups to understand this important phenomenon. The fact that there are more such invariants which fit into periodic patterns goes back to the seminal work of Kitaev,[2] see also Ref. 3. In Ref. 4, Teo and Kane accumulated the known topological invariants for systems with Time Reversal Symmetry (TRS) and/or Particle Hole Symmetry (PHS) depending on the dimension d of the system and the dimension of a defect D. The classes of quadratic Hamiltonians carrying TRS and PHS symmetries, aka. the tenfold way, were previously classified by Altland and Zirnbauer.[5]

Our approach goes back to Ref. 6 and uses variants of K-theory, in particular *KR* (Real K-theory) as introduced by Atiyah[7] and *KQ* (Quaternionic K theory) as introduce by Dupont.[8] A key role is played by the double indexed *KR*-theory and its reduction to the single indexed *KR* theory, which allows us to match to the physical classification of Ref. 4 that features the two parameters d and D mentioned above. The connection to the classification by Altland and Zirnbauer[5] comes through the work of Connes[9] that identifies the bi-indexed *KR*-theory that is described via Clifford algebras, see Ref. 10, with a reduced version that is described by symmetry operators; see also Ref. 11. These symmetry operators in the mathematical theory are Real and Quaternionic structures and are identified below with the TRS and PHS operators appearing in the physics literature. This description is in the spirit of the interpretation of the TKNN integers[12] in terms of Chern classes, see Ref. 13, complemented with the idea of using K-theory to describe topological phenomena that goes back to the foundational paper by Bellisard *et al.*[14]

This matching between the *KR*-theory indices and the dimension and defect indices on the one hand and the matching of the *KR*-theory indices with the presence of symmetry operators on the other hand provides a bridge between the mathematical and physical formulations. In particular, see Tables I and IV which give the key to the translation. *KR*-theory also neatly explains that the correct variable for the classification is $\delta = d - D$. This is the (1,1) periodicity of $KR^{p,q}$. Another important ingredient are the odd and even 8-h clocks which allow to raise and lower the odd and even indices by even and odd suspensions. The even suspensions are already in Ref. 15 and accounts for the period 8 of *KR* theory. It is based on the periodicity of Clifford representations[10] and as such appears in spin-geometry.[16] The odd clock can be found in Ref. 4. We

TABLE I. The KR/AZ classification and translation. The index j corresponds to KR^j theory, and with it to spin geometry and Clifford algebras, see Refs. 11 and 16 and Example VII.5. The translation to physical symmetries in the AZ classification is given by $D = H$, the Hamiltonian, $C = \Theta$, the TRS operator in the cases $j \neq 1, 5$ and $C' = \Pi$, the PHS operator for $j = 0, 2, 4, 6$, where $\varepsilon_\chi = \varepsilon_{C'}\varepsilon_C$. In the cases $j = 1, 5$, $C = \Pi$. In all cases $\Pi H = -H\Pi$ and $\Theta H = H\Theta$, $\chi D = -D\chi$. The type refers to the type of operator: $\mathbb{R}$ Real or $\mathbb{H}$ is quaternionic.

j mod 8	0	1	2	3	4	5	6	7
$C^2 = \varepsilon_C 1$	+	+	⋯	⋯	⋯	⋯	+	+
$C\chi = \varepsilon_\chi \chi C$	+		⋯		+		⋯	
$CD = \varepsilon_D DC$	+	⋯	+	+	+	⋯	+	+
$C'^2 = \varepsilon_{C'} 1$	+		+		⋯		⋯	
$C'\chi = \varepsilon_\chi \chi C'$	+		⋯		+		⋯	
$C'D = -\varepsilon_D DC'$	⋯		⋯		⋯		⋯	
$CC' = \varepsilon_\chi C'C$	+		⋯		+		⋯	
AZ name	BDI	D	DIII	AII	CII	C	CI	AI
Type of C	$\mathbb{R}$	$\mathbb{R}$	$\mathbb{H}$	$\mathbb{H}$	$\mathbb{H}$	$\mathbb{H}$	$\mathbb{R}$	$\mathbb{R}$
Type of C'	$\mathbb{R}$		$\mathbb{R}$		$\mathbb{H}$		$\mathbb{H}$	

present a general framework, which has a more streamlined classical "diagonal" version of these clocks as well a second "anti-diagonal" version that is used in examples and computations.

There are two flavors of K-theory at work here, a geometric theory and an operator C^*-algebra theory. The former naturally includes bundles such as the Bloch bundle over momentum space, and the latter is the natural home for Hamiltonians and Hilbert spaces. The two are directly related by considering the Hilbert space of sections of a bundle. There is a second relationship by using the theory of KR-homology and pairing of KR-cycles with KR classes. This is the most natural way to pair the bundle structure with Hamiltonians in a given symmetry class, as we explain. An approach using operator KR-theory was put forth in Ref. 17 and the articles[17–23] appeared more or less contemporaneously with the announcement.[6] In the interim there has been a lot of activity in this research area.[24–45] In Ref. 29 the authors follow the lead of the approach of Ref. 46, which presents another interesting access to the theory with possibly more symmetries using twisted representation rings and the Atiyah–Hirzebruch spectral sequence. Here we concentrate only on the symmetries coming from TRS and PHS, and show that they are naturally handled by the classical KR and KQ theory. All these contributions are valuable to the understanding of this complex subject.

The aim of the present article is to give a geometric interpretation of the full periodic table and to give an explanation of the dimension shift, see the first two columns of Table IV. The surprising upshot is that the periodicity of the table of Ref. 4, reproduced in Table IV, can be nicely summarized as saying that the strong invariants lie in $\widetilde{KR}^{-j-2}(\mathbb{S}^{D,d})$. Here KR is Real K-theory, that is the K-theory of so-called Real bundles as introduced in Ref. 7, $\widetilde{KR}$ is the reduced version, and $\mathbb{S}^{D,d}$ is the $D-d-1$ dimensional unit sphere in $\mathbb{R}^{D,d}$. This space is $\mathbb{R}^D \oplus \mathbb{R}^d$ equipped with the involution $\tau(x, y) = (x, -y)$. The index j in the first identification is related to the arrangements used in Refs. 2 and 4, in particular $s = j+1$ and $\delta = d - D$ in terms of Ref. 4. The index j is in its origin a suspension index used to define higher KR-groups. More deeply, in the theory of KR-cycles, after further reduction,[9,11,47] the index j can be seen as enumerating antiunitary symmetries which can be matched to the AZ classification. The corresponding symmetries, the index j and the AZ classification are given in Table I. This gives a straightforward, clear mathematical link between the cycle theory and the AZ classification. The invariants are summarized in Table IV. In one direction, this allows one to understand the symmetries in terms of (geometric) Real and Quaternionic structures. Conversely, this is the reason for the appearance of Real and Quaternionic theory. Note that previously several ways of counting off the AZ-classification were used, see Refs. 2–4 here we tie the enumeration to the KR index j. Note that the identification of the operators depends on this index. A doubling construction allows us to construct examples for all even j starting with an arbitrary Hamiltonian; see Corollary II.13. We furthermore construct examples with j odd from examples with j even; see Corollary II.15. These are the types of Hamiltonians for instance that appear in Refs. 3 and 4. Parameter dependent examples are given in Examples III.11, III.18, III.19, and VII.5.

To make the connection with the two parameters D, for the defect, and d, for the dimension, one has to use a bi-indexing of KR-theory and Clifford algebras corresponding to the action on $\mathbb{R}^{D,d}$ above.[7,48] The surprising aspect is that the two theories from completely different origin, physics and mathematics, meet in this formulation. There is a subtlety in the indexing and shifts. The main reason is that the sphere $\mathbb{S}^{D,d}$ is the one-point compactification of $\mathbb{R}^{D-1,d}$, so that by definition $KR^{-s}(\mathbb{R}^{D,d}) = \widetilde{KR}^{-s}(\mathbb{S}^{D+1,d}) \simeq \widetilde{KR}^{-j-2}(\mathbb{S}^{D,d})$ with $-s-1 = -j-2$. The point of contact with the usual theory from physics is that the invariants from Bloch theory lie in $KR^{-s}(\mathbb{T}^d)$, and T^d has the involution $k \to -k$. This contains a summand corresponding to $KR^{-s}(\mathbb{R}^{0,d}) = \widetilde{KR}^{-s}(\mathbb{S}^{1,d}) \simeq \widetilde{KR}^{-j-2}(\mathbb{S}^{0,d})$. To obtain the relevant summand, one can either decompose the torus into a product $\mathbb{T}^d = (\mathbb{S}^{1,1})^{\times d}$, see Example VI.3 or use a quotient map, see Sec. III A 2 for details. The torus $\mathbb{T}^d$ is the quotient of the unit cube $I^{0,d} \subset \mathbb{R}^{0,d}$ by periodic boundary conditions. As such, $\mathbb{T}^d$ has a natural projection to $\mathbb{S}^{1,d}$ by quotienting out by the image of the $\partial I^{0,d} \approx \mathbb{S}^{0,d}$. The strong summand, that is the one carrying the strong invariants, is now the pullback under the projection of $\widetilde{KR}^{-s}(\mathbb{S}^{1,d})$. After the shift one can view the invariants $\widetilde{KR}^{-j-2}(\mathbb{S}^{0,d})$ as invariants of the boundary, which is one interpretation of the bulk/boundary map, where now the bulk is the interior of the cube, which is not touched by the quotients. In the case with defects, the base manifold is $T^d \times S^{D4}$ and one can define a cell model with one top-dimensional cell $\mathbb{S}^{D+1,d}$.

In general, for a $\mathbb{Z}/2\mathbb{Z}$ equivariant CW complex X, the invariants lie in $KR^{-s}(X)$, and if there is a unique top-dimensional open cell $\mathbb{R}^{D,d}$, the strong invariants live in $KR^{-j-2}(\mathbb{S}^{D,d})$. For example, $\mathbb{S}^{1,d}$ is a d-dimensional sphere. Taking the cell models with two cells, a 0-cell $\{\infty\}$ and a d-cell $\mathbb{R}^{0,d}$ ($\mathbb{S}^{1,d}$ is the one-point compactification of $\mathbb{R}^{0,d}$), the strong summand is $\widetilde{KR}^{-j-2}(\mathbb{S}^{0,d})$ which coincides with the strong summand of $\mathbb{T}^d$.

The relationship to the general (weak) invariants, which are given by lower dimensional cells, can be made explicit by KR theory using exact sequences. These sequences have appeared in the literature in various approaches to compute the invariants, as we discuss. These also apply in the case that there is not a single top-dimensional cell, E.g. $X = \mathbb{S}^{0,d+1}$, that is the d-dimensional sphere with the antipodal map, which is another common base space considered in physics, has a decomposition where the cells are built up iteratively from the hemispheres. These kinds of spaces are considered in Sec. III.

Of particular interest are the cases AI, that is $s = 0$, which has no shifts on $\mathbb{T}^d$. In particular, this is the case $j = 7$ which has one bosonic TRS operator and an anti-unitary operator Θ with $\Theta^2 = 1$. The invariants lie in the Real K-theory of the torus $KR(\mathbb{T}^d)$. This is in line with the fact that $j = 7$ is the case of a bosonic TRS operator, and these operators are part of the structure of a Real vector bundle, see Sec. VI. In the case AII, that is $s = 4$, the relevant theory on $\mathbb{T}^d$ is $KR^{-4}(\mathbb{T}^d) \simeq KQ(\mathbb{T}^d)$, where KQ is the theory of Quaternionic bundles.[8] This is the case $j = 3$ which has one Fermionic TRS operator, and an anti-unitary operator Θ with $\Theta^2 = -1$. This was the original reason to study KQ-theory as the Quaternionic bundles have such an operator as part of the structure; see Sec. VI. The Kane–Mele invariant is then in $KR^{-4}(\mathbb{T}^2) = KQ(\mathbb{T}^2)$ whose strong summand is $KQ(\mathbb{S}^{0,2})$; by suspension this is the same as $KO^{-2}(pt) = \mathbb{Z}/2\mathbb{Z}$ that is the K-theory of vector bundles over the reals evaluated at a point. These groups are known, see Ref. 10 and Table III, and are the groups that appear in all periodic tables.

Going beyond the classification table, we realize the invariants as evaluations $KR^{-j-2}(X) \to KO^{D-d-j-1}(pt)$ through standard pairings coming from KR theory via so-called KK theory.[47,49] This is a kind of "reading out" of the invariants from the potential invariants to ones realized by a particular Hamiltonian. In the particular case of the torus $\mathbb{T}^d$, the pairing can be seen as given by a natural combination of maps including Poincaré duality and an assembly map.

It has been demonstrated, see e.g. Ref. 50 for an overview, that the invariants can be computed through local contributions given by Pfaffians or odd Chern characters. This involves bundle theory on CW complexes and local data in this situation. We include a detailed analysis of this geometry.

The paper is organized a follows. In Sec. II, we start by reviewing the basic notions in the detail needed in the paper. The physical interpretation is given in Sec. II B. We then combine the two classifications AZ and KR-cycle in Theorem II.10, which is summarized in Table I. A crucial structural result is Proposition II.6. We introduce examples via Pauli-matrices which are fundamental for the further constructions and examples, such as the construction of doubling detailed in Sec. II D 3.

Section III concerns families of Hamiltonians parameterized by a space—classically, momentum space. We give the basic examples of pertinent involutive spaces. We then review the theory Real and Quaternionic vector bundles, which are the mathematical description of the symmetry actions. The physical setup of Hilbert and Bloch bundles is discussed in Sec. III C. The section ends with general constructions and concrete examples Sec. III D. Using the analysis of Sec. II D 3, we can define the two 8-h clocks found in Refs. 4 and 15 which are connected to the Pauli-matrices via Clifford algebras,[11,16] see Theorem III.20.

Section IV studies the possible degeneracies and level crossings of the Bloch bundle. A signature of the fermionic theory, which is Quaternionic, in this description, is Kramers degeneracy, as we discuss. This leads to an interesting level crossing structure in the cases with $\Theta^2 = -1$ where in physics Θ is the TRS operator. We also introduce the sewing matrices, which transform the computations of the topological invariants into gauge-anomalies, which can be used to compute odd Chern classes.

In Sec. V, we analyze the geometry of the underlying space further. This gives restrictions on the spaces to be what we call tame equivariant CW-complexes. On these spaces, the sewing matrices, and spectral flow can be used to compute the invariants. It is also here that one can identify the doubling constructions and "effective boundary" of a theory.

In Sec. VI, we introduce the higher KR and KQ groups and explain the various long exact sequences used for computation pointing out where in the literature they have been used. This allows to identify the classification of Ref. 4 with the KR groups $KR^{-s}(\mathbb{S}^{D+1,d})$, see Theorem VI.15. The analysis allows to define the general invariants as $KR^{-s}(X)$. This recovers the weak invariants for $\mathbb{T}^3$. KR-cycles are also reviewed in this section which finalizes the identification in Table I. We then discuss discussion of how the local structure can be seen as a spectral flow combining the analysis of Sec. III with the classical theory of Ref. 15. The identification is more concrete in the basic example of $\mathbb{T}^d$ where it comes from the topological index of Ref. 51, see Sec. VI E.

The last Sec. VII reviews the theory of KR-cycles following Refs. 9 and 11. There is a natural pairing between cycles and KR-classes, which we identify as giving the strong invariants, see Theorem VII.7. Alternatively, in this case, the pairing is given by a combination of Poincaré duality and other maps using assembly maps and the Baum–Connes conjecture, in cases where it has been proven, as envisioned by Kitaev,[2] see Sec. VII C.

Conventions

We will only use separable Hilbert spaces and drop this extra adjective. A basis is understood to be a topological basis. Without extra mention, the Hilbert spaces are considered to be complex; if they are real, we add a subscript $\mathbb{R}$ as in $\mathscr{H}_\mathbb{R}$ and if they are quaternionic, $\mathscr{H}_\mathbb{H}$. If confusion may arise, we also write $\mathscr{H}_\mathbb{C}$ in the complex case. A non-zero element in a Hilbert space is called a state.

II. HILBERT SPACE DESCRIPTION OF TRS, PHS AND CHIRAL SYMMETRY

We will consider real, complex and quaternionic vector spaces and use the notation $\mathscr{H}_\mathbb{R}, \mathscr{H}_\mathbb{C}$ and $\mathscr{H}_\mathbb{H}$ to emphasize this. The presence of real and quaternionic structures and grading operators are then classified and when reinterpreted as TRS, PHS and chiral operators, used to match this classification to the AZ-classification. To make the connection one has to use that for particular pairs of such operators there is an equivalent formulation in terms of one of them and a grading operator, see Proposition II.6.

A. Mathematical setup

We will now collect results and consequences of dealing with grading operators and anti-unitaries. This leads to a translation between classifications of systems with these symmetries from mathematics and physics.

1. Anti-linear and anti-unitary operators

An anti-linear operator C satisfies $C(a\phi + b\psi) = \bar{a}C\phi + \bar{b}C\psi$. Such an operator can alternatively be thought of as a linear operator $C : \mathscr{H}_\mathbb{C} \to \bar{\mathscr{H}}_\mathbb{C}$ where $\bar{\mathscr{H}}_\mathbb{C}$ has the conjugate $\mathbb{C}$ action: $z \cdot \phi = \bar{z}\phi$.

An anti-unitary operator is an anti-linear operator which satisfies

$$\langle C\phi, C\psi\rangle = \langle \psi, \phi\rangle = \overline{\langle \phi, \psi\rangle} \tag{1}$$

This is commensurate with the sesqulinear form on $\bar{\mathscr{H}}$ being $\langle \phi, \psi\rangle_{\bar{\mathscr{H}}} = \overline{\langle \phi, \psi\rangle}_{\mathscr{H}}$. The adjoint of an anti-linear operator is defined by $\langle C^*\phi, \psi\rangle = \overline{\langle \phi, C\psi\rangle} = \langle C\psi, \phi\rangle$. If C is anti-unitary and $C^2 = \pm 1$, then $C^* = \pm C = C^{-1}$, since $\pm\langle C\phi, \psi\rangle = \langle C\phi, C^2\psi\rangle = \overline{\langle \phi, C\psi\rangle}$. In this way, one can write the adjoints as $C : \mathscr{H} \leftrightarrows \bar{\mathscr{H}} : C^*$ with $C^*C = CC^* = 1$. Note any anti-linear operator with $C^2 = \pm 1$ is anti-unitary. Anti-unitary operators may be rescaled by phases. That is, for C set $\tilde{C} = e^{i\alpha}C$, then one computes $\tilde{C}^*\tilde{C} = C^*C = 1$ and $\tilde{C}^2 = C^2$.

2. $\mathbb{Z}_2$ (aka. super) grading

A $\mathbb{Z}_2$ grading operator χ on $\mathscr{H} = \mathscr{H}_k$, $k = \mathbb{R}, \mathbb{C}, \mathbb{H}$ is a k-linear operator with $\chi^2 = 1$. This defines projectors to the plus and minus one eigenspaces of χ, which are classically denoted additively as $\mathscr{H}_0$ and $\mathscr{H}_1$; and $\mathscr{H}$ splits as $\mathscr{H} = \mathscr{H}_0 \oplus \mathscr{H}_1$. The projectors are $P_0 = \frac{1}{2}(1+\chi)$ and $P_1 = \frac{1}{2}(1-\chi)$ and the splitting is ordered. Reversing the order of the splitting correspondes to changing χ to $-\chi$.

A grading operator is balanced, if the spaces $\mathscr{H}_0$ and $\mathscr{H}_1$ are isomorphic. This is equivalent to the existence of an isomorphism of $\mathscr{H}$ that anti-commutes with χ. Choosing a basis such an isomorphism is a matching between basis elements. In the finite dimensional case the obstruction to the existence of such a matching is given by the signature $Tr(\chi) = r - s \in \mathbb{Z}$ where r is the number of positive and s is the number of negative Eigenvalues of χ. This flips sign under $\chi \to -\chi$ which is the exchange of H_0 and H_1. If a matching is possible then the obstruction vanishes and hence $r = s$. In this case, one can consider the value of $r = \frac{1}{2}(r+s) \bmod 2 \in \mathbb{Z}_2$. Here $r + s = sTr(\chi)$ is the supertrace. This is invariant under $\chi \to -\chi$ and only depends on the summands, not their orders.

3. Real structure on complex vector spaces

A real structure on a complex vector space is an *anti-linear* involution, i.e. an anti-linear operator C with $C^2 = 1$. This is the generalization of complex conjugation K in $\mathbb{C}$.

A vector is real, if $C\phi = \phi$ and purely imaginary if $C\phi = -\phi$. The vectors $\phi \pm C\phi$ are real respectively purely imaginary. Picking a basis ψ_k, the basis $\phi_k = \frac{1}{2}(\psi_k + C\psi_k)$ is a real basis. An operator D is real if it commutes with C and purely imaginary if it anti-commutes. If D is real, it preserves real and purely imaginary vectors and if it is purely imaginary then interchanges these. If D is real, then iD is purely imaginary and vice versa.

Remark II.1. Given one real structure K, any anti-linear operator C defines the linear invertible operator $L = CK$, and vice versa setting $C = LK$ defines a new real structure. If C and K are anti-unitary, $U_C := L$ is unitary and $C = U_CK$, this goes back to Ref. 52. Thus, if there is already a canonical (or chosen) unitary real structure K, we can interpret $C = U_CK$ as a unitary transformation of the standard real structure.

Example II.2. If $\mathscr{H}$ is just an abstract complex vector space, then there is no such canonical real structure. Choosing a basis ϕ_k fixes a real structure C defined by conjugating the coefficients as follows: $\sum_k z_k\phi_k \mapsto \bar{z}_k\phi_k$. Changing to a different base is implemented by a an invertible operator L and the new real structure $C = LKL^{-1}$. Note, $C = K$ precisely if L is real.

Example II.3. For any set or space X the space of maps $\mathrm{Map}(X, \mathbb{C})$ is a complex vector space and has a natural complex structure given by pulling back complex structures $\bar{\phi}(x) = \overline{\phi(x)}$. Thus on a vector space of functions or sections, and continuous, smooth or L^2 or all the usual versions of these, one has a canonical complex structure which we will call K and write $K(\phi) = \bar{\phi}$. In particular, the dual space $\mathscr{H}^* = \mathrm{Hom}(\mathscr{H}, \mathbb{C})$ has a canonical real structure. In a Hilbert space the morphism $\mathscr{H} \to \mathscr{H}^*$ given by $\phi \to \langle \phi, -\rangle$ is an injection and $\mathscr{H}$ has a canonical real structure by restriction.

Remark II.4. Restricting scalars to $\mathbb{R}$, the restriction $C_{\mathbb{R}}$ of C is $\mathbb{R}$ linear and is a grading operator. Hence there is a splitting $\mathscr{H}_{\mathbb{R}} = \mathscr{H}_{re} \oplus \mathscr{H}_{im}$ according to the $\pm$ eigenspaces. If ϕ_k is a real $\mathbb{C}$ basis for $\mathscr{H}$, it is an $\mathbb{R}$ basis for $\mathscr{H}_{re}$ and $C\phi_k$ is an $\mathbb{R}$ basis for $\mathscr{H}_{im}$. In the finite-dimensional case, it follows that $\dim_{\mathbb{R}}(\mathscr{H}) = 2\dim_{\mathbb{C}}(\mathscr{H})$, which accounts for the factor $\frac{1}{2}$ in the definition of the index ind_2, see Ref. 53.

4. Quaternionic structure

A quaternionic structure on a complex vector space is an anti-linear operator C with $C^2 = -1$. In this case, $\mathscr{H}$ is naturally a vector space $\mathscr{H}_{\mathbb{H}}$ over the quaternions $\mathbb{H}$ where C implements the left multiplication by $j : (z + jw)\phi = z\phi + Cw\phi = z\phi + \bar{w}C\phi$. For any non-zero ϕ, ϕ and $C\phi$ are linearly independent. Indeed, if $C\phi = \lambda\phi$ then $-\phi = C^2\phi = \bar{\lambda}\lambda\phi$ which is not possible as $\bar{\lambda}\lambda \geq 0$. The pair $(\phi, C\phi)$ is called a Kramers pair.

An operator D respects the quaternionic structure if it commutes with it, $CD = DC$. This means that the operator is $\mathbb{H}$ linear. If D anti-commutes with C, then iD commutes with C and vice versa.

If D is $\mathbb{H}$-linear, it follows that $\dim_{\mathbb{C}}(\ker(H(k)) = 2\dim_{\mathbb{H}}(\ker(H(k)))$ is even, as is the dimension $\dim_{\mathbb{C}}(\mathrm{coker}(H(k)))$ as well as the index of H. Since $\ker(iD) = \ker(D)$ and $\mathrm{coker}(iD) = \mathrm{coker}(D)$, these dimensions and the index are also even, if D anti-commutes with C.

Remark II.5. If $\mathscr{H}$ has a quaternionic structure, then we can view it as a quaternionic vector space $\mathscr{H}_{\mathbb{H}}$. Picking an $\mathbb{H}$ basis ϕ_k and then restricting scalars back to $\mathbb{C}$, $\mathscr{H}$ decomposes non-canonically as $\mathscr{H}_{\mathbb{C}} = \mathscr{H}'_{\mathbb{C}} \oplus \mathscr{H}''_{\mathbb{C}}$ where ϕ_k is a $\mathbb{C}$ basis for $\mathscr{H}'_{\mathbb{C}}$ and $C\phi_k$ is a $\mathbb{C}$ basis for $\mathscr{H}''_{\mathbb{C}}$. That is: $\mathscr{H}_{\mathbb{C}} = \mathscr{H}'_{\mathbb{C}} \oplus C\mathscr{H}'_{\mathbb{C}} \simeq \mathscr{H}'_{\mathbb{C}} \oplus \bar{\mathscr{H}}'_{\mathbb{C}}$ using that as an antilinear operator C provides an isomorphism $C : \mathscr{H}'_{\mathbb{C}} \to \bar{\mathscr{H}}'_{\mathbb{C}}$. Note choosing such a splitting is equivalent to choosing an anti-commuting grading operator χ.

In the finite-dimensional case the complex dimension of $\mathscr{H}$ is even. This is why some of the indices take values in $2\mathbb{Z}$.

Notice that once a quaternionic basis ϕ_k is fixed, restricting scalars all the way to $\mathbb{R}$ yields a decomposition $\mathscr{H}_{\mathbb{R}} = \tilde{\mathscr{H}}_{\mathbb{R}} \oplus i\tilde{\mathscr{H}}_{\mathbb{R}} \oplus j\tilde{\mathscr{H}}_{\mathbb{R}} \oplus k\tilde{\mathscr{H}}_{\mathbb{R}}$, where $\tilde{\mathscr{H}}_{\mathbb{R}}$ is the $\mathbb{R}$ vector space generated by the ϕ_k. The dimensions satisfy $\dim_{\mathbb{R}}(\tilde{\mathscr{H}}_{\mathbb{R}}) = 2\dim_{\mathbb{C}}(\mathscr{H}_{\mathbb{C}}) = 4\dim_{\mathbb{H}}(\mathscr{H}_{\mathbb{H}})$. This is why a factor $\frac{1}{4}$ appears in the definition of the index ind_4, see e.g. Ref. 53, to make it lie in $\mathbb{Z}$.

We will use the notation C_{ε_C} for an anti-linear operator with $C^2_{\varepsilon C} = \varepsilon_C$, viz. C_+ is a real structure and C_- is a quaternionic structure. The following proposition gives two equivalent formulations for the even cases in the classification, cf. Table I, either having two anti-unitary symmetry operators, or equivalently an anti-unitary symmetry operator and a grading operator.

Proposition II.6. The formulas $\chi_{\varepsilon_\chi} := C_{\varepsilon_C} C'_{\varepsilon_{C'}}$ and $C'_{\varepsilon_{C'}} := \varepsilon_C C_{\varepsilon_C}\chi_{\varepsilon_\chi}$ define one-to-one correspondences between the following sets.

1. *Pairs (C_+, C'_+) of commuting real structures and pairs (C_+, χ_+) of a real structure C and a commuting grading operator χ_+.*
2. *Pairs (C_-, C'_-) of commuting quaternionic structures and pairs (C_-, χ_+) of a quaternionic structure C_- and a commuting grading operator χ_+.*
3. *Pairs (C_-, C'_+) of a quaternionic structure C_- and an anti-commuting real structure C'_+ and pairs (C_-, χ_-) of a quaternionic structure C and an anti-commuting grading operator χ_-.*
4. *Pairs (C_+, C'_-) of a real structure C_+ and an anti-commuting quaternionic structure C'_- and pairs (C_+, χ_-) of a real structure C_+ and an anti-commuting grading operator χ_-.*

Proof. Consider $(C_{\varepsilon_C}, C'_{\varepsilon_{C'}})$ with $C^2_{\varepsilon_C} = \varepsilon_C 1$, $(C'_{\varepsilon_{C''}})^2 = \varepsilon_{C'}1$. Define ε_χ by $C_{\varepsilon_C}C'_{\varepsilon_{C'}} = \varepsilon_\chi C'_{\varepsilon_{C'}}C_{\varepsilon_C}$; in all the cases considered $\varepsilon_\chi = \varepsilon_C\varepsilon_{C'}$. Setting $\chi_{\varepsilon_\chi} = C_{\varepsilon_C}C'_{\varepsilon_{C'}}$, one computes $\chi^2_{\varepsilon_\chi} = C_{\varepsilon_C}C'_{\varepsilon_{C'}}C_{\varepsilon_C}C'_{\varepsilon_{C'}} = \varepsilon_\chi(C_{\varepsilon_C})^2(C'_{\varepsilon_{C'}})^2 = 1$. Furthermore, $\chi_{\varepsilon_\chi}C_{\varepsilon_C} = C_{\varepsilon_C}C'_{\varepsilon_{C'}}C_{\varepsilon_C} = \varepsilon_\chi C_{\varepsilon_C}C_{\varepsilon_C}C'_{\varepsilon_{C'}} = \varepsilon_\chi C_{\varepsilon_C}\chi_{\varepsilon_\chi}$. This establishes the correspondence in one direction.

Vice versa given χ_{ε_χ} and C_{ε_C} with $C^2_{\varepsilon_C} = \varepsilon_C 1$ and $C_{\varepsilon_C}\chi_{\varepsilon_\chi} = \varepsilon_\chi\chi_{\varepsilon_\chi}C_{\varepsilon_C}$, setting $C'_{\varepsilon_{C'}} = \varepsilon_C C_{\varepsilon_C}\chi_{\varepsilon_\chi}$ one computes: $(C'_{\varepsilon_{C'}})^2 = \varepsilon_C C_{\varepsilon_C}\chi_{\varepsilon_\chi}\varepsilon_C C_{\varepsilon_C}\chi_{\varepsilon_\chi} = \varepsilon_\chi C^2_{\varepsilon_C}\chi^2_{\varepsilon_\chi} = \varepsilon_\chi\varepsilon_C 1$ and thus $(C'_{\varepsilon_{C'}})^2 = \varepsilon_{C'_{\varepsilon_{C'}}}1$ with $\varepsilon_{C'} = \varepsilon_\chi\varepsilon_C$. This agrees with the claim as $\varepsilon_\chi = \varepsilon_C\varepsilon_{C'}$ for all cases. Furthermore, $C_{\varepsilon_C}C'_{\varepsilon_{C'}} = C_{\varepsilon_C}\varepsilon_C C_{\varepsilon_C}\chi_{\varepsilon_\chi} = \chi_{\varepsilon_\chi}$ and $C'_{\varepsilon_{C'}}C_{\varepsilon_C} = \varepsilon_C C_{\varepsilon_C}\chi_{\varepsilon\chi}C_{\varepsilon_C} = \varepsilon_\chi\chi$, so that $C_{\varepsilon_C}C'_{\varepsilon_{C'}} = \varepsilon_\chi C'_{\varepsilon_{C'}}C_{\varepsilon_C}$ as claimed.

The two opreations are clearly inversese of each other. □

Corollary II.7. In the presence of a canonical real structure K and a grading operator χ:

1. *If χ is K-real $(K\chi K = \chi)$, then $C = K\chi$ is a second real structure.*
2. *If χ is K-imaginary $(K\chi K = -\chi)$, then $C = K\chi$ is a quaternionic structure which anti-commutes with χ.* □

Example II.8. The following example is a good toy model and explains the ubiquitous appearance of the Pauli matrices. It is also at the base of the doubling construction Sec. II D 3. Consider the standard Pauli matrices acting on $\mathbb{C}^2$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad -i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

then as $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$, they are all grading operators. The choice σ_z corresponds to the splitting $\mathbb{C}^2 = \mathbb{C} \oplus \mathbb{C}$. If K is the diagonal real structure on $\mathbb{C}^2$, $K(z, w) = (\bar{z}, \bar{w})$, then the operators σ_x and σ_z are real, and thus $\sigma_x K$ and $\sigma_z K$ are also real structures. The operator σ_y is K-imaginary for K, so $\sigma_y K$ and $-i\sigma_y K$ are quaternionic structures. The standard quaternionic structure on $\mathbb{C}^2 = \mathbb{H}$ is $C_- = -i\sigma_y K$. Taking the real structure $C_+' = \sigma_z K$ these anti-commute, and (C_-, C_+') is of the form (3) in Proposition II.6. The grading operator anti-commuting with C_- is σ_x.

Choosing one of the operators and a commuting/anti-commuting grading operator one obtains the following examples:

1. $C_+ = \sigma_x K$ and $\chi_+ = \sigma_x$ commute and yield a pair of type (1). Here $C_+' = K$.
2. $C_+ = \sigma_x K$ and $\chi_+ = \sigma_y$ commute and yield a pair of type (1). Here $C_+' = -i\sigma_z K$.
3. $C_+ = \sigma_x K$ and $\chi_- = \sigma_z$ anti-commute and yield a pair of type (4). Here $C_-' = -i\sigma_y K$.
4. $C_+ = \sigma_z K$ and $\chi_- = \sigma_x$ anti-commute and yield a pair of type (4). Here $C_-' = i\sigma_y K$.
5. $C_+ = \sigma_z K$ and $\chi_+ = \sigma_y$ commute and yield a pair of type (1). Here $C_+' = i\sigma_x K$.
6. $C_+ = \sigma_z K$ and $\chi_+ = \sigma_z$ commute and yield a pair of type (1). Here $C_-' = K$.
7. $C_- = -i\sigma_y K$ and $\chi_- = \sigma_x$ anti-commute and are a pair of type (3). Here $C_+' = \sigma_z K$.
8. $C_- = -i\sigma_y K$ and $\chi_- = \sigma_y$ anti-commute and are a pair of type (3). Here $C_+' = -iK$.
9. $C_- = -i\sigma_y K$ and $\chi_- = \sigma_z$ anti-commute and are a pair of type (3). Here $C_+' = -\sigma_x K$.

The cases (3) and (9) as well as (4) and (7) have the same symmetry operators up to a sign. There is no type (2) combination of the operators, as $C_- = -i\sigma_y$ anti-commutes with σ_x, σ_y and σ_z.

B. Physics setup

According to Wigner,[52] time reversal symmetry (TRS) and particle hole symmetry (PHS) on a given Hilbert space $\mathscr{H}$ are both anti-unitary operators. The TRS and PHS operators are usually denoted by Θ, respectively Π. They satisfy $\Theta^2 = \epsilon_\Theta 1, \Pi^2 = \epsilon_\Pi 1$, where $\epsilon_\Theta, \epsilon_\Pi \in \{1, -1\}$ is a sign and hence the operators are either real or quaternionic. The sign ϵ_Θ depends on the particles; it is 1 for bosons and -1 for fermions.

If both these symmetries are present, by Wigner's Theorem[52] there is a chiral symmetry $\chi = \Theta\Pi$ which satisfies $\chi^2 = 1$, where for we used that one may rescale an anti-unitary by a phase. This is the grading operator in the mathematical setting. Since $1 = \chi^2 = \Theta\Pi\Theta\Pi$ it follows that $\Theta\Pi = \epsilon_\Theta\epsilon_\Pi\Pi\Theta$. Setting $\epsilon_\chi = \epsilon_\Theta\epsilon_\Pi$, like in the Proof of Proposition II.6, one obtains: $\chi\Theta = \Theta\Pi\Theta = \epsilon_\chi\Theta\Theta\Pi = \epsilon_\chi\Theta\chi$ and $\chi\Pi = \epsilon_\chi\Pi\chi$.

For convenience, we record the relations

$$\begin{gathered} \Theta^2 = \epsilon_\Theta 1, \quad \Pi^2 = \epsilon_\Pi 1, \quad \chi = \Theta\Pi, \quad \chi^2 = 1, \quad \Pi = \epsilon_\Theta\Theta\chi \\ \Theta\chi = \epsilon_\chi\chi\Theta, \quad \Pi\chi = \epsilon_\chi\Pi\chi, \quad \Theta\Pi = \epsilon_\chi\Pi\Theta, \quad \epsilon_\chi = \epsilon_\Theta\epsilon_\Pi \end{gathered} \tag{3}$$

A Hamiltonian H has TRS, respectively, PHS, respectively chiral symmetry, if

$$\Theta H = H\Theta \quad \text{resp.} \quad \Pi H = -H\Pi \quad \text{resp.}\ \chi H = -H\chi \tag{4}$$

Remark II.9. Note that if a state ϕ is Π symmetric $\phi = \Pi\phi$, then it is in the kernel of H. In fact $H|_{\ker(H)} \equiv 0$, the conditions (4) become vacuous, and so does the distinction between Θ and Π.

The possible choices of non-zero Hamiltonians with either TRS or PHS or both were classified by Altland-Zirnbauer[5] and lead to eight cases, cf. Table I. There are two additional cases, no symmetry (case A) or just a chiral symmetry (case AIII), which we will not focus on.

C. Symmetry classification

Theorem II.10. *The following two eight-case classifications agree under the specified identifications summarized in Table I.*

1. *The AZ classification for TRS and/or PHS.*
2. *The definition of KR^{-j} cycles obtained as reduced Clifford representations and Dirac operators, according to Refs. 9, 11, 16, and 47, also see Sec. VII A.*

   The Dirac Hamiltonian D in this correspondence is identified with the AZ Hamiltonian H. In the cases $j \neq 1, 5$ the operators are identified via $C = \Theta$, the TRS operator, $C' = \Pi$, the Particle Hole operator, and χ the chiral operator. In the cases $j = 1, 5 C = \Pi$.

Proof. This follows by inspection. The even cases, $j = 0, 2, 4, 6$, are the choices of pairs of a real or quaternionic structure and a commuting or anticommuting grading operator. These are taken to be unitary. According to Proposition II.6, the grading operator χ defines the anti-unitary $C' := \varepsilon_C C\chi$, which satisfies $C'^2 = \varepsilon_{C'} 1$ with $\varepsilon_{C'} = \varepsilon_\chi \varepsilon_C$. This is given in the fourth row of Table I. Vice versa the fourth row determines the second row by setting $\chi = CC'$ by Proposition II.6. The next rows give the properties of C' which are derived from those of C and χ according to Proposition II.6. The commutation relation with C' follows from $C'D = \varepsilon_C C\chi D = -\varepsilon_C CD\chi = -\varepsilon_C\varepsilon_D DC\chi = -\varepsilon_D C'$. Vice versa, defining $\chi = CC'$, $\chi D = CC'D = -\varepsilon_D\varepsilon_D DCC' = -D\chi$, a requirement for χ.

In the setting of TRS and PHS, one now identifies $C = \Theta$ as the time reversal symmetry, which commutes with the Hamiltonian, in all cases except $j = 1$ and 5. In these two cases, the sole operator $C = \Pi$ is the particle hole symmetry which anti-commutes with the Hamiltonian (4). Under this identification, if the grading operator χ is present, $j = 0, 2, 4, 6$, then $C = \Theta$ and $C' = \Pi$ and $\chi = CC' = \Theta\Pi$ is the chiral symmetry. Taking this dictionary translates the spin classification[11] to the Altland-Zirnbauer classification in the second to last row.[5] □

Remark II.11.

1. The last line indicates if the operators are is real, $\mathbb{R}$, or quaternionic, $\mathbb{H}$. The complex cases are the two remaining cases not treated here. The characterization -real, complex, or quaternionic—also holds for the Clifford algebras or the associated pinor representation, see e.g. Ref. 11.
2. The AZ classification has no natural cyclic ordering. The nomenclature was chosen to be analogous to Cartan's classification. The constructions of Refs. 2 and 4 have cyclic orders given by $s = j + 1$ and $q = j - 1$. The index j not only gives a cyclic order, but is tied more closely to Clifford representations and their periodicity. This is the correct index for KR-cycles. The index s gives the degree of KR-theory one is considering for the Bloch bundle, see Definition VI.12.
3. Dropping the reference to D, the 4 even cases are the content of Proposition II.6. In the four odd cases combinatorially one has one real operator $j = 1, 7$ or one quaternionic operator $j = 3, 5$ with the choice of sign ε_D to distinguish them.
4. In the cases $j = 1, 5$, the operator C gives a real/quaternionic structure, but the Hamiltonian does not respect this structure as it anti-commutes. If a real structure commutes with a Hamiltonian H, it is real. If it anti-commutes it is purely imaginary. If a quaternionic structure commutes with H, then it is an $\mathbb{H}$-linear operator.

D. Hamiltonians

In this section, we show how to move between the cases by forgetting symmetries and doubling. The latter construct Hamiltonians with symmetries $j \neq 0, 4$ from any given Hamiltonian by doubling. The cases $j = 0, 4$ are constructed by starting from a Hamiltonian having one of the symmetries—which is the case for the doubled Hamiltonians.

1. Structures in the j even cases

In the even cases, there is grading operator χ. This gives a decomposition of $\mathscr{H} = \mathscr{H}_0 \oplus \mathscr{H}_1$. The operators D anti-commute with χ and are hence in anti-diagonal form

$$D = \begin{pmatrix} 0 & D_1 \\ D_0 & 0 \end{pmatrix} \quad D_0 : \mathscr{H}_0 \leftrightarrows \mathscr{H}_1 : D_1 \tag{5}$$

Here D is chosen to be reminiscent of Dirac. In particular, $\ker(D) = \ker(D_0) \oplus \ker(D_1)$. D is self-adjoint if $D_0^* = D_1$ and skew-self adjoint if $D_0^* = -D_1$. By flipping a sign, these are two isomorphic theories, cf. Ref. 16,

$$D = \begin{pmatrix} 0 & D_0^* \\ D_0 & 0 \end{pmatrix} \quad \leftrightsquigarrow \quad D' = \begin{pmatrix} 0 & D_0^* \\ -D_0 & 0 \end{pmatrix} \tag{6}$$

Namely D is self-adjoint iff D' is skew-adjoint. In either case, $\ker(D_1) = \operatorname{coker}(D_0)$ and $\ker(D) = \ker(D_0) \oplus \operatorname{coker}(D_0)$. If these spaces are finite-dimensional, for instance if D is Fredholm, then $\operatorname{index}(D) = \dim_k(\ker(D_0)) - \dim_k(\operatorname{coker}(D_0))$.

Similarly if C anti-commutes with χ, $j = 2, 6$ then

$$C = \begin{pmatrix} 0 & C_1 \\ C_0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -C_0^* \\ C_0 & 0 \end{pmatrix}, \quad C' = \begin{pmatrix} 0 & -C_1 \\ C_0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & C_0^* \\ C_0 & 0 \end{pmatrix}, \quad \chi = \begin{pmatrix} \mathrm{id} & 0 \\ 0 & -\mathrm{id} \end{pmatrix} \tag{7}$$

where $C_0 = C|_{\mathscr{H}'_{\mathbb{C}}} : \mathscr{H}'_{\mathbb{C}} \to \bar{\mathscr{H}}'_{\mathbb{C}}$, $C_1 = C|_{\bar{\mathscr{H}}'_{\mathbb{C}}} : \bar{\mathscr{H}}'_{\mathbb{C}} \to \mathscr{H}'_{\mathbb{C}}$, and we used that if C, and hence C', is anti-unitary, then $C_0^* = -C_1$. Note that in this case C is also anti-Hermitian, while C' is anti-skew-Hermitian and they transform into each other by the sign flip of (6).

If C commutes with χ, then it is diagonal as is $C' = C\chi$

$$C = \begin{pmatrix} C_0 & 0 \\ 0 & C_1 \end{pmatrix}, \quad C' = \begin{pmatrix} C_0 & 0 \\ 0 & -C_1 \end{pmatrix}, \quad \chi = \begin{pmatrix} \mathrm{id} & 0 \\ 0 & -\mathrm{id} \end{pmatrix} \tag{8}$$

The following two constructions are a precursor to the spinorial clocks of Ref. 4 and the delooping of classifying spaces.[15]

2. Moving from even to odd: $2k-1 \leftarrow 2k \rightarrow 2k+1$ by forgetting symmetries

The class of a Hamiltonian in the AZ classification is fixed by specifying the symmetries. It is clear that in the even case, one can simply forget one of the two operators and move in the classification.

$j = 0$: Forgetting χ, and retaining C, moves to the cases $j = 7$.
Forgetting C and retaining C' moves to the case $j = 1$.
$j = 2$: Forgetting χ while retaining C moves to the cases $j = 3$.
Forgetting C while retaining C' moves to the case $j = 1$.
$j = 4$: Forgetting χ while retaining C moves to the cases $j = 3$.
Forgetting C while retaining C' moves to the case $j = 5$.
$j = 6$: Forgetting χ while retaining C moves to the cases $j = 7$.
Forgetting C while retaining C' moves to the case $j = 5$.

Note that there is an asymmetry in the moves. Physically this is explained by the fact that $C' = \Pi$ is the PHS operator, and if this is the only operator after forgetting C, then we are in the cases $j = 1, 5$. Similarly retaining only $C = \Theta$ leaves only a TRS operator and then we are in the cases $j = 3, 7$.

3. Doubling and construction of classes of Hamiltonians with symmetries

Given *any Hamiltonian* H on a Hilbert space $\mathscr{H}$, with an anti-unitary operator C with $C^2 = \varepsilon_C 1$, we can add symmetries by the following doubling construction: Consider $\mathscr{H}_d = \mathscr{H} \oplus \mathscr{H} = \mathbb{C}^2 \otimes \mathscr{H}$ and the following anti-linear operators on it:

$$\begin{aligned} \hat{C}_{\mathrm{id}} &= \mathrm{id} \otimes C = \begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix}, & \hat{C}_z &= \sigma_z \otimes C = \begin{pmatrix} C & 0 \\ 0 & -C \end{pmatrix} \\ \hat{C}_x &= \sigma_x \otimes C = \begin{pmatrix} 0 & C \\ C & 0 \end{pmatrix} & \hat{C}_{iy} &= -i\sigma_y \otimes C = \begin{pmatrix} 0 & -C \\ C & 0 \end{pmatrix} \end{aligned} \tag{9}$$

These satisfy $\hat{C}_{\mathrm{id}}^2 = \hat{C}_x^2 = \hat{C}_z^2 = \varepsilon_C \mathrm{id}$ and $\hat{C}_{iy}^2 = -\varepsilon_C \mathrm{id}$. The operator $\hat{C}_{\mathrm{id}}$ commutes with the other ones, while any two of the other operators anti-commute with each other. $\hat{C}_{\mathrm{id}}$, $\hat{C}_x$ and $\hat{C}_z$ are of the same type as C, that is real or quaternionic, while $\hat{C}_{iy}$ is of the opposite type, quaternionic or real.

Let the Pauli matrices operate as block matrices on $\mathscr{H} \oplus \mathscr{H}$, then define

$$\begin{aligned} \hat{H} &= \begin{pmatrix} H & 0 \\ 0 & CHC^* \end{pmatrix} & \hat{H}_z &= \begin{pmatrix} H & 0 \\ 0 & -CHC^* \end{pmatrix} \\ \hat{H}_x &= \begin{pmatrix} 0 & CHC^* \\ H & 0 \end{pmatrix} & \hat{H}_{-iy} &= \begin{pmatrix} 0 & -CHC^* \\ H & 0 \end{pmatrix} \end{aligned} \tag{10}$$

Lemma II.12. The Hamiltonians above satisfy the commutation or anti-commutation relations with the operators $\hat{C}_{\mathrm{id}}$, $\hat{C}_x$, $\hat{C}_{iy}$ and $\hat{C}_z$ listed in Table II. The entries with ± 1 hold for any Hamiltonian H, the entries with $\pm\varepsilon_D$ hold for Hamiltonians already possessing a symmetry $CHC^* = \varepsilon_D H$.

Proof. It suffices to prove this for $\hat{H}$, then the rest follows from the commutation relations of the sigma matrices.

$$\begin{pmatrix} C & 0 \\ 0 & \pm C \end{pmatrix} \begin{pmatrix} H & 0 \\ 0 & \varepsilon_D H \end{pmatrix} \begin{pmatrix} C^* & 0 \\ 0 & \pm C^* \end{pmatrix} = \begin{pmatrix} CHC^* & 0 \\ 0 & \varepsilon_D CHC^* \end{pmatrix} = \begin{pmatrix} \varepsilon_D H & 0 \\ 0 & H \end{pmatrix} = \varepsilon_D \hat{H} \tag{11}$$

and

$$\begin{pmatrix} 0 & \pm C \\ C & 0 \end{pmatrix} \begin{pmatrix} H & 0 \\ 0 & CHC^* \end{pmatrix} \begin{pmatrix} 0 & C^* \\ \mp C^* & 0 \end{pmatrix} = \begin{pmatrix} CCHC^*C^* & 0 \\ 0 & CHC^* \end{pmatrix} = \begin{pmatrix} H & 0 \\ 0 & CHC^* \end{pmatrix} = \hat{H} \tag{12}$$

□

TABLE II. The type of the operators $\hat{C}_{\mathrm{id}}$, $\hat{C}_z$, $\hat{C}_x$, and $\hat{C}_{iy}$ and their commutation relations with the Hamiltonians, where $CHC^* = \varepsilon_D H$; "+" means commute and "−" means anti-commute.

C	$\mathbb{R}$	$\mathbb{H}$
$\hat{C}_{\mathrm{id}}$	$\mathbb{R}$	$\mathbb{H}$
$\hat{C}_z$	$\mathbb{R}$	$\mathbb{H}$
$\hat{C}_x$	$\mathbb{R}$	$\mathbb{H}$
$\hat{C}_{iy}$	$\mathbb{H}$	$\mathbb{R}$

	$\hat{C}_{\mathrm{id}}$	$\hat{C}_z$	$\hat{C}_x$	$\hat{C}_{iy}$
$\hat{H}$	ε_D	ε_D	+	+
$\hat{H}_z$	ε_D	ε_D	−	−
$\hat{H}_x$	ε_D	$-\varepsilon_D$	+	−
Hy	ε_D	$-\varepsilon_D$	−	+

Corollary II.13. Given $\mathscr{H}$ with any Hamiltonian H and an antilinear unitary C with $C^2 = -\varepsilon_C \mathrm{id}$, every one of the Hamiltonians in (10) has a real and a quaternionic structure that anticommute with each other. Picking one of these operators and a doubled Hamiltonian this directly establishes examples of type $j = 1, 3, 5, 7$. Picking two operators that have opposite commutation properties, one obtains examples of $j = 2$ and $j = 6$.

Example II.14. If there is a given real structure $C^2 = \mathrm{id}$, e.g. a canonical real structure, $C = K$, and *any Hamiltonian* one can directly construct all odd symmetry classes by doubling:

$j = 1$: $C = \hat{C}_x$ and $D = \hat{H}_z$.
$j = 3$: $C = \hat{C}_{iy}$ and $D = \hat{H}_{-iy}$.
$j = 5$: $C = \hat{C}_{iy}$ and $D = \hat{H}_z$.
$j = 7$: $C = \hat{C}_x$ and $D = \hat{H}$.

One can also construct the following two even classes:

$j = 2$: $C = \hat{C}_{iy}$, $C' = \hat{C}_x$ and $D = \hat{H}_{-iy}$.
$j = 6$: $C = \hat{C}_x$, $C' = \hat{C}_{iy}$ and $D = \hat{H}_x$.

Note that the cases $j = 0, 4$ are not accessible this way. For this one needs to involve $\hat{C}_{\mathrm{id}}$. This is possible if H already satisfies the compatibility equation $CHC^* = \varepsilon_D H$, see Corollary II.15.

4. Moving from odd to even $2k \leftarrow 2k+1 \rightarrow 2k+2$ by doubling

If the Hamiltonian is already symmetric or anti-symmetric by reading off from the table, one can move from the odd cases $2k+1$ to $2k$ and $2k+2$.

Corollary II.15. Given a pair (H, C) for $j = 2k+1$, a type of a Hamiltonian H and an anti-unitary C with $C^2 = \varepsilon_C C$ and $CHC^* = \varepsilon_D H$, doubling results in two triples $(\hat{H}, \hat{C}, \hat{C}')$ of types $j = 2k$ and $j = 2k+1 \bmod 8$ as follows:

For $j = 1$: $\varepsilon_D = -1$, and $\varepsilon_C = 1$:
The Hamiltonian $\hat{H}$ together with $\hat{C} = \hat{C}_x$ and $\hat{C}' = \hat{C}_{\mathrm{id}}$, with $\chi = \sigma_x$, is of type $j = 0$.
The Hamiltonian $\hat{H}$ with $\hat{C} = \hat{C}_{iy}$, $\hat{C}' = \hat{C}_z$, with $\chi = \sigma_x$, is of type $j = 2$.
For $j = 3$: $\varepsilon_D = 1$, $\varepsilon_C = -1$:
The Hamiltonian $\hat{H}_z$ with $\hat{C} = \hat{C}_z$ and $\hat{C}' = \hat{C}_{iy}$, with $\chi = \sigma_x$, is of type $j = 2$.
The Hamiltonian $\hat{H}_z$ together with $\hat{C} = \hat{C}_{\mathrm{id}}$ and $\hat{C}' = \hat{C}_x$, with $\chi = -\sigma_x$, is of type $j = 4$.
For $j = 5$: $\varepsilon_D = -1$, $\varepsilon_C = -1$:
The Hamiltonian $\hat{H}$ together with $\hat{C} = \hat{C}_x$ and $\hat{C}' = \hat{C}_{\mathrm{id}}$, with $-\chi = -\sigma_x$, is of type $j = 4$.
The Hamiltonian $\hat{H}$ with $\hat{C} = \hat{C}_{iy}$, $\hat{C}' = \hat{C}_z$, with $\chi = -\sigma_x$, is of type $j = 6$.
For $j = 7$: $\varepsilon_D = 1$, $\varepsilon_C = 1$:
The Hamiltonian $\hat{H}_z$ with $C = \hat{C}_z$ and $C' = \hat{C}_{iy}$, with $\chi = -\sigma_x$, is of type $j = 6$.
The Hamiltonian $\hat{H}_z$ together with $\hat{C} = \hat{C}_{\mathrm{id}}$ and $\hat{C}' = \hat{C}_x$, with $\chi = \sigma_x$, is of type $j = 0$.

Remark II.16.

1. In the cases above, we have that the Hamiltonian is always of the form $\hat{H} = \sigma_z \otimes H$.
2. These doubling and reductions also appear in the construction of a reduced KR cycle from an unreduced KR cycle, see Ref. 11 and Sec. VII A.
3. The doubling has a natural interpretation in the bundle setting. This is at the heart of the 8-hour clocks in *KR* theory[11,15,16] for mathematical sources and Ref. 4 for a physics source, as well as Sec. VI.
4. There are similar statements involving the anti-diagonal Hamiltonians. This is used in Refs. 54 and 55. These are the Hamiltonians $\hat{H}_x$ for $j = 3, 7$ and $\hat{H}_{-iy}$ for $j = 1, 5$ which in the studied cases are $\sigma_x \otimes H$. They are anti-diagonal and are of the Dirac form as studied in Sec. II D 1. The symmetry operators are the combinations: $(\hat{C}_z, \hat{C}_{\mathrm{id}})$ to descend from $j = 1, 5$; $(\hat{C}_{iy}, \hat{C}_x)$ to ascend from $j = 1, 5$; $(\hat{C}_x, \hat{C}_{iy})$ to descend from $j = 3, 7$; and $(\hat{C}_{\mathrm{id}}, \hat{C}_x)$ to ascend from $j = 3, 7$. In all cases this yields $\chi = \pm\sigma_z$.
5. By combining Corollary II.13 with Corollary II.15, starting from any Hamiltonian H one can construct a Hamiltonian of any given type $j = 0, \ldots, 7$ by doubling or quadrupling, where doubling suffices in the cases $j \neq 0, 4$.

III. GEOMETRY OF TRS AND KR/KQ THEORY

A. Involutive spaces and real and quaternionic bundles over them

We give the basic definitions and examples used in the identification of the topological invariants. Under time reversal $t \to -t$ momenta transform as $k \to -k$ and spacial coordinates as $x \to x$.[52] Mathematically, this is an involution on the base aka. parameter space $\tau : X \to X, \tau^2 = \mathrm{id}$.

Consider a (compact) parameter space X together with an involution τ. As in applications X will be often be viewed as generalized momentum space, we will denote its elements by k to indicate a possibly non-trivial involution. These are also the spaces that underlie so-called Real K-theory as defined in Ref. 7. Bloch bundles in physics are bundles over the momentum space X, see e.g. Ref. 14. The extra structure of PHS or TRS makes them into Real of Quaternionic bundles. If both structures are present, this corresponds to a grading.

1. Involutive spaces

Definition III.1. An involutive space (X, τ) is a space X equipped with an involution, i.e., a homeomorphism $\tau : X \to X$ such that $\tau^2 = id_X$. A morphism between two involutive spaces (X', τ') and (X, τ) if a continuous map $f : X' \to X$ which intertwines the inclusions: $\tau f = f\tau'$.

A standard example for such an involution τ is complex conjugation in $\mathbb{C}$, which defines its real structure. In analogy, (X, τ) is also called a Real space in general. This nomenclature was introduced by Atiyah[7] in his study of *KR*-Theory, aka. Real *K*-theory-note the capital letter *R*. The fixed points of an involution τ is the set of points $X^\tau := \{x \in X | \tau(k) = k\}$ which will often be assumed to be a finite set for simplicity in the following.

2. Examples

The following are structural examples used in the theory and calculations: define $\mathbb{R}^{p,q} := \mathbb{R}^p \oplus i\mathbb{R}^q$ together with the involution τ by complex conjugation, i.e., $\tau : (x, y) \to (x, -y)$, or equivalently $\tau|_{\mathbb{R}^p} = 1$ and $\tau|_{i\mathbb{R}^q} = -1$. $\mathbb{R}^{1,1}$ is $\mathbb{C}$ with complex conjugation. In standard notation, the sphere $\mathbb{S}^{p,q} \subset \mathbb{R}^{p,q}$ of points with $|x| + |y| = 1$ is the $p + q - 1$ sphere in $\mathbb{R}^{p+q}$ with the induced involution.[56] This is the boundary of $\mathbb{B}^{p,q}$ which is the unit ball in $\mathbb{R}^{p,q}$. For example, $\mathbb{S}^{1,1} \subset \mathbb{R}^{1,1}$ are the points $e^{i\theta}, \theta \in [-\pi, \pi]$ with involution $\tau(\theta) = -\theta$. The $q - 1$ sphere with the antipodal map is $\mathbb{S}^{0,q}$ while the $p - 1$-sphere with the trivial involution is $\mathbb{S}^{p,0}$.

The torus $\mathbb{T}^d$ thought of as the momentum space (Brillouin zone) of a periodic system—the Pontryagin dual of a lattice in $\mathbb{R}^d$—has the involutive structure $k \to -k$. Realizing $S^1 \subset \mathbb{C}$, the parametrization by angles is

$$\mathbb{T}^d = \{(e^{i\theta_1}, \ldots, e^{i\theta_d}) \mid \theta_i \in [-\pi, \pi] \bmod 2\pi, \quad i = 1, \ldots, d\} \tag{13}$$

This allows us to think of the torus as a cube I^d, $I = [-\pi, \pi]$ modulo periodic boundary conditions. The time reversal transformation τ is given by

$$\tau : \mathbb{T}^d \to \mathbb{T}^d; \quad (e^{i\theta_1}, \ldots, e^{i\theta_d}) \mapsto (e^{-i\theta_1}, \ldots, e^{-i\theta_d}) \tag{14}$$

This identifies it with $\mathbb{T}^d = (\mathbb{S}^{1,1})^{\times d}$ as an involutive space. It has 2^d fixed points, $(\mathbb{T}^d)^\tau = \{(\pm1, \pm1, \ldots, \pm1)\}$ when $\theta_i = 0, \pi$. The one-point compactification of $\mathbb{R}^{p,q}$, that is $\mathbb{B}^{p,q}/\mathbb{S}^{p,q}$, is $\mathbb{S}^{p+1,q}$. In particular, the continuum model for the momentum space of a lattice is the one-point compactification of $\mathbb{R}^{0,d}$, which is

$$\mathbb{S}^{1,d} = \{(x_0, x_1, \ldots, x_d) \in \mathbb{R}^{d+1} \mid x_0^2 + x_1^2 + \cdots + x_d^2 = 1\} \tag{15}$$

where the time reversal transformation τ on $\mathbb{S}^{1,d}$ is defined by

$$\tau : \mathbb{S}^{1,d} \to \mathbb{S}^{1,d}; \quad (x_0, x_1, \dots, x_d) \mapsto (x_0, -x_1, \dots, -x_d) \tag{16}$$

It has two fixed points under the time reversal transformation, $(\mathbb{S}^{1,d})^\tau = \{(\pm 1, 0, \dots, 0)\}$ corresponding to the North and South Pole.

Thinking of T^d as a d-cube I^d with periodic boundary conditions as above, i.e. $T^d = I^d/\sim$, as $S^d = I^d/\partial I^d$, and the equivalence relation $\sim$ is only on the boundary, there is an induced quotient map $T^d \to S^d$. Let $\mathbb{I}^{0,d}$ be the cube $[-\pi,\pi]^{\times d}$ in $\mathbb{R}^{0,d}$; taking the involutions into account yields the diagram of quotient maps:

$$\begin{tikzcd}
\mathbb{I}^{0,d} \arrow[r, tail, two heads] \arrow[d, tail, two heads] & \mathbb{S}^{1,d} \\
\mathbb{T}^d \arrow[ur, tail, two heads] &
\end{tikzcd} \tag{17}$$

For $d = 2$ this is the quotient of T^2 by $S^1 \vee S^1$. In general, to obtain a sphere one collapses the $d-1$ skeleton of $\mathbb{T}^d$ of the CW model inherited from the natural CW decomposition of the cube. In coordinates, if T^d is taken to be $[-\pi,\pi]^d$ with periodic boundary conditions, then the map to S^d is given by collapsing all of the boundary points to the point at infinity for the sphere. In coordinates, $(0,0,\dots,0)$ gets sent to $(-1,0,\dots,0)$, and infinity is taken to be $(1,0,\dots,0)$. One concrete map is to rescale the cube to $\mathbb{R}^d$ and then use inverse stereographic projection. This identifies the result with the one-point compactification S^d of $\mathbb{R}^d$. It is straightforward to check that all morphisms in (17) are $\mathbb{Z}/2$-equivariant morphisms. The fixed point $(0,\dots,0)$ gets sent to the South Pole, and all of the other fixed points are sent to the point at infinity, which is the North Pole.

3. Real and quaternionic bundles

Definition III.2. A Real, respectively Quaternionic vector bundle (E,χ) over an involutive space (X,τ) is a complex vector bundle $\pi : E \to X$ equipped with an anti-linear isomorphism $C : E \to \tau^* E$ which satisfies $C^2 = \varepsilon_C 1$ with $\varepsilon_C = 1$ in the Real case and $C^2 = -1$ in the Quaternionic case. Note that conjugating the bundles $\tau^* E$, the map $C : E \to \tau^* \bar{E}$ is a linear isomorphism.

The fact that C is a bundle map means that if $\pi : E \to B$ is the structure map, $\pi \circ C = \tau \circ \pi$. Hence C acts on fibers as an anti-linear isomorphism $C(k) : E_k \to E_{\tau(k)}$ which squares to $\varepsilon_C \mathrm{id}(k) : E_k \to E_k$. Another way of stating this is that $C : E \to \overline{\tau^* E}$ is a bundle isomorphism.

We will choose a fiberwise Hermitian inner product, which is always possible.[57] As $C(k)^2 = \pm 1$ it is an anti-unitary.

Remark III.3. The standard nomenclature is to use capital "Real" respectively "Quaternionic" to indicate that τ may not trivial. If $\tau = \mathrm{id}$, the bundles are called real, respectively quaternionic (symplectic).

If *τ is trivial*, a Real bundle E is the complexification of a real bundle. A Quaternionic bundle is a quaternionic bundle, which means that each fiber is a quaternionic vector space, or, more precisely, it has the structure group reducible to $\mathrm{GL}_n(\mathbb{H})$. Adding a Hermitian form further reduces this group to $\mathrm{Sp}_n(\mathbb{H})$. Namely, if a Hermitian inner product is chosen on the quaternionic vector bundle, it naturally gives rise to a symplectic structure ω so that $(i^* E, \omega) \to X^\tau$ becomes a symplectic vector bundle, i.e., each fiber is a symplectic vector space, see e.g. Ref. 50, 3.3.1. Similarly in the case of a real bundle (Real with trivial τ), choosing an inner product will reduce the structure group to $O(n)$.

Given a morphism of involutive spaces $f : (X', \tau') \to (X, \tau)$ and a bundle $\pi : E \to X$ with fiber F and a Real/Quaternionic structure C, define the operator $f^*(C)$ locally by $f^* C(x, v) = (x, Cv) : U' \times F \to U' \times \bar{F}$. Fiberwise, for $k = f(k')$, it acts as a morphism from $f^* C(k') : f^*(E_k) = E_k \xrightarrow{C(k)} \overline{\tau^* E_{\tau(k)}} = \overline{\tau}'^*(f^*(E))$. The following is then straightforward.

Lemma III.4. Given a Real or Quaternionic structure C, its pull-back is a Real or Quaternionic structure as an isomorphism $f^* C : f^*(E) \to \overline{f^*(\tau^*(E))} = \overline{\tau'^*(f^*(E))}$. □

Definition III.5. A grading operator on a bundle E is a continuous family of grading operators $\chi(k) : E_k \to E_k$. A grading operator is compatible with a Real or Quaternionic bundle structure C if it commutes or anti-commutes with C. That is, $\chi C = \varepsilon_\chi C \chi$ globally. Fiberwise this is an equation of anti-linear isomorphisms $\chi(\tau(k)) C(k) = \varepsilon_\chi C(k) \chi(k) : E_k \to E_{\tau(k)}$.

A grading operator splits the bundle $E = E_+ \oplus E_-$ according to the ± 1 Eigenspaces of χ.

Remark III.6. We have the same six-case classification of real and quaternionic bundles with a commuting/anti-commuting or no grading operator as in Remark II.11 (3). The last two cases are distinguished by adding a Hamiltonian.

Grading operators are also pull-backs under morphisms of involutive spaces. The fiberwise action is $f^*(\chi(x)) : f^*(E_{k'}) = E_k \to E_k = f^*(E_{k'})$.

B. Adding a Hamiltonian to the geometry

Given a Real or Quaternionic bundle $(p : E \to X, \tau, C)$, a continuous family of linear operators $D(k)$ depending on $k \in X$ that acts fiberwise is compatible with C if:

$$C(k)D(k)C^*(k) = \epsilon_D D(\tau(k)) \tag{18}$$

We assume that the $D(k)$ are self-adjoint and in the graded case that D anti-commutes with χ. This leads to the eight-case classification of Table I, where now in the ungraded case one has the two choices that D commutes or anti-commute with the sole operator C. in the graded case $\epsilon_D = 1$, which implies that the one operator C' anti-commutes.

The Dirac Hamiltonians of a spin manifold are examples, see Example VII.5 for details. Physically these Hamiltonians appear in the standard lists,[3,4] also see and Examples III.18 and III.19 below.

C. Physics setup

1. Bundles and Hilbert space

For a physical theory the Hilbert space will be the space of sections of a complex vector bundle E over a parameter space X which is acted upon by a family of Hamiltonians acting fiberwise $H(k) : E_k \to E_k$. Endowing E with a Hermitian metric the space of L^2-sections $\mathscr{H} = \Gamma_{L^2}(X, E)$ becomes a Hilbert space with fiber-wise inner product $\langle \phi, \psi \rangle = \int_X \langle \phi(k), \psi(k) \rangle_k dk$, where $\langle \phi(k), \psi \rangle_k$ is the Hermitian inner-product on the fiber over k. The L^2-sections will be called states.

A complex vector bundle is said to be a Hilbert bundle, if it is equipped with a complete continuously varying Hermitian inner product so that each fiber is a Hilbert space. The completeness is automatic in the finite dimensional case. In the infinite dimensional case this is an extra condition. For example, given an effective Hamiltonian of a topological insulator, one considers the Hilbert bundle $E \to X$, which describes the band structure of the topological insulator over the momentum space X.

A typical situation is that one has a family of Hamiltonians acting on the same Hilbert space $H(k) : \mathscr{H}_F \to \mathscr{H}_F$, with a parameter k in a base space X which has an involution. Typically these spaces are $\mathbb{T}^d, \mathbb{S}^{1,d}$ or $\mathbb{T}^d \times S^D$ and $\mathscr{H}_F = \mathbb{C}^n$ so that $H : X \to \mathrm{Herm}_n$ where Herm_n are Hermitian $n \times n$ matrices and the family results from Fourier transform. Examples are in Sec. III D and Examples III.18 and III.19. To connect to the discussion above, one considers the trivial bundle $E = X \times \mathscr{H}_F$ on which the family $H(k)$ act fiberwise. Note that although the bundle E is trivial, subbundles, like Eigenbundles of the Hamiltonian family (see e.g. Refs. 58 and 59) or bundles given by projection onto energies below a given gap, see Ref. 14, need not be—see e.g. Example III.11 and Sec. IV.

Remark III.7. The Hilbert space as a space of sections also has an action of the C^*-algebra of $\mathbb{C}$-valued continuous functions $\mathscr{A} := C^0(X, \mathbb{C})$ and the whole k-dependent family $H(k)$ yields a Hamiltonian on the Hilbert space of sections $H : \mathscr{H} \to \mathscr{H}$. One can also impose more smoothness conditions, but from the point of view of C^*-geometry, that is noncommutative topology, continuous functions are most natural. Following Bellissard,[14] we will ultimately use Connes' noncommutative geometry approach based on C^*-algebras, see Ref. 11.

In classical geometry one considers the sheaf of continuous sections and likewise in quantum mechanics one is interested in continuous or differentiable wave functions or sections, see also Remark V.2. This leads to the known complications and solutions using rigged Hilbert spaces, see e.g. Ref. 60. We will not make this explicit here.

2. TRS and PHS

Physically, TRS and PHS act trivially on space-like variables $\Theta(r) = r$, but using Bloch theory or Fourier transform, one obtains that as $t \mapsto -t$, on momenta k, TRS and PHS send k to $-k$.[52] This is an involution on the momentum space $\tau(k) = -k, \tau^2 = \mathrm{id}$.

The action of a TRS or PHS operator C is coupled to the involution on X: $C(k) : E_k \to E_{\tau(k)}$ and is precisely an isomorphism $C : E \to \overline{\tau^*(E)}$, that is a Real or Quaternionic structure depending on the sign of $C^2 = \epsilon_C 1$. The total Hilbert space is given by L^2-sections of the bundle.

$$\Theta(k)H(k)\Theta^*(\tau(k)) = H(\tau(k)), \quad \Pi(k)H(\tau(k))\Pi^*(k) = -H(k) \tag{19}$$

The chiral operator $\chi = \Theta\Pi$ then operates fiberwise $\chi(k) : E_k \to E_k$ and χ anti-commutes with H.

If there is only a TRS operator Θ, this can be identified with the operator C in the case $AI, j = 7$, which corresponds to Real bundles, and $AII, j = 3$ which corresponds to Quaternionic bundles.

If there is only a PHS operator Π, this can be identified with the operator C in the case $D, j = 1$, which corresponds to Real bundles, and $C, j = 5$ which corresponds to Quaternionic bundles.

If there are both, a TRS Θ and a PHS operator Π, then they define the chiral operator χ. These match with the even cases for $C = \Theta$ and $C' = \Pi$. In DII, $j = 2$ and CII, $j = 4$, Θ is a Quaternionic structure with which χ anti-commutes in the first case and commutes in the second case. In BDI $j = 0$ and CI, $j = 6$, Θ is a Real structure with which χ commutes in the first case and anti-commutes in the second case.

D. Constructing examples

1. Constructions via pull-back

The following is straightforward:

Proposition III.8. Given an example (C, D) for j odd or (C, χ, D) for j-even on a bundle E base space (X, τ) and a morphism of involutive spaces $f : (X', \tau') \to (X, \tau)$, the pull backs $f^*(C), f^*(D)$ and, if present, $f^*(\chi)$ are a structure of type j on the bundle $f^*(E)$. □

A function f on an involutive space is even if $f(k) = \bar{f}(\tau(k))$ and odd if $f(k) = -\bar{f}(\tau(k))$.

Lemma III.9. Given a tuple (C, D) for j odd or (C, χ, D) for j even for a bundle E over an involutive space (X, τ):

1. *for even functions f the tuples (C, fD) or (C, χ, fD) are also of type j.*
2. *for odd functions f the tuples (C, fD) or (C', χ, fD) are of type $-j$.*

Notice that in the j-even cases the roles of the operators C and $C' = \varepsilon_c C\chi$ are switched.

Proof. This is a straightforward calculation. For $f(k) = \varepsilon\bar{f}(\tau(k))$ ($\varepsilon = 1$ even, $\varepsilon = -1$ odd):

$$C(k)f(k)D(k) = \varepsilon_D\bar{f}(k)D(\tau(k))C(k) = \varepsilon\varepsilon_D\, f(\tau(k))D(\tau(k))C(k) \tag{20}$$

so that $\varepsilon_{fD} = \varepsilon\varepsilon_D$. As χ is linear, $\chi f D = f\chi D = -fD\chi$. The change in sign for the Hamiltonian is indeed $j \to -j$ by inspection of Table I. □

Given an example (C_0, D_0) for j odd or (C_0, χ_0, D_0) for j-even, acting on $F = \mathscr{H}$, consider this as a bundle over the one point space with trivial involution. Given any involutive space (X, τ), consider the trivial bundle $E = X \times F$. This is the pull back of $F \to pt$ via the map $\pi : X \to pt$. The pulled back structures $\pi^* C_0$ and $\pi^*\chi$ are constant.

Corollary III.10.

1. *for any even function $f(k) = \bar{f}(\tau(k))$ the tuples $(\pi^* C_0, f(k)D_0)$, respectively $(\phi^* C_0, \chi_0, f(k))$ are families of the form j.*
2. *For any odd function $f(\tau(k)) = -\bar{f}(x)$ the tuples $(\pi^* C_0, f(k)D_0)$, respectively $(\pi^* C_0, \chi_0, f(k))$ are families of the form $-j$.*

Proof. Notice that as T only acts on the base coordinate, $C_0 T(k, v) = (\tau(k), C_0(v)) = TC_0(k, v)$. Similarly $D_0 T = TD_0$ and $\chi T = T\chi$. If $\bar{f}(k) = \varepsilon f(\tau(k))$,

$$C(k)D(k) = TC_0(k)f(k)D_0(k) = \varepsilon_{D_0}\bar{f}(k)TD_0(k)C_0(k) = \varepsilon\varepsilon_{D_0}\, f(\tau(k))D_0(\tau(k))TC_0(k) \tag{21}$$

so that $\varepsilon_D = \varepsilon\varepsilon_{D_0}$. This proves the odd cases. In the even cases: $\chi D = \chi f(k)D_0 = -f(k)D_0\chi = -D\chi$ and $\chi C = \chi TC_0 = T\chi C_0 = \varepsilon_\chi C\chi$. Since ε_χ is invariant under $j \to -j$ this proves the claim. □

Note that if the same C respectively χ a compatible with several Hamiltonians H_i, then one can build linear combinations.

This allows to construct the following standard families from Example II.8. Some of these are considered in Ref. 4.

Example III.11 (Paradigmatic Example). The three Hamiltionians $\sigma_x, \sigma_y, \sigma_z$ acting on $\mathbb{C}^2$ all anti-commute with $C_- = -i\sigma_y K$, which is a PHS with $C^2 = -1$. Pull back this family to $\mathbb{R}^{0,3}$ using the odd functions k_x, k_y, k_z, we obtain the paradigmatic Hamiltonian and Quaternionic TRS operator

$$H(k) = k \cdot \boldsymbol{\sigma} = k_x\sigma_x + k_y\sigma_y + k_z\sigma_z, \quad C = -i\sigma_y K \tag{22}$$

which is of type AII, $j = 3$. It remains of type AII, if one adds an imaginary mass term $im\sigma_z$ for instance, as $f(k) = im$ is odd.

The family can be restricted to the compact $\mathbb{B}^{0,3}$ or $\mathbb{S}^{0,3}$, which is S^2 with the antipodal map or tampered at ∞ to yield a bundle on $\dot{\mathbb{R}}^{0,3} = \mathbb{S}^{1,3}$. Further interesting restrictions are to the different coordinate planes and their $\mathbb{S}^{0,2}$'s as well as to intervals passing through 0. These give standard models, cf. e.g. Refs. 58 and 59.

Although on S^2 the bundle E is trivial by construction, it is well known, see e.g. Refs. 13, 58, and 61, that the bundle on $S^2 = \mathbb{S}^{0,3}$ decomposes into the ± 1 eigenbundles for the family $H(k)$ as $B_H \oplus \bar{B}_H$. Here B_H is the Hopf bundle. Now $c_1(E) = 1 - 1 = 0$, which explains the triviality of the sum. Thus the total bundle is a doubling of B_H which explains its vanishing first Chern class. What is not trivial is the splitting.

Choosing a different involution for instance considering the family on $\mathbb{R}^{3,0}$, the functions k_x, k_y, k_z are even and hence $-i\sigma_y K$ anti-commutes and is a Quaternionic PHS operator, yielding the case C, $j = 5$. Now one can add mass term like $m\sigma_z$ as real constants are even functions.

Switching the operator to $C = \sigma_x K$, we have that σ_x commutes and σ_y, σ_z anti-commute. Thus considering the family (22) on $\mathbb{R}^{1,2}$, we obtain $C = \sigma_x K$ which is a Real TRS operator, and we are in case AI, $j = 7$, while on $\mathbb{R}^{2,1}$, with coordinates (k_y, k_z, k_x), C is a Real PHS operator, and we are in case D, $j = 1$. The case of $\mathbb{R}^{1,2}$ is interesting as it contains the sphere $S^{1,2} = \dot{\mathbb{R}}^{0,2}$.

Example III.12. Pulling back to $\mathbb{R}^{0,2}$ and considering only

$$H(k) = k_x\sigma_x + k_y\sigma_y \tag{23}$$

we have the Quaternionic TRS operator $-i\sigma_y K$ and the anti-commuting grading operator $\chi = \sigma_z$ to obtain an example of type DIII, $j = 2$. Adding an imaginary mass term of the form $im\sigma_x$ or $im\sigma_y$ is still possible. Adding a term $\varepsilon\sigma_z$ breaks the grading operator and one has a BdG Hamiltonian for a 2D, aka. a 2d spinless chiral p-wave, cf. e.g. Ref. 54.

Similarly, one can use $H(k) = k_y\sigma_y + k_z\sigma_z$, which has an anti-commuting grading operator σ_x. Pulling back to $\mathbb{R}^{2,0}$, for (23), we have a Quaternionic PHS operator and anti-commuting grading operator, which puts us in the case CI, $j = 6$.

Considering (23) with the operator $C = \sigma_z K$, which anti-commute with σ_x and commutes with σ_y, and the commuting grading operator $\chi = \sigma_x$ (23), this case is of type BDI, $j = 0$ when considered on $\mathbb{R}^{1,1}$, where the TRS operator is K and $\sigma_z K$ is the PHS operator. It is possible to add a real mass term $m\sigma_x$ or $m\sigma_z$.

Example III.13. The Jackiw–Rebbi model[62] and the related Su–Schrieffer–Heeger model[63] is of the form $vk\sigma_x + m\sigma_y$ with additional term $\varepsilon k^2\sigma_y$ considered on $\mathbb{R}^{0,1}$. It is an odd function times σ_x and an even function times σ_y; this has TRS $\sigma_z K$ and anti-commuting $\chi = \sigma_z$ and is in class BDI, $j = 0$.

Example III.14. One can also use more sophisticated odd and even functions. The Bogoliubov–de Gennes Hamiltonian (BdG) for the 1D Kitaev super-conductor model, see e.g. Ref. 54, is given by

$$H(k) = (t\,\cos(k) - \mu)\sigma_z + \Delta\,\sin(k)\sigma_x \tag{24}$$

on $R^{0,1}$, with t and Δ being parameters. This is of type D, $j = 1$ with the Real PHS operator $C = \sigma_x K$. C commutes with σ_x and $\sin(k)$ is odd, while it anti-commutes with σ_z and $\cos(k)$ is even, so that both terms satisfy $CH(k)C^* = -CH(\tau(k))$.

2. Doubling construction for families of Hamiltonians

The doubling and restriction operations of Sec. II D also work fiberwise. Given an anti-unitary operator C with $C^2 = \varepsilon_C\mathrm{id}$ acting as $C(k) : E_k \to \bar{E}_k$, consider the natural diagonal families of Hamiltonians $\hat{H}_\varepsilon(k)$ acting on the fibers of $E \oplus \tau^* E$ given by

$$\hat{H}(k) = \begin{pmatrix} H(k) & 0 \\ 0 & CH(k)C^* \end{pmatrix} \quad \hat{H}_z(k) = \begin{pmatrix} H(k) & 0 \\ 0 & -CH(k)C^* \end{pmatrix} \tag{25}$$

These have the same symmetry operators as given in Lemma II.12, see Table II.

Proposition III.15. Doubling gives examples of bundles with symmetries of the six types $j \neq 0, 4$ with the operators specified in Corollary II.13 on the same base space.

If additionally $CH(k)C^* = \varepsilon_D H(\tau(k))$, then $\mathscr{H}_+$ also furnishes examples for the cases $j = 0, 4$ with the operators specified according to Corollary II.15.

Proof. The claims are a straightforward calculations, parallel to those of Lemma II.12. □

Remark III.16. The anti-diagonal action of $\hat{C}_x$ and $\hat{C}_{iy}$ is natural as $(E \oplus \tau^*\bar{E})(k) = E_k \oplus \bar{E}_{\tau(k)}$ while $(E \oplus \tau^*\bar{E})(\tau(k)) = E_{\tau(k)} \oplus \bar{E}_k$.

Remark III.17.

1. We used the definition of the Hamiltonians Sec. II D 3 of $\hat{H}$ which, when $CH(k) = \varepsilon_H H(\tau(k))C$, are $\begin{pmatrix} H(k) & 0 \\ 0 & -H(\tau(k)) \end{pmatrix}$. Another option is to use the Hamiltonian $\sigma_z \otimes H = \begin{pmatrix} H(k) & 0 \\ 0 & -H(k) \end{pmatrix}$.
2. As in Remark II.16, there are similar statements using the anti-diagonal Hamiltonians $\hat{H} = \begin{pmatrix} 0 & H(\tau(k)) \\ H(k) & 0 \end{pmatrix}$ and $\sigma_x \otimes H = \begin{pmatrix} 0 & H(k) \\ H(k) & 0 \end{pmatrix}$, used for instance in Ref. 54.

Example III.18. As in Ref. 54 consider the massless 3 + 1D Dirac Hamiltonian $H = \sum_\mu(-i\sigma_x \otimes \sigma_\mu\partial_\mu)$, $\mu = x, y, z$, which in momentum form is $H = \sigma_x \otimes (k \cdot \boldsymbol{\sigma})$. This is the doubling of (22). Considering the quaternionic $C = \hat{C}_{\mathrm{id}} = \mathrm{id} \otimes (-i\sigma_y K)$ and grading operator $\chi = \sigma_z$, this is of type CII, $j = 5$. If one adds an extra mass term $m\sigma_z \otimes \mathrm{id}$, since m is an even function, this breaks the grading operator and

$$H(k) = \sigma_x \otimes (k \cdot \boldsymbol{\sigma}) + m\sigma_z \otimes \mathrm{id} = \begin{pmatrix} m & k\cdot\sigma \\ k\cdot\sigma & -m \end{pmatrix} \tag{26}$$

is of type AII $j = 3$. This is the momentum space version of the massive 3 + 1D Dirac Hamiltonian. $H = \sum_\mu(-i\sigma_x \otimes \sigma_\mu\partial_\mu + m\sigma_\mu \otimes \mathrm{id})$, $\mu = x, y, z$,

Changing to a chiral mass term $H = -i\sigma_x \otimes \sigma_\mu\partial_\mu - m\sigma_y \otimes \mathrm{id}$, $\mu = x, y, z$, which in momentum form is

$$H(k) = \begin{pmatrix} 0 & k\cdot\sigma - im \\ k\cdot\sigma + im & 0 \end{pmatrix} \tag{27}$$

this is of the type (6). It is the doubling of (22) with the TRS operator $\hat{C}_{-iy}$ and the grading operator σ_z, together with an additional term $m\sigma_y \otimes \mathrm{id}$ that anti-commutes with σ_z and is an even function times an anti-commuting operator.

Example III.19. Doubling (26), that is $D = k_\mu\sigma_x \otimes \sigma_\mu + m\sigma_z \otimes \mathrm{id}$, by tensoring with σ_x, as $D^\dagger = D$, one obtains $H = \begin{pmatrix} 0 & D \\ D & 0 \end{pmatrix}$ which is of the form CII, $j = 4$ with $C = \hat{C}_{\mathrm{id}}$ and $\chi = \sigma_z$. This is an example of an 8-component 3 + 1D Dirac Hamiltonian.

E. Moving around the $\mathbb{Z}/8\mathbb{Z}$-clocks by suspension

There are even and odd suspension operations on families of Hamiltonians, which change the index j to $j + 1$ or $j - 1$, see Sec. VI D for the original construction[15] of the even suspension, and[4] for a construction of the odd suspension. Here we adaptRef. 15 to the reduced case and tweak the construction of Ref. 4. Recall that for $I = [-1, 1]$ the suspension SX of a space X is the quotient of $X \times I$ by the relations $(x, -1) \sim (x', -1)$ and $(x, 1) \sim (x', 1)$. For the suspension of an involutive space (X, τ) one needs to specify the involution on the new coordinate t. We will say t is even if $\tau(t) = t$ and t is odd if $\tau(t) = -t$ as an involutive subset $I \subset \mathbb{R}^{1,0}$ or $I \subset \mathbb{R}^{0,1}$.

Theorem III.20. *For j even, given a family of Hamiltonians $H(k)$ over X with a chiral symmetry χ consider the following family defined over the suspension SX*

$$H(k,t) = \cos\left(\frac{\pi}{2}t\right)H(k) + \sin\left(\frac{\pi}{2}t\right)\chi, \quad t \in [-1, 1] \tag{28}$$

If t is even this is of type $j - 1 \bmod (8)$, and if t is odd this is of type $j + 1 \bmod (8)$, where depending on j, we retain the operators C or C' parallel to Sec. II D 2.

For j odd, doubling H to $\hat{H} = \begin{pmatrix} H(k) & 0 \\ 0 & -H(\tau(k)) \end{pmatrix}$ according to Corollary II.15 and using the symmetry operators given there consider

$$H(k,t) = \cos\left(\frac{\pi}{2}t\right)\hat{H}(k) + \sin\left(\frac{\pi}{2}t\right)\sigma_y, \quad t \in [-1, 1] \tag{29}$$

Extending the involutive structure by $\tau(t) = t$, the system is of type $j - 1 \bmod (8)$.

Extending the involutive structure by $\tau(t) = -t$, the system is of type $j + 1 \bmod (8)$.

Proof. This is again a case-by-case analysis. Define the sign ε_t by $\tau(t) = \varepsilon_t t$.

In all j-even cases label the two terms $H(k,t) = H_0(k,t) + H_1(k,t)$ then as $\varepsilon_D = 1$ and $\cos(\varepsilon_t t) = \cos(t)$, on the one hand,

$$\begin{aligned} CH_0(k,t)C^* &= C\,\cos\left(\frac{\pi}{2}t\right)H(k)C = \cos\left(\frac{\pi}{2}t\right)H(-\tau(k)) = H_0(\tau(k), \tau(t)) \\ C'H_0(k,t)(C')^* &= C'\,\cos\left(\frac{\pi}{2}t\right)H(k)(C')^* = -H_0(\tau(k), \tau(t)) \end{aligned} \tag{30}$$

for both extensions. On the other hand, since $C'\chi = \varepsilon_\chi C'$ and $\sin(\varepsilon_t(t)) = \varepsilon_t \sin(t)$, for H_1 one obtains:

$$\begin{aligned} CH_1(k,t)C^* &= C\,\sin\left(\frac{\pi}{2}t\right)\chi C^* = \varepsilon_\chi\varepsilon_t H_1(\tau(k), \tau(t)) \\ C'H_1(k,t)(C')^* &= C'\,\sin\left(\frac{\pi}{2}t\right)\chi(C')^* = \varepsilon_\chi\varepsilon_t H_1(\tau(k), \tau(t)) \end{aligned} \tag{31}$$

Using the forgetting technique as in Sec. II D 2, the claim follows. For example, starting at $j = 2$, $\varepsilon_\chi = -1$, we have that if $\varepsilon_t = 1$, C' anti-commutes with $H(k,t)$, and we are in the case $j = 1$; while if $\varepsilon_t = -1$, C commutes with $H(k,t)$.

In the j-odd case, again splitting up $H(k,t)$ and considering the cases according to Corollary II.15, $H_0(k,t)$ anti-commutes with χ and commutes with $\hat{C}$, regardless of the choice of ε_t. Independently of j or ε_t, H_1 anti-commutes with $\chi = \pm\sigma_x$. In the case $\varepsilon_t = 1$, H_1 and hence σ_y has to commute with C as specified in Corollary II.15. This means for $j = 1,5$ with $\hat{C}_x$ and for $j = 3,7$ with $\hat{C}_z$. As σ_y is purely imaginary, it does this.

For $\varepsilon_t = -1$, H_1 has to commute C which means that σ_y has to anti-commute with C. In the case of $j = 1,5$ this is $\hat{C}_{iy}$, and for $j = 3,7$ this is $\hat{C}_{\mathrm{id}}$. These anti-commute with σ_y as σ_y is purely imaginary. □

Remark III.21.

1. We used the variable t as in Ref. 4. To get the polar angle used in Refs. 16, 53, and 64 one uses the transformation $t' = 1 - t$. Note $\sin\left(\frac{\pi}{2}t'\right) = \cos\left(\frac{\pi}{2}t\right)$ and $\cos\left(\frac{\pi}{2}t'\right) = \sin\left(\frac{\pi}{2}t\right)$.
2. As in Remark III.17, one can alternatively use the anti-diagonal Hamiltonians or the Hamiltonians $H \otimes \sigma_z, H \otimes s_x$.
3. One can also choose σ_a in H_1 for $a \in \{x,z\}$ depending on j and the extension of the involution as follows if $\tau(t) = t$, then $a = y$ for $j = 1,5$ and $a = x$ for $j = 3,7$. If $\tau(t) = -t$, then $a = z$ for $j = 1,5$ and $a = y$ for $j = 3,7$. This type of setup was used in Ref. 4 and the examples in Sec. III D and the Examples III.18 and III.19.

Example III.22. The paradigmatic Example III.11 can be built up using odd suspensions. Using an odd suspension on the DIII, $j = 2$ example (23) restricted to $\mathbb{S}^{0,2}$, that is $k_x = \cos(\theta), k_y = \sin(\theta)$, with grading operator $\chi = \sigma_z$, the base space is $\mathbb{S}^{0,3}$ and using the polar angle $\phi = \frac{\pi}{2}t'$ the Hamiltonian becomes

$$H(\theta,\phi) = \cos(\theta)\sin(\phi)\sigma_x + \sin(\theta)\sin(\phi)\sigma_y + \cos(\phi)\sigma_z \tag{32}$$

on $\mathbb{S}^{0,3}$ which is of type AII, $j = 2 + 1 = 3$.

If one starts out with $H(k) = k\mathrm{id}$ where $\mathrm{id} = \mathrm{id}_{\mathbb{C}}$ on $S^{0,1}$, with PHS given by σ_y using the odd suspension with σ_x, as in Remark II.16 (4) one obtains the Hamiltonian $H(k,\theta) = \cos(\theta)k\sigma_x + \sin\theta k\sigma_y$ where $k = \pm 1, \theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$. This has the global form

$$H(k,\theta) = \cos(\theta)k\sigma_x + \sin\theta\, k\sigma_y, \theta \in [-\pi,\pi] \tag{33}$$

which is of type DIII, $j = 1 + 1 - 2$ with TRS operator $-i\sigma_y K$ grading operator σ_z.

IV. EIGENBUNDLES AND BAND CROSSINGS

A. Non-degenerate families

One interesting type of family is one in which none of the $H(k)$ has degenerate Eigenvalues. This is the case for the paradigmatic family (22) when restricted to S^2. In this case, one can split the bundle $E = \oplus_{i=1}^r \mathscr{L}_i$, r is the rank of E, where $\mathscr{L}_i$ are line bundles, which are ordered according to their real Eigenvalues. Notice that they cannot cross, since then the Hamiltonian would be degenerate. Fiberwise this means that $H(k)|_{\mathscr{L}_i} = \lambda_i(k) id_{\mathbb{C}}$. An Eigenstate ϕ satisfies $(H\phi)(k) = \lambda_\phi(k)\phi$ where $\lambda_\phi = \lambda_i$ for some i.

The usual integer topological invariants in this case are the Chern classes $c_1(\mathscr{L}_i)$. Note since E is trivial $c_1(E) = \sum_i c_1(\mathscr{L}_i)$. If the fiber is $\mathbb{C}^2$, this means that $E = \mathscr{L} \oplus \bar{\mathscr{L}}$ with $c_1(\mathscr{L}) = -c_1(\bar{\mathscr{L}})$. For the family (22) this splitting corresponds to the grading operator. Physically speaking the Eigenvalues are energies, and we will also write E_i.

B. Kramers degeneracies

If there are symmetry operators C present, then they act on states where $(C\phi)(k) = C(\phi(\tau(k))) \in E_k$. Note that if ϕ has support V, then $C\phi$ has support $\tau(V)$. Such symmetries can force degeneracies over fixed points of τ.

Lemma IV.1. Let C be symmetry a operator for $H(k)$: $CH(k)C^* = \varepsilon_H H(\tau(k))$. If $\varepsilon_H = 1$, this is a TRS operator and if $\varepsilon_H = -1$, this is a PHS operator. For an Eigenstate $\phi \in \mathscr{H}$, with $H(k)\phi(k) = \lambda_\phi(k)\phi(k)$, the state $C\phi$ is an Eigenstate with $H(k)(C\phi)(k) = \lambda_{C\phi}(k)(C\phi)(k)$ where $\lambda_{C\phi}(k) = \varepsilon_H\lambda_\phi(\tau(k))$.

Proof. Unraveling definitions:

$$\begin{aligned} H(k)(C\phi)(k) &= H(k)C(\phi(\tau(k))) = \varepsilon_H CH(\tau(k))\phi(\tau(k)) \\ &= \varepsilon_H C\lambda_\phi(\tau(k))\phi(\tau(k)) = \varepsilon_H\lambda_\phi(\tau(k))(C\phi)(k) =: \lambda_{C\phi}(k)(C\phi)(k) \end{aligned} \tag{34}$$

where we used fact that $\lambda_\phi(k)$ is real. □

If $C^2 = 1$, then either ϕ and $C\phi$ are linearly independent, or $C\phi = \lambda\phi$ with $\lambda\bar{\lambda} = 1$. In particular, this is the case for C-real and C-imaginary vectors. After a phase shift one can assume that ϕ is real. If $\varepsilon_D = -1$, i.e. C is a PHS operator, then if ϕ is an Eigenstate of H which is not in the kernel, ϕ and $C\phi$ are linearly independent. This holds in particular fiberwise over the fixed point set.

For a Quaternionic TRS, each energy level is at least doubly degenerate as ϕ and $C\phi$ are linearly independent, see Sec. II A 4. This is called Kramers degeneracy in physics, and the pair $(\phi, C\phi)$ is called a Kramers pair. Commensurate with the definition in Sec. II A 4, we also allow C to be a Quaternionic PHS operator.

Remark IV.2. The rotated basis $\phi \pm C\phi$ obtained from Kramers pairs is related to the double Hamiltonians. If ϕ is an Eigenstate with Eigenfunction E_ϕ, then writing

$$\hat{H}(k)\begin{pmatrix}\phi\\ C\phi\end{pmatrix}(k) = \begin{pmatrix}H(k)\phi(k)\\ CH(k)C^*C\phi\end{pmatrix} = \lambda_\phi(x)\begin{pmatrix}\phi\\ C\phi\end{pmatrix}(k) \text{ and } \begin{pmatrix}0 & \varepsilon_C C\\ C & 0\end{pmatrix}\begin{pmatrix}\phi\\ C\phi\end{pmatrix} = \begin{pmatrix}\varepsilon_C C^2\phi\\ C\phi\end{pmatrix} = \begin{pmatrix}\phi\\ C\phi\end{pmatrix} \tag{35}$$

Corollary IV.3. Given an operator C with $CH(k)C^* = \varepsilon_H H(\tau(k))$ at each fixed point $k \in X^\tau$ a basis of the eigenspaces can be given by Kramers pairs. If $\varepsilon_H = 1$ (j = 2, 3, 4), each Eigenvalue of $H(k) = H(\tau(x))$ has even multiplicity, and if $\varepsilon_H = -1$ (j = 4, 5, 6), the multiplicity of $\lambda \neq 0$ is that of $-\lambda$ and the multiplicity of 0 is even.

At a fixed point, E_k is a quaternionic space and thus $\dim_{\mathbb{C}}(E_k) = 2\dim_{\mathbb{H}}(E_k)$ is an even integer, and $\dim_{\mathbb{C}}(\ker(H(k)) = 2\dim_{\mathbb{H}}(\ker(H(k)))$ and $\dim_{\mathbb{C}}(coker(H(k)))$ are even.

Proof. If there is a Real or Quaternionic structure C with $C^2 = -1$, by Lemma IV.1 the rank of the fiber at any fixed point is even, as every basis element ϕ has a linearly independent Kramers partner $C\phi$. As the rank is constant, if there is any such fixed point on X, the rank of the bundle is even. Furthermore, over the fixed points locus, Lemma IV.1 specifies the indicated multiplicities. As H commutes with Θ, the kernel is fixed by Θ and has the structure of a quaternionic vector space.

If $\varepsilon_H = 1$, H is $\mathbb{H}$-linear, it follows that $\dim_{\mathbb{C}}(\ker(H(k)) = 2\dim_{\mathbb{H}}(\ker(H(k)))$ is also even as is $\dim_{\mathbb{C}}(\text{coker}(H(k)))$. If $\varepsilon_H = -1$, then for each fixed point E_k is a quaternionic space, and as iH is $\mathbb{H}$-linear, the statement follows from the discussion in Sec. II A 4. □

1. Kramers structures in the *j*-even cases

In the j-even cases, as $CC' = \varepsilon_\chi C'C$, the smallest subspace for both operators to act upon is the subspace spanned by $(\phi, C\phi, C'\phi, CC'\phi)$. There are several relations:

Lemma IV.4. The pair ϕ and $C\phi$ is linearly independent iff the pair $C'\phi$ and $CC'\phi$ is linearly independent. Similarly, the pair ϕ and $C'\phi$ is linearly independent iff the pair $C\phi$ and $CC'\phi$ is linearly independent.

If ϕ and $C\phi$ are linearly dependent, then $C^2 = \text{id}$. If ϕ and $C'\phi$ are linearly dependent, then $(C')^2 = \text{id}$, and, moreover if ϕ is an Eigenstate, then $\phi \in \ker(H)$.

If $C\phi$ and $C\phi$ are linearly dependent, then $CC'\phi = \chi\phi = \pm\phi$.

If $\phi \notin \ker(H)$ is an Eigenstate, then on the open set where $\lambda(k) \neq 0$, $(\phi, C\phi, C'\phi, CC'\phi)$ has rank 2 or 4.

Proof. The first two statements follow by applying the correct operator. E.g. if $C\phi = \mu\phi$, $C'C\phi = \varepsilon_\chi CC'\phi = \bar{\mu}C'\phi$. Recall from Sec. II A 4 that if $C^2 = -1\phi$ and $C\phi)$ are linearly independent. Moreover, if $C'\phi = \mu\phi$ and $D\phi = \lambda\phi$ with real λ, then $DC'\phi = \mu\lambda\phi$ and $DC'\phi = -C'D\phi = -\mu\lambda\phi$, so that $\lambda = -\lambda = 0$.

If $C\phi = \lambda C'\phi$, then $\varepsilon_C\phi = \bar{\lambda}CC'\phi$ and ϕ is an Eigenstate for χ.

For the final statement assume that $D(k)\phi(k) = \lambda(k)\phi(k)$ and $(c_1\phi + c_2C\phi + c_3C'\phi + c_4CC'\phi)(k) = 0$ then $0 = D(c_1\phi + c_2C\phi + c_3C'\phi + c_4CC'\phi)(k) = \lambda(k)c_1\phi(k) + \lambda(k)c_2C\phi(k) - \lambda(k)c_3C'\phi(k) - \lambda(k)c_4CC'\phi(k)$. If $\lambda(k) \neq 0$, then dividing by $\lambda(k)$ and adding the two equations, we find $(c_1\phi + c_2C\phi)(k) = 0$ and ϕ and $C\phi$ are either linearly dependent or $c_1 = c_2 = 0$. Similarly by subtracting, $C'\phi$ and $CC'\phi$ are linearly dependent or $c_3 = c_4 = 0$. But ϕ and $C\phi$ being linearly dependent is equivalent to $C'\phi$ and $C'C\phi$ being linearly independent. Thus if $\lambda(k) \neq 0$, the vectors cannot be linearly dependent unless ϕ and $C\phi$ are, in which case the dimension drops by 2. It can be 1 only if also ϕ and $C'\phi$ are linearly dependent, in which case ϕ must lie in the kernel. □

This gives the following taxonomy for the dimension of $span(\phi, C\phi, C'\phi, CC'\phi)$.

1. $j = 0$. Here both operators are real and commute. All dimensions, 1–4, are possible. The vectors ϕ and $C\phi$ can be linearly dependent if the support of ϕ τ-invariant. The same for $\phi, C'\phi$. If ϕ is an Eigenstate and $C'\phi$ is linearly dependent, then also $H\phi = 0$. In particular, if at a fixed point $\phi(k)$ and $C'\phi(k)$ are linearly independent, then $\phi(k) \in \ker(H(k)$. Thus, if the dimension is 1 and ϕ is an Eigenstate, ϕ is in the kernel and $\chi\phi = \phi$. If the dimension is 2, then either ϕ and $C\phi$ are linearly dependent, but ϕ and $C'\phi$ are not, or vice versa. If ϕ is not in the kernel, then the dimension is either 2 or 4 by Lemma IV.4.
2. $j = 2$. Here C is quaternionic, and the dimension is either 2 or 4. It is at least 2 and if it is not 4, it is at most 2 by Lemma IV.4. It is 2 if ϕ and $C'\phi$ are linearly dependent, which implies that if ϕ is an Eigenstate, it lies in the kernel.

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3. $j = 4$. In this case the dimension is 2 or 4. Since ϕ and $C\phi$ are linearly independent, then being dimension 2 implies that $C\phi$ and $C'\phi$ are linearly dependent and $\chi\phi = \pm\phi$. If the rank is at least 3, it is 4 if ϕ is not in the kernel.
4. $j = 6$. Here again the dimension is at least 2 and if ϕ is not in the kernel, then the dimension is 4.

Lemma IV.5. Assume that there is a Real/Quaternionic structure $\Pi^2 = \pm 1$ which anticommutes or, respectively, commutes with a TRS invariant Hamiltonians $H(k)$ (j = 2, 4). Then for an eigenstate ϕ the quartet of states $\phi(k), \Theta\phi(k), \Pi\phi(k), \Theta\Pi\phi(k)$ can be linearly dependent only if $\phi(k) \in \ker(H(k))$.

Proof. Assume that $H\phi = \lambda\phi$ and $(c_1\phi + c_2\Theta\phi + c_3\Pi\phi + c_4\Theta\Pi\phi)(k) = 0$ then $0 = H(c_1\phi + c_2\Theta\phi + c_3\Pi\phi + c_4\Theta\Pi\phi)(k) = \lambda(k)c_1\phi(k) + \lambda(k)c_2\Theta\phi(k) - \lambda(k)c_3\Pi\phi(k) - \lambda(k)c_4\Theta\Pi\phi(k) = 0$ and if $\lambda(k) \neq 0$, then dividing by $\lambda(k)$ and adding the two equations, we find $(c_1\phi + c_2\Theta)(k) = 0$ which means that $c_1 = c_2 = 0$ as these vectors are linearly independent. Similarly $\Pi\phi$ and $\Theta\Pi\phi$ are linearly independent, so that if $\lambda(k) \neq 0$, the vectors cannot be linearly dependent. □

Assumption IV.6. We will assume that the bundle E has even rank (this is automatic, if there is a fixed point), and we will assume that H is maximally non-degenerate in the sense that there are no degenerate eigenvalues of $H(k)$ (aka. no level crossings) except at the fixed points X^τ and that these crossings are due to Kramers degeneracy.

Under this assumption the kernels of $H(k)$ at fixed points are described as follows:

Proposition IV.7. In the quaternionic cases $j = 2, 3, 4$, if the levels ϕ_1, ϕ_2 (this means that ϕ_1, ϕ_2 are two eigensections that are non-vanishing near the fixed point and have distinct eigenvalues away from the fixed point), cross at a fixed point (this means that their eigenvalues coincide at k), two Kramers pairs $(\phi_1, \Theta\phi_1)$ and $(\phi_2, \Theta\phi_2)$ have to become linearly dependent. This means that the quaternionic basis elements ϕ_1 and ϕ_2 become linearly dependent.

In the presence of PHS, that is Π, the Kramers pairs $(\phi_1, \Theta\phi_1)$, $(\Pi\phi_1, \Theta\Pi\phi_1)$ can cross only at $\lambda(k) = 0$, that is they are in $\ker(H(k))$. The dimension of the space spanned by these vectors is not continuous and drops by two at the fixed point. If two independent Kramers pairs $(\phi_1, \Theta\phi_1)$ and $(\phi_2, \Theta\phi_2)$ cross at $\lambda_k = 0$, then so do their independent PHS partners $(\Pi_1\phi, \Theta\Pi_1\phi)$ and $(\Pi\phi_2, \Theta\Pi\phi_2)$; then the dimension of the space spanned by these vectors drops by 4.

This is depicted in Fig. 1.

Proof. All statements except the dimension drop have been shown previously. The dimension drop is due to the fact that the rank of the subbundle spanned by the indicated vectors is constant. In the first case, this is 2, and hence the drop is from 4 to 2. In the second case, the drop is from 8 to 4. □

This is best understood by considering the bundle $E \oplus \overline{\tau^*(E)}$. At the fixed points the inclusion $E(k) \to E(k) \oplus \bar{E}(k)$ is the diagonal map considered above.

A consequence of this assumption is that near an isolated fixed point there exists a decomposition

$$E = \bigoplus_{i=1}^{N} E_i \tag{36}$$

where $E_i \to X$ is a non-trivial rank-2 subbundle. We set $\mathscr{H}_i = \Gamma(X, E_i)$, then $\mathscr{H} = \oplus_{i=1}^{N} \mathscr{H}_i$ and C respects this decomposition. This means that we can also restrict the operators (9) to the bundle $E_i \oplus \tau^*(\overline{E_i})$.

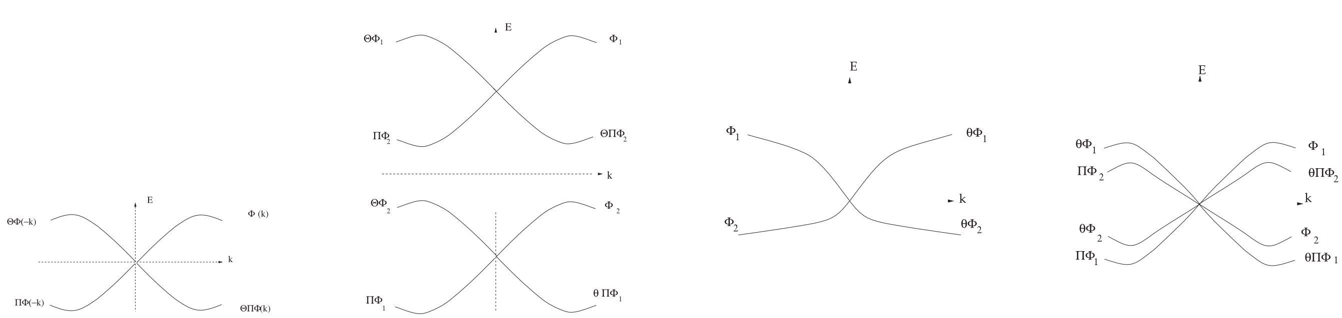

FIG. 1. Different possibilities for level crossings at a fixed point taken as $k = 0$ for illustration. The cases are a self—crossing for $j = 2$, two pairs crossing outside the zero level as a deformation, a crossing for two Kramers pairs in $j = 3$, and a crossing of two Kramers pairs in $j = 4$.

Another consequence is that on $X\backslash X^\tau E$ is trivializable by ordering the eigenvalues $E_1(k) < E_2(k) < \cdots < E_{2N}(k)$ as $H(k)$ is assumed to be nondegenerate outside the fixed points X^τ, and thus the bundle splits into line bundles

$$E|_{X\backslash X^\tau} = \bigoplus_{j=1}^{2N} \mathscr{L}_j \text{ with } E_i = \mathscr{L}_{2i} \oplus \mathscr{L}_{2i+1} \tag{37}$$

To do the computations, one needs to look at the local geometry, which we present in Sec. V. This also allows to "see" the index computations by using the spectral flow. This is what one intuitively reads off from Fig. 1.

2. Sewing matrices

If the global bundle is trivializable and choosing global sections e_i, $E = X \times \mathbb{C}^{2N}$, as in the paradigmatic example, the unitary matrix $w = CK$ representing C can be given by the matrix coefficients, see Ref. 65

$$w_{ij}(k) = \langle e_i(\tau(k)), C\bar{e}_j(k)\rangle \tag{38}$$

The action is from $E_k \to E_{\tau(k)}$. The fact that $C^2 = -1$ means that this matrix satisfies

$$w(\tau(k)) = -w(k)^T \tag{39}$$

If e_{2i} and e_{2i+1} are a Kramers pair, viz. $e_{2i} = Ce_{2i+1}$, then this matrix takes on the form $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

Based on w^i, the parity anomaly of the topological $\mathbb{Z}_2$ invariant is translated into a gauge anomaly of the topological band theory, see Ref. 65.

V. LOCAL AND GLOBAL GEOMETRY FOR MOMENTUM SPACES

A. Fundamental domains and conditions for the action

We will now decompose the underlying space X according to the action by the time reversal transformation τ. In the general setting, this decomposition can be quite wild, but in concrete situations it is usually well behaved. For instance, as we explain in Sec. VI B, in case this decomposition is suitably "nice," we can apply different long exact sequences to compute the invariants. This is a bit more subtle than one would initially expect.

We will assume that the Real space (X, τ) is *tame*. For a connected X this means that there are closed connected fundamental domains $V_\pm$, such that $\tau(V_\pm) = V_\mp$, $X = V_+ \cup V_-$ and $B = V_+ \cap V_-$ is the closed boundary of both V_+ and V_-. That is $V_\pm = V_\pm^o \sqcup B$ as sets, with $\tau(V_\pm^o) = V_\mp^o$ open and B is closed of codimension greater or equal to 1. Such B separates, namely, V_+^o and V_-^o occupy different components of $X\backslash X^\tau$. Here and in the following $\sqcup$ means the disjoint union. For a general X, being tame means that each connected component of X is tame. This is for instance the case for a Riemannian manifold X where $V_\pm$ are given by Dirichlet fundamental domains, a.k.a. Voronoi cells. We call a tame space *regular*, if we can find a decomposition $X = X_+ \sqcup X_- \sqcup X^\tau$ where $\tau(X_\pm) = X_\mp$ such that $\bar{X}_\pm = V_\pm$, $X_\pm$ and $X\backslash X^\tau$ are locally compact. This is the case for all the examples that we will consider including the examples given above, see Fig. 2.

The case where (X, τ) is a finite $\mathbb{Z}_2$-equivariant regular CW complex is the most important for applications. For such a complex, there exists a $\mathbb{Z}_2$-equivariant cellular decomposition of X. This means that for all cells C of dimension k, $\tau(C)$ is also a cell of dimension k. Such an equivariant cellular decomposition is also very useful in the computation of K-theory. In this case, we can decompose $X = V_+ \cup V_-$ as above where now $V_\pm$ are sub-CW complexes. Moreover, $V_\pm = \bar{O}_\pm$ where $O_\pm = \sqcup_{C\in V_\pm} C^o$ is the union of all the interiors of the top dimensional cells in $V_\pm$, that is, those that are not at the boundary of any other cell. We denote the closed cells by C and write C^o for their open interior. Vice versa, starting with the fixed points X^τ, X can be built up by gluing cells that carry a free $\mathbb{Z}_2$ action, i.e., $\mathbb{Z}_2$-cells. This construction is closely related to the stable homotopy splitting of X into spheres respecting the time reversal symmetry[46] and Sec. VI.

There is also another decomposition that we will use: $X = X_+ \sqcup X_- \sqcup X^\tau$. To do this, we assign $+$, $-$ or *fix* to all cells, inductively, by choosing fundamental domains as above starting with the dimension zero cells and using induction on the k-skeleton. We choose $+$ and $-$ for the cells interchanged by τ and *fix* for all the cells fixed by τ. We will call them $+$, $-$ or fixed cells. The induction ensures that no $+$ cell

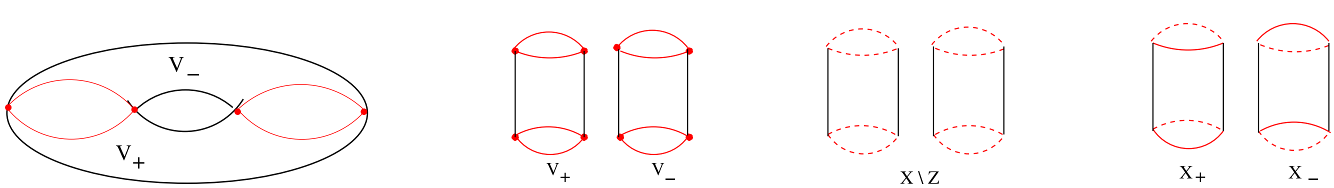

FIG. 2. From the left to right: (a) the torus with two fundamental domains V_+, V_- with $Z = V_+ \cap V_- = \mathbb{S}^{1,1} \sqcup \mathbb{S}^{1,1}$ in red, (b) the disjoint union of V_+ and V_-, (c) the complement of Z, and (d) the subsets $X_\pm$. Dotted lines indicate open boundaries.

lies at the boundary of only − cells. Notice that fixed points do not lie in the interior of any + or − cell, moreover, $X^\tau = \sqcup_{C:\text{fixed cell}} C^o$. Set $X_+ = \sqcup_{C:+\text{ cell}} C^o$, $X_- = \sqcup_{C:-\text{ cell}} C^o$. We call such a CW complex *weak* $\mathbb{Z}_2$*-space* if there is a choice of ± such that each skeleton X^k is regular, as defined above, with respect to the decomposition above. This is for instance the case, if X is a compact manifold and X^τ is discrete, which encompasses all the examples from the literature. In particular, this means that if $Z = V_+ \cap V_-$, then Z is again a weak $\mathbb{Z}_2$-space and one can use induction.

Example V.1. All the $\mathbb{T}^d$ and $\mathbb{S}^{1,d}$ are of this type. For $d = 0$ the space consists of two points, marked by *fix*. For $d = 1$ one adds two intervals joining the points, marked by + and −. For $\mathbb{S}^{1,d}$, we realize it as $\mathbb{R}^{0,d} \cup \{\infty\}$. Mark ∞ by *fix* and then mark $\mathbb{R}^{0,d}$ by decomposing it w.r.t. the iterated upper and lower half spaces, marking the upper half space by + and the lower by −. This agrees with the decomposition as $\mathbb{R}^{0,d} = \mathbb{R}^{0,1} \times \cdots \times \mathbb{R}^{0,1}$. Similarly, we can define the decomposition of $\mathbb{T}^d = \mathbb{S}^{1,1} \times \cdots \times \mathbb{S}^{1,1}$, see Fig. 3.

1. Fundamental domain and Hilbert space

The fundamental domains allows us to split the bundle and perform a "halving" using a grading operator. Under the tameness assumption above we can embed $\mathscr{H} \subset \mathscr{H}_+ \oplus \mathscr{H}_-$ where $\mathscr{H}_\pm = \Gamma(V_\pm, E)$ and the map $\phi \mapsto (\phi_+, \phi_-)$ comes from the restrictions $\phi_\pm = \phi|_{V^\pm}$. To test whether a given pair glues to a section, we can check if $\phi_+|_{V_+\cap V_-} - \phi_-|_{V_+\cap V_-} = 0$. Setting $\mathscr{H}' = \Gamma(V_+ \cap V_-, \mathscr{H})$, we get the exact sequence

$$\mathscr{H} \xrightarrow{i_{\mathscr{H}}} \mathscr{H}_+ \oplus \mathscr{H}_- \xrightarrow{diff} \mathscr{H}' \tag{40}$$

Remark V.2. For the embedding, it actually plays a role what types of sections we use. For continuous sections, the embedding is proper, since the condition for gluing two sections is that they agree on the intersection. If we use L^2 sections, then the embedding is an equality, since as classes any two L^2 sections glue, as the intersection is of measure 0. Finally, if one uses differentiable sections such as C^1, or C^∞ sections, then one actually needs to glue over open sets. This slightly changes the definition of $\mathscr{H}_\pm$. Namely, choose two neighborhoods $U_\pm$ of $V_\pm$ with $\tau(U_+) = U_-$, then X is covered by the two open sets U_+ and U_-. Now, $\mathscr{H}_\pm := \Gamma_{C^1,C^\infty}(U_\pm, E)$. In the usual situation, we can choose the neighborhoods so that they retract onto $V_\pm$. In practice, physical states should be continuous integrable sections.

Given a symmetry operator C, it interchanges the two spaces $C : \mathscr{H}_\pm \to \mathscr{H}_\mp$, that is, it takes on the matrix form

$$C_\pm = \begin{pmatrix} 0 & C|_{\mathscr{H}_-} \\ C|_{\mathscr{H}_+} & 0 \end{pmatrix} = \begin{pmatrix} 0 & C_- \\ C_+ & 0 \end{pmatrix}$$

There is a standard pairing on $\mathscr{H}_+ \oplus \mathscr{H}_-$ given by

$$((\phi_+, \phi_-), (\psi_+, \psi_-)) := \int_{V_+} (\phi_+, \psi_+)_x \, dx + \int_{V_-} (\phi_-, \psi_-)_x \, dx \tag{41}$$

This allows us to view $\mathscr{H}_-$ as $\bar{\mathscr{H}}_+$ and $\mathscr{H}$ becomes the doubled Hilbert space of Sec. II D 3. The splitting corresponds to the grading operator χ with $\mathscr{H}_\pm$ being the eigenspaces to ±1. The operator C which anticommutes with χ then takes on the diagonal form σ_z. Alternatively using the doubling point of view $\hat{C} = \begin{pmatrix} 0 & \epsilon_C C_+^* \\ C_+ & 0 \end{pmatrix}$.

The action of C makes $\mathscr{H}_+ \oplus \mathscr{H}_-$ into a real/quaternionic space and makes $i_{\mathscr{H}}$ into a morphism of real/quaternionic Hilbert spaces. We can identify $\mathscr{H}_+ \oplus \mathscr{H}_-$ as the sections of the bundle $E^{\text{sum}} = E \oplus \overline{\tau^* E}$ over V_+ (or V_-)

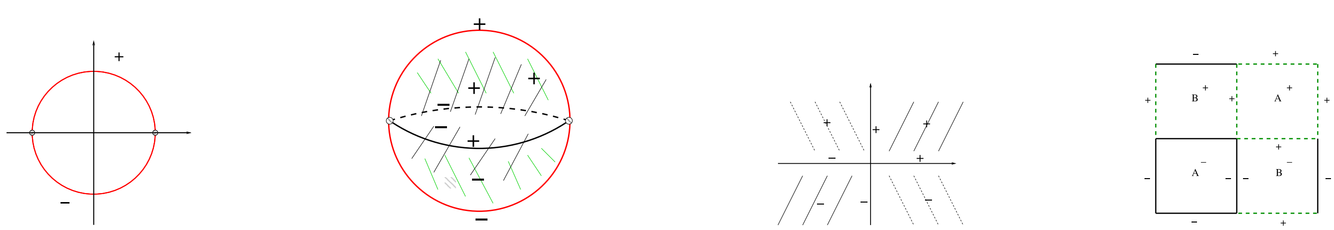

FIG. 3. The $\mathbb{Z}_2$-CW decompositions of (a) $\mathbb{S}^{1,1}$,(b) $\mathbb{S}^{1,2}$, with 2 0-cells, 4 1-cells and 4 2-cells, corresponding to the one-point compactification of $\mathbb{R}^{0,2}$ decomposed into quadrants and half lines depicted in (c), and (d) the decomposition of $\mathbb{T}^2$.

$$\begin{aligned} \tau^* : \Gamma(V_-, E|_{V_-}) &\xrightarrow{\sim} \Gamma(V_+, \tau^*(E|_{V_-})) = \Gamma(V_+, \overline{(\tau^* E)|_{V_+}}) \\ \phi_- &\mapsto \tau^*\phi_-, \quad (\tau^*\phi_-)(k) = \phi_-(\tau(k)) \end{aligned} \tag{42}$$

and $\mathscr{H}_+ \oplus \mathscr{H}_- \simeq \Gamma(V_+, E^{\text{sum}})$. The operator $\hat{C}$ now operates on E^{sum}. Taking this point of view, we define $\hat{H}$ by (25), but now acting on $\mathscr{H}_+ \oplus \mathscr{H}_-$.

Remark V.3. Notice that we could have equally well chosen V_- or $\mathscr{H}_-$ in the place of V_+ and $\mathscr{H}_+$ above.

2. Doubling the sum

We can of course consider both $\mathscr{H} \oplus \overline{\mathscr{H}} = \Gamma(\overline{E\oplus \tau^*(E), X})$ and the decomposition $\mathscr{H} \to \mathscr{H}_+ \oplus \mathscr{H}_-$. In this case, we have

$$\mathscr{H} \oplus \overline{\mathscr{H}} \xrightarrow{i} \mathscr{H}_+ \oplus \mathscr{H}_- \oplus \overline{\mathscr{H}_+ \oplus \mathscr{H}_-} = \mathscr{H}_+ \oplus \mathscr{H}_- \oplus \overline{\mathscr{H}_+} \oplus \overline{\mathscr{H}_-} \tag{43}$$

If $\Phi = (\phi, C\phi)$ is a Kramers pair, then we have that $i(\Phi) = (\phi_+, \phi_-, C\phi_-, C\phi_+)$. To accommodate the anti-linearity of Kramers pairs, it is hence useful to consider the following arrangement of summands

$$\mathscr{H}_{quad} := \mathscr{H}_+ \oplus \overline{\mathscr{H}_-} \oplus \mathscr{H}_- \oplus \overline{\mathscr{H}_+}$$

and the inclusion $i \quad : \mathscr{H} \oplus \overline{\mathscr{H}} \to \mathscr{H}_{quad}$. Then for a Kramers pair

$$i_{\text{quad}}(\phi, C\phi) = (\phi_+, C\phi_+, \phi_-, C\phi_-)$$

On the level of bundles this corresponds up to permutation of summands to considering

$$E_{\text{quad}} \simeq \Gamma\big(V_+, (E \oplus \tau^*\overline{E})|_{V_+} \oplus (E \oplus \tau^*\overline{E})|_{V_-}\big) \tag{44}$$

The structures now are the ones discussed in Sec. II D 3.

3. Splitting further

Restricting further to $X\backslash Z$, by the assumption, we can split $\mathscr{H}_+$ and $\mathscr{H}_-$ into the positive and negative eigenvalues of H. Note that we assumed that there is only level crossing at fixed points. Then there is a quadruple Hilbert space $\mathscr{H}_{++} \oplus \mathscr{H}_{+-} \oplus \mathscr{H}_{-+} \oplus \mathscr{H}_{--}$. If there is also a grading operator χ or equivalently a PHS operator C', the tuples $(\phi, C'\phi, C\phi, CC'\phi)$ discussed in Sec. V A 4 naturally live in this space. Outside of Z, by the assumption, the bundle can be trivialized. The bundle itself is then given by clutching across Z. The classical construction is $\mathbb{S}^{d,1} = \dot{\mathbb{R}}^{d,0}$ where the bundle on the upper hemisphere is clutched to the bundle on the lower hemisphere by a sewing, cf. Refs. 7 and 10.

Taking a tubular neighborhood $Tub(X^\tau)$ of Z^τ, one can restrict the bundle, and under the assumption that the fixed points are isolated, this is given just by a collection of balls. The bundle itself is trivializable, but the important information is in the Eigenbundle decomposition, just like in Example III.11. This allows one to regard the spectral flow of eigenvalues along a curve through the fixed point. More generally, one could choose a normal direction to the 0-section.

4. Kramers pairs and the Hilbert bundle

Since C respects the decomposition of the Hilbert bundle (36), we can further decompose $\mathscr{H}_i \subset \mathscr{H}_{i,+} \oplus \mathscr{H}_{i,-}$ as a block matrix consisting of blocks

$$C_i = \begin{pmatrix} 0 & C|_{\mathscr{H}_{i,-}} \\ C|_{\mathscr{H}_{i,+}} & 0 \end{pmatrix}$$

If there was no time reversal symmetry, then under the assumption of non-degeneracy each band can be modeled by a complex line bundle $\mathscr{L}_i \to X$. When the time reversal symmetry is switched on, each band locally around Z is modeled by a rank-2 Hilbert subbundle π: $\mathscr{H}_i \to X$. By the existence of a Kramers pair $(\phi_i, C\phi_i)$, $\mathscr{H}_i$ can be locally decomposed into

$$E_i = \mathscr{L}_i \oplus C\mathscr{L}_i, \quad \text{with} \quad C\mathscr{L}_i \cong \tau^*(\overline{\mathscr{L}_i}), \tag{45}$$

where $\tau^*(\overline{\mathscr{L}_i})$ is the pullback of the conjugate bundle, since C is an anti-linear bundle isomorphism. The decomposition of $\mathscr{H}_i$ is similar to a spinor bundle, since the time reversal operator C switches the chirality of a Kramers pair. In the literature, some authors assume the total Hilbert bundle is a globally trivial complex vector bundle, for example see Ref. 65. This is in line with Example III.11. By our assumption, the bundle is at least trivial on $X\backslash Z$.

Outside of the fixed points X^τ, we can locally trivialize the bundle using Kramers pairs. By assumption Kramers degeneracy is the only degeneracy. It follows that on $X\backslash X^\tau$ the bundle $\mathscr{H}_i$ splits into a direct sum of two line bundles: $\mathscr{H}_i|_{X\backslash X^\tau} = \mathscr{L}_{2i-1}\oplus\mathscr{L}_{2i}$. Thus if we choose trivializing sections ψ_{2i-1}, ψ_{2i} on some neighborhood U with $U\cap\tau(U) = \emptyset$, then we obtain a Kramers pair (ψ_I, ψ_{II}), $\psi_{II} = C\psi_I$ given by

$$\psi_I|_U = \psi_{2i-1}, \quad \psi_I|_{\tau(U)} = C\psi_{2i} \text{ and } \psi_{II}|_U = -\psi_{2i}, \quad \psi_{II}|_{\tau(U)} = C\psi_{2i-1}. \tag{46}$$

These are the two Kramers pairs $\phi_{1,2}$ that cross in Fig. 1. On X^τ, by definition, Kramers pairs are linearly independent and any one of them trivializes the bundle $\mathscr{H}_i|_{X^\tau}$.

A Kramers pair $(\psi_{I,i}, \psi_{II,i})$ is also commonly written as $(\phi_i, C\phi_i)$ if we randomly choose $\phi_i = \psi_{I,i}$ or $\phi_i = \psi_{II,i}$, since there is no *a priori* ordering between the chiral states $\psi_{I,i}$ and $\psi_{II,i}$.

A Kramers pair that crosses the 0 level at a fixed point will be called a Majorana zero mode. If there is an additional PHS operator $\Pi = C'$, or, mathematically, an additional grading operator χ, then in the basis above one can further assume that $\phi_{2i} = \Pi\phi_{2i-1}$. Note that this choice is symmetric in the case $j = 2$, but not in the case $j = 4$.

5. Kramers pairs and the decomposition

In $\mathscr{H}_+\oplus\mathscr{H}_-$, we can regard Kramers pairs as above,

$$(\phi, C\phi) = ((\phi_+, \phi_-), ((C\phi)_+, (C\phi)_-)) = ((\phi_+, \phi_-), (C(\phi_-), C(\phi_+)))$$

There are now several choices. Indeed there are four obvious pairs,

$$\begin{array}{cc} ((\psi_{2i-1,+}, 0), (0, C\psi_{2i-1,+})) & ((\psi_{2i,+}, 0), (0, C\psi_{2i,+})) \\ ((C\psi_{2i-1,-}, 0), (0, -\psi_{2i-1,-})) & ((C\psi_{2i,-}, 0), (0, -\psi_{2i,-})) \end{array}$$

These are not linearly independent though, the relations will be given by the transition functions below. By mixing and matching, this leads to the following choice of two Kramers pairs, whose elements give a local basis,

$$(\psi_{I,i}, \psi_{II,i}) = ((\psi_{2i-1,+}, C\psi_{2i,+}), (-\psi_{2i,+}, C\psi_{2i-1,+}))$$
$$(\tilde{\psi}_{I,i}, \tilde{\psi}_{II,i}) = ((\psi_{2i-1,+}, -C\psi_{2i,+}), (\psi_{2i,+}, C\psi_{2i-1,+}))$$

The first is the basis of the description of Ref. 66 as it is possible to choose ψ_{2i}, ψ_{2i-1} in such a fashion that they glue to be a section over certain subdomains,[50,66] that is on X^τ: $\psi_{I/II,i,+} - \psi_{I/II,i,-} = 0$. The sections in the second pair do not glue, but rather their difference generates the fiber, that is on X^τ: $(\psi_{I,i,+} - \psi_{I,i,-}, \psi_{II,i,+} - \psi_{II,i,-}) = (\phi_i, C\phi_i)$. This is a manifestation of Majorana zero modes, see Refs. 4 and 6. The corresponding configurations are sketched in Fig. 1.

B. Effective boundary/bulk-boundary

One can regard Z or X^τ as an effective boundary. In particular, for $\mathbb{S}^{D,d}$, $Z = \mathbb{S}^{D-1,d}$, and if $d = 0$, this is just the equator. Taking Z as a reflection plane, this explains the doubling construction of Ref. 55. Looking at the spectral flow at the fixed point locus is discussed in Sec. VI D. Note that the fixed point locus on $\mathbb{S}^{D,d}$ is $\mathbb{S}^{0,d} = S^{d-1}$, so that another way to look at the bulk/boundary correspondence is as the (1,1)-periodicity in Table I.

VI. *KR* AND *KQ* THEORY

A. Real and quaternionic K-theory

The vector bundles that support TRS/PHS invariant Hamiltonians have to come equipped with the antilinear operators C that allow to write the Eq. (19). This is the setting of Real and Quaternionic bundles as discussed in Sec. III. The corresponding Real K-groups were first introduced by Atiyah[7] and the Quaternionic K-groups by Dupont.[8] We recollect the basic facts here. A good reference is Ref. 16. Real and Quaternionic bundles, see Definition III.2, afford a direct sum construction, viz. if E_1 and E_2 are Real, respectively Quaternionic, bundles with operators C_1 and C_2, then the Whitney sum $E_1\oplus E_2$, is also Real, respectively Quaternionic, by taking the fiberwise direct of the symmetry operators $C = C_1\oplus C_2$.

Definition VI.1. For a compact Hausdorff Real space (X, τ), the Real K-group $KR(X, \tau)$, respectively, the Quaternionic K-group $KQ(X, \tau)$ are defined to be the Grothendieck group of finite rank Real, respectively Quaternionic vector bundles (E, C) over (X, τ).

When the involution τ is understood, the Real/Quaternionic K-group $KR(X, \tau)$, respectively $KQ(X, \tau)$, is denoted simply by $KR(X)$, respectively $KQ(X)$.

Recall that the Grothendieck group for an Abelian monoid, here isomorphism classes of vector bundles with $\oplus$ as the monoid structure, is the group completion whose elements are formal differences, here $[E_1\ominus E_2]$. These are constructed as pairs of isomorphisms classes $([E_1], [E_2])$ modulo the cancellation law $([E_1], [E_2]) \sim ([F_1], [F_2])$ if there is a G such that $[E_1\oplus F_2\oplus G] = [F_1\oplus E_2\oplus G]$.

Like in K theory, KR-theory (and parallelly KQ-theory) can be extended to locally compact spaces. For a pointed space $(X, x_0 \in X)$, the reduced Real K-group $\widetilde{KR}(X)$ is defined as the kernel of the restriction map $i^* : KR(X) \to KR(x_0) = \mathbb{Z}$ and similarly for the Quaternionic K-group. If X is only a locally compact Hausdorff space, then the convention is that the K-theory is the relative K-theory of its one-point compactification X^+: $KR(X) := \widetilde{KR}(X^+)$. The relative KR groups are defined as $KR(X,Y) = \widetilde{KR}(X/Y)$.

Parallel to topological K-theory, one can equivalently define the reduced KR and KQ groups, denoted by $\widetilde{KR}$ and $\widetilde{KQ}$ via stabilization, viz. isomorphism classes after possibly adding trivial bundles $[E] \sim [F]$ if there are trivial bundles τ_1, τ_2 such that $[E \oplus \tau_1] = [F \oplus \tau_2]$. For this notice that on a trivial bundle, respectively, an even rank trivial bundle, there exists a natural Real, respectively Quaternionic, structure acting on the fibers,[67] cf. Sec. II A 4, and thus stabilization is well defined. The reduced versions of the theory are the kernel of the rank map induced by the inclusion of the base-point. Note that stabilization makes sense in the physical setting, as adding a trivial bundle that is not occupied does not change the physics of a topological insulator.

The higher KR groups are defined as $KR^{-i}(X) := \widetilde{KR}(\Sigma^i(X))$ where Σ is the reduced suspension. For a pointed space $(X, x_0 \in X)$: $\Sigma X = (X \times I)/(X \times \{0\} \cup X \times \{1\} \cup \{x_0\} \times I)$, where $I = [0,1]$. In particular, for the spheres S^n: $\Sigma S^n = S^{n+1}$. There are completely parallel definitions for KQ.

A fundamental fact is that there exists a canonical isomorphism[8]

$$KQ^{-j}(X) \cong KR^{j-4}(X), \tag{47}$$

Thus these theories are isomorphic up to a shift and all properties of KQ can be deduced from those of KR.

Bott periodicity of KR-theory is 8,

$$KR^{-i-8}(X) \cong KR^{-i}(X) \tag{48}$$

and the Bott periodicity of KQ-theory is easily derived from that of KR-theory. This allows to define these theories for all $j \in \mathbb{Z}$.

These theories satisfy the axioms of a generalized cohomology theory, that is the Eilenberg–Steenrod axioms with the exception of the dimension axiom. This provides a long exact sequence for a pair (X, Y) of involutive spaces. The sequence reads:

$$\cdots \to \widetilde{KR}^{-i-1}(Y) \to \widetilde{KR}^{-i}(X/Y) \to \widetilde{KR}^{-i}(X) \to \widetilde{KR}^{-i}(Y) \to \cdots \tag{49}$$

If Z is a retract of X, there is a splitting

$$\widetilde{KR}^{-i}(X) = \widetilde{KR}^{-i}(X,Y) \oplus \widetilde{KR}^{-i}(Y) \tag{50}$$

For two spaces with base points (X, x_0) and (Y, y_0), their wedge sum is defined as $X \vee Y = (X \sqcup Y)/(x_0 \sim y_0)$. The smash product is defined as $X \wedge Y = (X \times Y)/(X \vee Y)$. In this case, (50) yields

$$\widetilde{KR}^{-i}(X \times Y) = \widetilde{KR}^{-i}(X \wedge Y) \oplus \widetilde{KR}^{-i}(X) \oplus \widetilde{KR}^{-i}(Y) \tag{51}$$

There exists a natural link between KR-theory and complex K-theory,[7] given by

$$KR^{-i}(Y \times \mathbb{S}^{0,1}) \cong K^{-i}(Y) \tag{52}$$

By Bott periodicity two for complex K-theory:

$$KQ^{-i}(Y \times \mathbb{S}^{0,1}) \simeq KR^{4-i}(Y \times \mathbb{S}^{0,1}) \simeq K^{4-i}(Y) \simeq K^{-i}(Y) \tag{53}$$

This can be used to treat the two other cases, the complex cases A and AIII, appearing in the AZ classification.

When the involution τ on the base space X in KR-theory is trivial, it is the real K-theory of X, that is the Grothendieck group of real vector bundles, which is called KO-theory,

$$KR^{-i}(X, \tau = \mathrm{id}) = KO^{-i}(X) \tag{54}$$

which also has the Bott periodicity 8: $KO^i(X) \cong KO^{i+8}(X)$. The KO-theory of a point is given in Table III. This can be computed using the construction of Atiyah–Bott–Shapiro[10] which uses Clifford algebras. This also explains the periodicity 8. In the case of trivial involution, $KQ^{-i}(X, \tau = \mathrm{id}) = KSp^{-i}(X)$ is known as symplectic K-theory, that is the K-theory of symplectic bundles.

These are the groups that appear in the KR groups of the standard spaces; see the examples below. They also correspond to the known topological insulator classifications, see Theorem VI.15 below.

TABLE III. The *KO* groups of a point for *i* mod 8.

i	0	1	2	3	4	5	6	7
$KO^{-i}(pt)$	$\mathbb{Z}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	0	$\mathbb{Z}$	0	0	0

What is special in Real K-theory are the bi-indexed groups which are defined as

$$KR^{p,q}(X,Y) := KR(X \times \mathbb{B}^{p,q}, X \times \mathbb{S}^{p,q} \cup Y \times \mathbb{B}^{p,q}) \tag{55}$$

In particular, $KR^{i,0}(X) = KR^{-i}(X)$. There exists an isomorphism, called the (1,1)-periodicity of KR-theory given by multiplication by $\xi = [B_H] - [\tau_1]$ where B_H is the Hopf bundle and τ_1 a trivial bundle.

$$KR^{p,q}(X) \cong KR^{p+1,q+1}(X) \tag{56}$$

It follows that $KR^{p,q}(X) \simeq KR^{q-p}$.

Example VI.2. Since $\mathbb{S}^{1,d}$ is the one-point compactification of $\mathbb{R}^{0,d}$:

$$KR^{-i}(\mathbb{S}^{1,d}) = KO^{-i}(pt) \oplus KR^{-i}(\mathbb{R}^{0,d}) = KO^{-i}(pt) \oplus KO^{-i+d}(pt) \tag{57}$$

$\mathbb{S}^{D,d}$ has an equivariant CW-structure with one 0-cell and one top cell of dimension $D + d - 1$. This also corresponds to the decomposition of the sphere $\mathbb{S}^{1,d} = \mathbb{R}^{0,d} \cup \{\infty\}$, one fixed point of the time reversal symmetry is $\{0\} \in \mathbb{R}^{0,d}$ and the other is $\{\infty\}$. The two summands can be identified with the contributions from these two cells and the top cell summand is $KO^{-i+d}(pt)$.

More generally, by suspension one obtains

$$\widetilde{KR}^{-i}(\mathbb{S}^{D,d}) = KR^{-i}(\mathbb{R}^{D-1,d}) = KO^{-i+d-D-1}(pt) \tag{58}$$

which is the summand corresponding to the top cell. In particular,

$$\begin{aligned} KQ(\mathbb{S}^{1,2}) &= KR^{-4}(\mathbb{S}^{1,2}) = KO^{-4}(pt) \oplus KO^{-2}(pt) = \mathbb{Z} \oplus \mathbb{Z}_2 \\ KQ(\mathbb{S}^{1,3}) &= KR^{-4}(\mathbb{S}^{1,3}) = KO^{-4}(pt) \oplus KO^{-1}(pt) = \mathbb{Z} \oplus \mathbb{Z}_2 \end{aligned} \tag{59}$$

Example VI.3. The KQ-groups of $\mathbb{T}^d$ are iteratively computed as

$$KR^{-i}(\mathbb{T}^d) = \oplus_{k=0}^{d} \binom{d}{k} KO^{-i+k}(pt) = \oplus_{k=0}^{d} \binom{d}{k} KO^{-i+k}(pt) \tag{60}$$

As KQ is given by shifting KR by 4:

$$\begin{aligned} KQ(\mathbb{T}^2) &= KR^{-4}(\mathbb{T}^2) = KO^{-4}(pt) \oplus KO^{-2}(pt) = \mathbb{Z} \oplus \mathbb{Z}_2 \\ KQ(\mathbb{T}^3) &= KR^{-4}(\mathbb{T}^3) = KO^{-4}(pt) \oplus 3KO^{-2}(pt) \oplus KO^{-1}(pt) \quad = \mathbb{Z} \oplus 4\mathbb{Z}_2 \end{aligned} \tag{61}$$

Alternatively, one can decompose $\mathbb{T}^d = (\mathbb{S}^{1,1})^{\times d}$ into fixed points plus involutive Euclidean spaces $\mathbb{R}^{0,k}$ $(0 \le k \le d)$ and use this for the computation.

From the above example, notice that $KQ(\mathbb{T}^3)$ has $\mathbb{Z}_2$-components from both $KO^{-1}(pt)$ and $KO^{-2}(pt)$ corresponding to the weak and the strong invariants. These can be read out by KR cycles, see below.

Example VI.4. Taking products with the spheres $\mathbb{S}^{D,d}$ from (51) and using the definition of shifts, recall $(\mathbb{R}^{d,D-1})^+ = \mathbb{S}^{d,D}$,

$$\widetilde{KR}^{-i}(X \times \mathbb{S}^{D,d}) = \widetilde{KR}^{-i+d-D+1}(X) \oplus \widetilde{KR}^{-i}(X) \oplus KO^{-i+d-D+1}(pt) \tag{62}$$

In particular, as $S^D = \mathbb{S}^{0,D+1}$

$$\widetilde{KR}^{-i}(T^d \times S^D) = \widetilde{KR}^{-i+d-D}(T^d) \oplus \widetilde{KR}^{-i}(T^d) \oplus KO^{-i-D}(pt) \tag{63}$$

The product has a CW model by using the decomposition of the torus from Example VI.3 and the model of the sphere with one 0-cell and one cell in top dimension.

The summand $K0^{-i+d-D}(pt)$ in the first term is the term coming from the top cell, which has dimension $d + D$.

Remark VI.5. Another way to compute the KR-theory of $\mathbb{T}^d$ is to use the stable homotopy splitting of the torus into spheres, see Ref. 46. This uses the periodicity under suspension and the formula $\Sigma(X \times Y) = \Sigma X \vee \Sigma \vee \Sigma(X \wedge Y)$ for connected X, Y.

The Baum–Connes isomorphism for the free Abelian group $\mathbb{Z}^d$ provides yet another method to compute the KR-theory of $\mathbb{T}^d$.

B. Examples of long exact sequences used in defining invariants

As a first upshot of our treatment, we can use several long exact sequences in K-theory, that corresponds to the different ways to introduce the $\mathbb{Z}_2$ invariant found in the physics literature. These correspond to different ways topological invariants have been computed.

There is long exact sequence in KR/KQ-theory corresponding to the "exact sequence"[48] [II, 4.17] $Z \dashrightarrow X \dashrightarrow X\backslash Z$ for a closed Z. Here the dashed arrows indicate that we are looking at locally compact spaces and the morphisms in that category which are defined via their one point compactifications. In KQ the sequence reads:

$$\cdots KQ^{-i-1}(Z) \to KQ^{-i}(X\backslash Z) \to KQ^{-i}(X) \to KQ^{-i}(Z) \to \cdots \tag{64}$$

Lemma VI.6. For a regular space X with $Z = V^+ \cap V^-$, we have the long exact sequence

$$\begin{aligned} \cdots\ &\to K^{-i-1}(V_+^o) \to KQ^{-i-1}(X) \to KQ^{-i-1}(Z) \\ &\to K^{-i}(V_+^o) \to KQ^{-i}(X) \to KQ^{-i}(Z) \to \cdots \end{aligned} \tag{65}$$

Proof. By assumption Z separates, so that $X\backslash Z = V_+^o \sqcup V_-^o = V_+^o \times \mathbb{S}^{0,1}$ and we can apply (53) and (57). ◻

If we are in the case of a weak $\mathbb{Z}_2$-space, one can now further decompose Z iteratively. This explains the effective boundary used in Ref. 50.

Example VI.7. In the case of $\mathbb{T}^2$, we have $V_+^o \sim \mathbb{S}^1 \times \mathbb{R}$, $Z = \mathbb{S}^{1,1} \sqcup \mathbb{S}^{1,1}$,

$$K(V_+^o) \to KQ(X) \to KQ(Z) \tag{66}$$

where $K(V_+^o) = K(\mathbb{S}^1 \times \mathbb{R}) = K^{-1}(\mathbb{S}^1) = \mathbb{Z}$, $KQ(\mathbb{T}^2) = \mathbb{Z} \oplus \mathbb{Z}_2$ and $KQ(\mathbb{S}^{1,1}) = KQ(pt) \oplus KQ^1(pt) = \mathbb{Z}$. In other words, the above exact sequence gives

$$\mathbb{Z} \to \mathbb{Z} \oplus \mathbb{Z}_2 \to \mathbb{Z} \oplus \mathbb{Z} \tag{67}$$

or in reduced K-theory,

$$\widetilde{K}^{-1}(\mathbb{S}^1) \to \widetilde{KQ}(\mathbb{T}^2) \to 2\widetilde{KQ}(\mathbb{S}^{1,1}), \quad \mathbb{Z} \to \mathbb{Z}_2 \to 0 \tag{68}$$

This explains the reduction from $\mathbb{Z}\ (= \widetilde{K}^{-1}(\mathbb{S}^1) \cong \widetilde{K}(\mathbb{T}^2))$ to $\mathbb{Z}_2\ (= \widetilde{KQ}(\mathbb{T}^2))$, that is, the $\mathbb{Z}_2$ invariant results from the time reversal symmetry while the complex K-theory becomes the Quaternionic K-theory.

When X is a weak $\mathbb{Z}_2$-space, there exists a decomposition $X = X_+ \sqcup X_- \sqcup X^\tau$, one has a long exact sequence involving different K-theories.

Lemma VI.8. If X is a weak $\mathbb{Z}_2$-space, then there exists a long exact sequence

$$\begin{aligned} \cdots\ &\to KQ^{-j-1}(X_+ \cup X_-) \to KQ^{-j-1}(X) \to KSp^{-j-1}(X^\tau) \\ &\to KQ^{-j}(X_+ \cup X_-) \to KQ^{-j}(X) \to KSp^{-j}(X^\tau) \to \cdots \end{aligned} \tag{69}$$

where $X_+ \cup X_-$ has a free $\mathbb{Z}_2$-action interchanging the spaces. If X_+ and X_- are in different components of $X\backslash X^\tau$, then the above long exact sequence is reduced to

$$\begin{aligned} \cdots\ &\to K^{-j-1}(X_+) \to KQ^{-j-1}(X) \to KSp^{-j-1}(X^\tau) \\ &\to K^{-j}(X_+) \to KQ^{-j}(X) \to KSp^{-j}(X^\tau) \to \cdots \end{aligned} \tag{70}$$

Proof. Using $X^\tau \dashrightarrow X \dashrightarrow X\backslash X^\tau$, we get the first sequence by noticing that when restricting the involution τ to the fixed points, $\tau|_{X^\tau}$ becomes trivial, so $KQ^{-j}(X^\tau, \tau|_{X^\tau}) = KSp^{-j}(X^\tau)$. Now under the assumption that X_+ and X_- are in different components of $X\backslash X^\tau$, we have $X\backslash X^\tau = X_+ \sqcup X_- = X_+ \sqcup \tau(X_+) = X_+ \times \mathbb{S}^{0,1}$, it follows that $KQ^{-j}(X\backslash X^\tau) = KQ^{-j}(X_+ \times \mathbb{S}^{0,1}) \simeq K^{-j}(X_+)$. ◻

We can also replace the middle terms by $KQ^{-j}(X) \simeq KR^{-j+4}(X)$. This sequence is at the heart of the description of Ref. 66.

Example VI.9. When $X = \mathbb{S}^{1,3}$, $X^\tau = \mathbb{S}^{0,1}$ and the open set is chosen to be $\mathbb{S}^{1,3}\backslash\mathbb{S}^{0,1} = \mathbb{R}^{0,3}\backslash\{0\} = X_+ \cup X_-$, where $X_+ \sim 3\mathbb{R} \cup 6\mathbb{R}^2 \cup 4\mathbb{R}^3$. Here and below for an object A (space or group) we take $nA = A \oplus \cdots \oplus A$ n-times where for a space $\oplus = \sqcup$, the disjoint union. We extract two parts from the long exact sequence, the first part is

$$KSp^{-6}(\mathbb{S}^{0,1}) \to K^{-5}(X_+) \to KQ^{-5}(\mathbb{S}^{1,3}) \to KSp^{-5}(\mathbb{S}^{0,1}) \tag{71}$$

that is,

$$2\mathbb{Z}_2 \to 3\mathbb{Z} \oplus 4\mathbb{Z} \to \mathbb{Z}_2 \to 2\mathbb{Z}_2 \tag{72}$$

And the second part is

$$KSp^{-2}(\mathbb{S}^{0,1}) \to K^{-1}(X_+) \to KQ^{-1}(\mathbb{S}^{1,3}) \to KSp^{-1}(\mathbb{S}^{0,1}) \tag{73}$$

that is,

$$0 \to 3\mathbb{Z} \oplus 4\mathbb{Z} \to \mathbb{Z}_2 \to 0 \tag{74}$$

Another sequence is the Mayer–Vietoris sequence for a regular space X covered by two fundamental domains, i.e., $X = V_+ \cup V_-$,

$$\cdots \to KQ^{-i-1}(V_+ \cap V_-) \xrightarrow{\Delta} KQ^{-i}(X) \xrightarrow{u} KQ^{-i}(V_+) \oplus KQ^{-i}(V_-) \xrightarrow{v} KQ^{-i}(V_+ \cap V_-) \to \cdots \tag{75}$$

where $u(\alpha) = (\alpha|_{V+}, \alpha|_{V_-})$ and $v(\alpha_1, \alpha_2) = \alpha_1|_{V_+\cap V_-} - \alpha_2|_{V_+\cap V_-}$.

Example VI.10. This is the long exact sequence at the heart of the argument of Ref. 68. When $X = \mathbb{T}^2$, $V_+ = V_- = C = \mathbb{S}^{1,1} \times \mathbb{R}^{0,1}$, where C is an open cylinder with the time reversal $\mathbb{Z}_2$-action and $Z = V_+ \cap V_- = \mathbb{S}^{1,1} \sqcup \mathbb{S}^{1,1}$.

$$2KQ^{-1}(\mathbb{S}^{1,1}) \to KQ(\mathbb{T}^2) \to 2KQ(C) \to 2KQ(\mathbb{S}^{1,1}) \tag{76}$$

Since $KQ(\mathbb{T}^2) \cong KQ(\mathbb{S}^{1,2})$, the above sequence is the same as

$$2KQ^{-1}(\mathbb{S}^{1,1}) \to KQ(\mathbb{S}^{1,2}) \to 2KQ(C) \to 2KQ(\mathbb{S}^{1,1}) \tag{77}$$

The KQ-theory of the cylinder C is,

$$KQ(C) = KR^{-4}(\mathbb{S}^{1,1} \times \mathbb{R}^{0,1}) = KR^{-3}(\mathbb{S}^{1,1}) = KO^{-3}(pt) \oplus KO^{-2}(pt) = \mathbb{Z}_2 \tag{78}$$

so that,

$$\mathbb{Z} \oplus \mathbb{Z} \to \mathbb{Z} \oplus \mathbb{Z}_2 \to \mathbb{Z}_2 \oplus \mathbb{Z}_2 \to \mathbb{Z} \oplus \mathbb{Z} \tag{79}$$

Hence the $\mathbb{Z}_2$ invariant living in $\widetilde{KQ}(\mathbb{S}^{1,2})$ can also be found in $KQ(C)$.

Finally, there is the relative sequence, for a closed subspace Y in X

$$KQ^{-j-1}(X, Y) \to KQ^{-j}(X) \to KQ^{-j}(Y) \to KQ^{-j}(X, Y) \tag{80}$$

as $KQ^{-n}(X, Y) = \widetilde{KQ}(\Sigma^n(X/Y)))$, where S^n is the n-fold suspension, then the first map is induced by the quotient $q : X \to X/Y$.

Example VI.11. Using this for $\mathbb{T}^2$ and $\mathbb{S}^{1,1} \vee \mathbb{S}^{1,1}$, one obtains the collapse map $q : \mathbb{T}^2 \to \mathbb{S}^2$ and similarly for $\mathbb{T}^3$. This is what is used in Ref. 46.

C. Identifications of invariants as bivariant *KR*-groups

Definition VI.12. We define the *topological invariants* of a system with symmetry $j = s + 1$ on an involutive space (X, τ) to be $KR^{-s}(X)$. If (X, τ) is a $\mathbb{Z}/2\mathbb{Z}$ equivariant CW complex with one top-dimensional cell in dimension k, let X^{k-1} be its $k-1$-skeleton, we define the *strong topological invariants* of (X, τ) to be the image of $\widetilde{KR}^{-s}(X, X^{k-1}) \to \widetilde{KR}^{-s}(X)$ coming from the long exact sequence (49).

Note that if the top dimensional cell has as open part is $\mathbb{R}^{D,d}$, (k = D + d), then $X/X^{k-1} = \mathbb{S}^{D+1,d}$ and $\widetilde{KR}^{-s}(X, X^{k-1}) = \widetilde{KR}^{-s}(\mathbb{S}^{D+1,d}) = KO^{-s+d-D-1}(pt) = KO^{-j-2-\delta}(pt)$ where $\delta = D - d$ and $j = s + 1$. Suspending only once, we see that $\widetilde{KR}^{-s}(X, X^{k-1}) = \widetilde{KR}^{-s-1}(\mathbb{S}^{D,d}) = \widetilde{KR}^{-j-2}(\mathbb{S}^{D,d})$.

Remark VI.13. Note that the cases of the sphere $\mathbb{S}^{D,d}$ (Example VI.2), the torus T^d (Example VI.3) and $T^d \times S^D$ (Example VI.4) with the given examples are of this type and moreover the strong invariants are split as a summand as discussed in Examples VI.2, VI.3 and VI.4 and Remark VI.5.

Remark VI.14. The cases where there is only one symmetry operator, that is a TRS operator, are AII, i.e. $j = 3$ $(s = 4)$ with $\Theta^2 = -1$ and AI $j = 7$ $(s = 0)$ with $\Theta^2 = 1$. For AII, $KR^{-s}(X) = KR^{-4}(X) = KQ(X)$, which was the original motivation for considering KQ-theory in Ref. 6. The case AI corresponds to the bosonic TRS and the relevant topological invariants are the un-shifted $KR(X)$. This can thus be seen as the origin of considering KR and KQ theory.

Theorem VI.15. *Setting $j = s + 1$, the Teo–Kane classification of strong topological invariants in Table IV can be identified with the KR groups $\widetilde{KR}^{-j-2}(\mathbb{S}^{D,d})$.*

In particular, this is the split summand consisting of the classes in $KR^{-s}(\mathbb{T}^d \times S^D)$ pulled-back from $\mathbb{S}^{D+1,d}$ to $KR^{-j-2}(\mathbb{S}^{D,d})$ via the map $\pi : (\mathbb{T}^d \times S^D) \to \mathbb{S}^{D+1,d}$ defined in (17).

Proof. First notice that the entries indeed are equal to $\widetilde{KR}^{-j-2}(\mathbb{S}^{D,d})$. Setting $s = j + 1, \delta = d - D$, since $-j - 2 + d - (D - 1) = -j - 1 + (d - D) = \delta - s$

$$\widetilde{KR}^{-j-2}(\mathbb{S}^{D,d}) \simeq KR^{-j-2}(\mathbb{R}^{D-1,d}) \simeq KR^{-j-1+d-D}(pt) = KO^{\delta-s}(pt) \tag{81}$$

Due to the (1,1) periodicity of the table, one sees that one only has to check one row or column to find the result. This is now clear from comparing Table III with Table IV. In particular, the column $\delta = 1$ reads as $KO^{-j}(pt)$ which corresponds to the sequence of groups $KO^{-i}(pt), i \equiv -7, 0, -1, -2, \dots, -6$ in Table III.

The fact that $\widetilde{KR}^{-j-2}(\mathbb{S}^{D,d})$ is a split summand of $\widetilde{KR}^{-j-2}(\mathbb{T}^d \times S^{D-1})$ under pull-back follows from Remark VI.13. Inspection of the table shows that using the parameters s and δ we have agreement with the table from Ref. 4. Note that the present argument legitimizes their shift of focus from $\mathbb{T}^d \times S^{D-1}$ to S^{D-1+d} or, including the $\mathbb{Z}/2$ action, $\mathbb{S}^{D,d}$.

To compare the construction of the invariants, note that since in each row/column the sequence of KR-groups is that of the $KO^{-i}(pt)$—up to a shift—and the construction of the clocks of Ref. 4 agrees with the construction of periodicity in KR theory–see Refs. 7, 16, and 11—it is actually enough for the matching that the entry for the Kane–Mele invariant, that is $s = 4$, $\delta = 2$ is $\widetilde{KR}^{-4}(\mathbb{T}^2) = \widetilde{KQ}(\mathbb{T}^2) = KO^{-2}(pt)$. The identification of the Kane–Mele invariant is done by looking at the AII case in 2d which boils down to Remark VI.14 and (61) for the group. The identification for the actual invariant follows from the Example VI.10 for the version of the $\mathbb{Z}/2$ invariant defined in Ref. 68. For other physical definitions the identification is made in the other examples of Sec. VI B. □

Remark VI.16. There are several ways to understand this result. One is that the standard sequence for point defects is in the column $\delta = 1$. Point defects are what one can naturally enclose by a sphere, and they are the most easy to understand as giving rise to charges, cf. Ref. 58. As $\delta - s = 1 - j - 1 = -j$, the invariants lie in $KO^{-j}(pt)$. This explains the shift between j and s, where the latter is the preferred parameter in the physics literature. The standard sequence in the column $\delta = 0$ is $KO^{-s}(pt)$. Likewise one can study the rows. Fixing j and varying d for the spheres $\mathbb{S}^{1,d}$, the topological invariants are in $\widetilde{KR}^{-j-2}(\mathbb{S}^{1,d}) = KO^{d-1-s}(pt)$ which corresponds to the one special TRS point of the point defect, see (57). For $s = 0$ (AI) starting at $d = 1, \delta = 0$, we obtain the sequence of the first column cyclically read right to left. This means that the invariant just comes from that of a point by suspension, see Theorem III.20. For $s = 4$ (AII) this is shifted by 4, as expected from the arguments in Remark VI.14.

TABLE IV. The classification of insulators in dimension d with defects in dimension D according to Ref. 4. Note that we also used the convention $2\mathbb{Z}$ which helps to distinguish this group from the group $\mathbb{Z}$. Mathematically, the isomorphism is given by $\frac{1}{2} : 2\mathbb{Z} \to \mathbb{Z}$. The index j is the Clifford/KR-index. The entry is $\widetilde{KR}^{-s}(\mathbb{S}^{D+1,d}) \simeq \widetilde{KR}^{-j-2}(\mathbb{S}^{D,d}) \simeq KO^{\delta-s}(pt)$. The index s is the index of the eight hour clock of Ref. 4, which is related to Kitaev's index q by $s = q + 2$.

	$s \equiv j + 1(8)$					$\delta = d - D$				
j	s	AZ	0	1	2	3	4	5	6	7
7	0	AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
0	1	BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
1	2	D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
2	3	DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
3	4	AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
4	5	CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
5	6	C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
6	7	CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

The defects of the theory can be identified with the fixed point locus X^τ. That is, the spheres S^{D-1} times the isolated fixed points of momentum space. This is a reduced situation from the point of view of physics. From the pure geometric point of view, the fixed points are naturally given by $(\mathbb{S}^{d,D})^\tau = \mathbb{S}^{0,D}$, which is the $\mathbb{S}^{D-1}$ carrying the parameters in real space in physics parlance.

In the considerations of Ref. 4, the base manifolds considered are $\mathbb{T}^d \times S^D$ or $\mathbb{S}^{1,d} \times \mathbb{S}^{D,0}$-note that $\mathbb{S}^{D,0} = \mathbb{S}^{D-1} \subset \mathbb{R}^D$. Both spaces can be seen as the quotient of the ball $\mathbb{B}^{D-1,d} \subset \mathbb{R}^{D-1,d}$ as in Sec. III A 2. To see this, consider the Cartesian product of the cubes $I^{D-1,0} \times I^{0,d} = I^{D,d} \approx \mathbb{B}^{D,d}$. One can now quotient by either periodic boundary conditions or the full ∂I^d to obtain the two spaces $\mathbb{T}^d \times \mathbb{S}^{D,0}$ or $\mathbb{S}^{1,d} \times \mathbb{S}^{D,0}$. To obtain $\mathbb{S}^{D,d}$, one can take a further quotient by the wedge product of the spaces which gives the one-point compactification $I^{D-1,d}/\partial(I^{D-1,d}) = \dot{\mathbb{R}}^{D-1,d} = \mathbb{S}^{D,d}$. This gives a natural interpretation of the physical construction of taking the boundary of a tubular neighborhood of the defects used in Ref. 4.

Example VI.17. In the case of $\mathbb{T}^d$, we obtain that $\widetilde{KR}^{-s}(\mathbb{T}^d) = \oplus_{k=1}^{d}\binom{d}{k}KO^{-s+k}(pt)$. In particular, for $j = 3, s = 4, d = 2$, as $KO^{-3}(pt) = 0$, this is $KO^{-2}(pt)$. This is the case of the original Kane-Mele invariant.

For $j = 3, s = 4, d = 3$, we have $3KO^{-2}(pt) \oplus KO^{-1}(pt)$ which corresponds to the three weak and the strong Kane–Mele invariants. Notice that we can also see that three weak invariants are given by the three coordinate inclusions of $\mathbb{T}^2$ into $\mathbb{T}^3$ by pulling back along the three coordinate inclusions.

D. Spectral flow

There is a way to see the indices as given by spectral flow, see e.g. Ref. 53. In particular, choosing a transversal direction to a fixed point, one can now regard the spectral flow of the operator. Heuristically, the spectral flow of a one-parameter family of self-adjoint Fredholm operators is just the net number of eigenvalues (counting multiplicities) which pass through zero in the positive direction from the start of the path to its end. More precisely, let $B : [0,1] \to \mathscr{F}^{sa}_*$ be a continuous path of self-adjoint Fredholm operators. Writing B_t for $B(t)$, one defines eigenprojections by functional calculus $E_a(t) := \chi_{[-a,a]}(B_t)$, and then the spectral flow of $\{B_t\}$, denoted by $sf(B)$, can be defined as the dimension of the nonnegative eigenspace at the end of this path minus the dimension of the nonnegative eigenspace at the beginning, for details see Ref. 69.

1. Background from Ref. 15

The space of self-adjoint Fredholm operators $\mathscr{F}^{sa}$ has three components, the first component $\mathscr{F}^{sa}_+$ has essential spectrum $\{+1\}$, the second component $\mathscr{F}^{sa}_-$ has essential spectrum $\{-1\}$, and the third component is the complement $\mathscr{F}^{sa}_* = \mathscr{F}^{sa} \backslash (\mathscr{F}^{sa}_+ \sqcup \mathscr{F}^{sa}_-)$.[15] Atiyah and Singer[15] define subsets $\mathscr{F}^{sa,k}_* \subset \mathscr{F}^{sa}$ and show that they are classifying spaces for KR^{-k}. The space $\mathscr{F}^{sa,k}$ is given by those real skew-adjoint operators A that anti-commute with a given set of Clifford elements

$$J_i^2 = -1, \quad \{J_i, J_j\} = 0, \quad \{J_i, A\} = 0, \quad i = 1, \ldots k-1, \quad J_k^* = J_k; \tag{82}$$

This is understood to be a nested collection depending on k. In the case $k = -1(4)$ one also postulates that $w(A) := J_1 J_2 \cdots J_{k-1} A = w(A)^*$. Setting $J_0 = 1$, the (de)looping morphism is

$$\mathscr{F}^{sa,k}_* \to \Omega_{-J_{k-1},J_{k-1}}(\mathscr{F}^{sa,k-1}_*), \quad A \mapsto \sin(\pi t)A + \cos(\pi t)J_{k-1}, \quad t \in [0,1] \tag{83}$$

Where $\Omega_{-J_{k-1},J_{k-1}}$ are the paths from $-J_{k-1} \to J_{k-1}$, which is the adjoint functor to the suspension S.

The indices ind_j, $j = 0, 1, 2, 4$ having values in $KO^{-j}(pt)$ defined in Ref. 10 can be seen as counting Eigenvalues.[53] The definition is first as a map $\mathrm{ind}_k : \mathscr{F}^{sa,k}_* \to A_k$, where A_k is the Grothendieck group of graded C_k-modules modulo those extendable to C_{k+1} modules, given by $A \mapsto [Ker(A)]$. Note $\ker(A)$ is a C_k module for $A \in \mathscr{F}^k_*$. This map is continuous and gives and isomorphism between $\pi_0(\mathscr{F}^{sa,k}_*) \simeq A_k$. The latter is isomorphic to $KO^{-k}(pt)$, see Ref. 10. In this setup, $\mathrm{ind}_0(B) = \mathrm{index}(B_0)$, where now B acts on a $\mathbb{Z}/2\mathbb{Z}$ graded Hilbert space $\mathscr{H} = \mathscr{H}_0 \oplus \mathscr{H}_1$, $\mathrm{ind}_1(A) = \dim_{\mathbb{R}}(\ker(A)) \bmod 2$, $\mathrm{ind}_2(A) = \dim_{\mathbb{C}}(\ker(A)) = \frac{1}{2}\dim_{\mathbb{R}}(\ker(A)) \bmod 2$ (note the kernel has a complex structure using J_1), and $\mathrm{ind}_4(A) = \mathrm{index}_{\mathbb{H}}(A_+)$, where now the action of $Cl_2 = \mathbb{H} \oplus \mathbb{H}$, decomposes $\mathscr{H} = \mathscr{H}_+ \oplus \mathscr{H}_-$ into two quaternionic spaces. Notice that the isomorphism $A_k \simeq KO^{-k}(pt)$ can alternatively be given by delooping $\pi_0(\mathscr{F}^{as,k}_*) \simeq \pi_k(\mathscr{F}^{sa,0}_*) \simeq \widetilde{KR}(S^k) = KR^{-k}(pt)$.

2. Computing the indices via spectral flow

Using the property for the classifying spaces of KR^{-k} theory, that $\mathscr{F}^{sa,k} \simeq \Omega_{-J_{k-1},J_{k-1}}\mathscr{F}^{sa,k-1}$, the indices can be computed by the spectral flow, see Ref. 53 for details. Running through all the fixed points, we count all switchings of Eigenvalues from negative to positive by adding those spectral flows together. In the end, the total flow is the the collective result of those spectral flows. Namely, a Hamiltonian H is a self-adjoint Fredholm operator parametrized by $x \in X$. For each Eigenstate with zero energy around a fixed point x_k, one takes a transversal path $H : I_k = [0,1] \to \mathscr{F}^{sa}_*$ such that the fixed point x_k is located at $t = \frac{1}{2}$, so the spectral flow of a chiral zero mode is the same as the spectral flow of $\{H_t\}$ for $t \in I_k$. Note that the spectral flow of $\{H_t\}$ is independent of the choice of intervals I_k as long as such interval passes through x_k. One can find sketches of such spectral flows for example in Ref. 70. For each fixed point with a real (Majorana) zero mode, one considers a path $\{H_t\}$ for $t \in I_k$ and its local spectral flow, where k labels the fixed points with zero modes. So the spectral flow of the Hamiltonian $H(x)$

for $x \in X$ is the sum of all local spectral flows of $\{H(t), t \in I_k\}$ for all k, which counts all the sign changes of those local zero modes running over all the fixed points. Therefore, the spectral flow of the Hamiltonian $H(x)$ is the analytical index $\mathrm{ind}_a(H)$. In the case of $j = 2, 3$ the count is mod (2), and for $j = 4$ the count comes up with an even number, so to obtain an integer, one divides by 2. This corresponds to taking the quaternionic dimension, see Ref. 15.

This is commensurate with the discussion of level crossings in Sec. IV B.

Remark VI.18. In the symplectic setting, if one models a chiral state by some Lagrangian submanifold, then the intersection number between this Lagrangian and the zero energy level is given by the Maslov index, which is used to define an edge $\mathbb{Z}_2$ index in Ref. 71. The Maslov index can be geometrically realized by the spectral flow of a family of Dirac operators,[50] so that the edge $\mathbb{Z}_2$ index can be computed by a mod 2 spectral flow. Our approach has essentially the same idea using spectral flow, but it is not necessary to set up the model in symplectic topology.

E. Topological index

The definitions and shifts in degree can be understood by looking at the diagonal corresponding to $KO^{-2}(pt)$ with the examples $\mathbb{T}^d$ and $s = d + 2$ using the Atiyah–Singer index theorem which states that the analytical index can be computed by the topological index. In this subsection, we will compute the mod 2 analytical index corresponding to $KO^{-2}(pt)$ by a mod 2 topological index. This is the observation that the parity anomaly of the topological $\mathbb{Z}_2$ invariant can be translated into a gauge anomaly, and the local formula is basically given by the odd topological index of a specific gauge representing time reversal symmetry.[4,50,65] The new tool here is to use the Thom isomorphism.

Given a skew-adjoint elliptic operator P with the symbol class $[\sigma(P)] \in KR^{-2}(T^*X)$, the topological index of $[\sigma(P)]$ was constructed by Atiyah,[51]

$$ind_t : KR^{-2}(T^*X) \to KO^{-2}(pt) = \mathbb{Z}_2 \tag{84}$$

where $\pi : T^*X \to X$ is the cotangent bundle over X. For a d-dimensional involutive space (X, τ), the Thom isomorphism in KR-theory is given by

$$KR^{-j}(X) \cong KR^{d-j}(T^*X) \tag{85}$$

Combining these two maps gives a map from KR-theory (or KQ-theory) to $K\,O^{-2}(pt)$, and we still call it the topological index map.

Example VI.19. Considering $X = \mathbb{T}^d$ and $j = d$, this is the map

$$KQ^{-d+2}(\mathbb{T}^d) = KR^{-d-2}(\mathbb{T}^d) \to KR^{-2}(T\mathbb{T}^d) \to KO^{-2}(pt) \,\text{for}\, j = d \tag{86}$$

When $X = \mathbb{T}^2$, the topological index map is the map $ind_t : KQ(\mathbb{T}^2) = KR^{-4}(\mathbb{T}^2) \cong KR^{-2}(T^*\mathbb{T}^2) \to KO^{-2}(pt)$ which represents the Kane–Mele invariant for $j = 2$ in 2d.

When $X = \mathbb{T}^3$, the topological index map is a map from $KQ^{-1}(\mathbb{T}^3)$ to $\mathbb{Z}_2$, $ind_t : KQ^{-1}(\mathbb{T}^3) = KR^{-5}(\mathbb{T}^3) \cong KR^{-2}(T^*\mathbb{T}^3) \to KO^{-2}(pt)$. This is the case $j = 3$ and corresponds to the WZW type invariant.

VII. CONNES' C^* VERSION, *KR*-CYCLES AND INDEX PAIRINGS

In this section, we will interpret the results in terms of Connes' C^* version of KR-theory and the dual theory of cycles, which allows one to read out the KR classes. The dual theory is essentially a theory formulated in operators.

We will recall some basic facts about KR-cycles.[9,11,47] The motivation for the dual theory of KR-cycles comes from spin geometry.[16] In the C^* approach, the K-theory is given by a Grothendieck group of classes of idempotents in the matrix ring over a C^*-algebra. The main fact is that $K^0(X) = K_0(C^*(X))$, where $C^*(M) = C(M, \mathbb{C})$ with complex involution. Note there is a shift from an upper to a lower index as using functions changes the variance.

If one defines the real function algebra on the Real space (X, τ),

$$C_0(X, \tau) := \{f \in C_0(X) \,|\, \overline{f(x)} = f(\tau(x))\} \tag{87}$$

then the KR-theory of (X, τ) is identified with the topological K-theory of the above real function algebra,[72]

$$KR^{-i}(X, \tau) = KR_i(C_0(X, \tau)) \tag{88}$$

Note, some authors write $KO_i(C_0(X, \tau)$, which we avoid to not confuse this with the case of a trivial involution.

A. KR-cycles

There is a bit of notation involved for the dual KR cycles. This turns out to be the same data as used for AZ-classification. The main reference used is Ref. 11.

Definition VII.1. An (unbounded) K-cycle for a $*$-algebra of operators $\mathscr{A}$ is a triple $(\mathscr{A}, \mathscr{H}, D)$, commonly called a spectral triple in noncommutative geometry, where $\mathscr{H}$ is a complex Hilbert space, and $\mathscr{A}$ has a faithful $*$-representation on $\mathscr{H}$ as bounded operators, i.e., $\pi : \mathscr{A} \to B(\mathscr{H})$. D is a self-adjoint (typical unbounded) operator with compact resolvent such that the commutators $[D, \pi(a)]$ are bounded operators for all $a \in \mathscr{A}$.

In practice, $\mathscr{A}$ is always assumed to be a unital (pre-)C^*-algebra. When the representation π is understood, it is always skipped from the notation.

From a K-cycle $(\mathscr{A}, \mathscr{H}, D)$, one obtains the corresponding Fredholm module $(\mathscr{A}, \mathscr{H}, F)$ by setting $F = \text{sign}(D) := D(1 + D^2)^{-1/2}$. By definition, the set of equivalence classes of Fredholm modules modulo unitary equivalence and homotopy equivalence defines the K-homology group, for details see Refs. 73 and 74.

A K-cycle $(\mathscr{A}, \mathscr{H}, D)$ is even (or graded) if there exists a grading operator χ with $\chi^* = \chi$ and $\chi^2 = 1$ such that $D\chi = -\chi D$ and $\chi a = a\chi$ for all $a \in \mathscr{A}$. Otherwise, a K-cycle is odd (or ungraded). If there exists a grading χ, then the Hilbert space $\mathscr{H}$ is also assumed to be $\mathbb{Z}_2$-graded.

For the KR version, one postulates that $\mathscr{A}$ has an involution τ. In the original definition, one also uses a Clifford algebra action. We follow Ref. 11 in the notation for $Cl_{p,q}$ being the algebra generated by γ^k, $k = 1, \ldots, p + q$

$$(\gamma^k)^2 = 1, \quad k = 1 \ldots p; \quad (\gamma^k)^2 = -1; k = p + 1, \ldots, p + q; \quad \gamma^j\gamma^k = -\gamma^k\gamma^j, j \neq k \tag{89}$$

Remark VII.2. Note the differences to the definition in Sec. VI D: first of all, even Clifford elements are used and secondly there is one more odd Clifford element. This is due to the fact that in Sec. VI D the operator was real, so that the complex structure when extending scalars to $\mathbb{C}$ is the extra operator.

The following definition goes back to Ref. 47. We use the conventions of Ref. 11.

Definition VII.3. An unreduced KR^j-cycle is a quintuple $(\mathscr{A}, \mathscr{H}, D, C, \chi)$, where $\mathscr{A}$ is short for an involutive algebra $(\mathscr{A}, \tau)$, $(\mathscr{A}, \mathscr{H}, D)$ is a K-cycle, C is an antilinear isometry C on $\mathscr{H}$ that commutes with D and implements the involution τ, and χ is a grading operator, commuting with C and anti-commuting with D

$$CD = DC, \quad C^2 = \varepsilon_C \text{id}, \quad CaC^* = \tau(a), \quad C\chi = \chi C, \quad D\chi = -\chi D \tag{90}$$

where a stands for multiplication by a together with an action of the Clifford algebra $Cl_{p,q}$ which commutes with $\mathscr{A}$ and C and anti-commutes with D.

$$a\gamma^k = \gamma^k a, a \in \mathscr{A}; \quad D\gamma^k = -\gamma^k D, \quad C\gamma^k = \gamma^k C, \quad \chi\gamma^k = -\gamma^k\chi \tag{91}$$

Reduced real structures on a spectral triple were first introduced by Connes.[9] This allows to reduce away the action of the Clifford algebra, but introduces a more complex taxonomy, which, however, matches up with the classification of symmetry classes. Let $(\mathscr{A}, \mathscr{H}, D)$ be an unbounded K-cycle, with involutive $(\mathscr{A}, \tau)$, C an operator implementing τ and χ a grading operator.

Definition VII.4. A reduced KR^{2k-1}-cycle (for $j = 2k - 1 \bmod 8$) is a quadruple $(\mathscr{A}, \mathscr{H}, D, C)$ while a reduced KR^{2k}-cycle ($j = 2k \bmod 8$) is a quintuple $(\mathscr{A}, \mathscr{H}, D, C, \chi)$ for which the operators satisfy the relations in Table I.

The two notions of reduced and unreduced KR^j cycles are equivalent. This equivalence is given by explicit constructions using grading operators and projections to reduce a KR^j cycle, and vice versa doubling and quadrupling the Hilbert space to unreduce such a cycle, cf. Ref. 11.

Example VII.5. The following example is the classical Dirac geometry modeling Majorana spinors in spin geometry.[11,16] Let M be a compact spin manifold of dimension $2k$, its Dirac geometry is defined as the unbounded K-cycle $(C^\infty(M), L^2(M, \not{S}), \not{D})$, where $L^2(M, \not{S})$ is the Hilbert space of spinors and $\not{D}$ is the Dirac operator. The grading operator γ, or $c(\gamma)$ for the Clifford multiplication by γ, is defined as usual in an even-dimensional Clifford algebra. In addition, the canonical real structure is given by the charge conjugation operator C acting on the Clifford algebra. Thus the quintuple $(C^\infty(M), L^2(M, \not{S}), \not{D}, C, \gamma)$ defines a KR_{2k}-cycle of spinors. In spin geometry, when a spinor $\psi \in L^2(M, \not{S})$ satisfies the real condition $C\psi = \psi$ (generalizing $\psi^\dagger = \psi$ used in physics), it is called a Majorana spinor, the space of Majorana spinors is denoted by $L^2(M, \not{S}; C)$.

B. Pairing

There is a pairing between KR cycles and KR theory.[9,11] This is induced by so-called KK theory and its Real version KKR.[47] This can be seen parallel to the pairing between cohomology and homology or deRham comomology and deRham cohomology with compact support.[75]

This is given by considering the K-theory of the function C^*-algebra $C^*(X) = C^0(X, \mathbb{C})$. This changes the variance of the construction which is dual to the topological theory: $KR^{-j}(X) = KR_j(C^*(X))$—likewise, we dualize $KR^j(C^*((X,\tau))) = KR_{-j}(X)$. The cap product becomes a map:

$$KR^i(X) \times KR_j(X) \to KR^{i-j}(pt) = KO^{i-j}(pt) \tag{92}$$

The "reading out" of invariants comes from paring with the fundamental class in top super-degree $KR_{-\delta}(X)$ if X is an $\mathbb{Z}/2\mathbb{Z}$ equivariant CW complex whose top dimensional cells are all of the form $\mathbb{S}^{D+1,d}$ which has super-dimension $-\delta = D - d$.

Definition VII.6. The index pairing for topological invariants on an $\mathbb{Z}/2\mathbb{Z}$-equivariant CW complex (X, τ) with super dimension $-\delta = d - D$ the index map is defined to be the cap product

$$KR^{-s}(X) \times KR_{-\delta}(X) \to KO^{\delta - s}(pt) \tag{93}$$

Theorem VII.7. *The strong Teo–Kane classification of topological insulators with a top cell $\mathbb{S}^{D+1,d} = \dot{\mathbb{R}}^{D,d}$ can be identified with the KR pairing with the fundamental class*

$$KR^{-s}(\mathbb{S}^{D+1,d}) \times KR_{-\delta}(\mathbb{S}^{D+1,d}) \to KO^{\delta - s}(pt) \tag{94}$$

which is dual notation for the pairing $KR_s(C^*(X)) \times KR^{\delta}(C^*(X)) \to KR_{s-\delta}(\mathbb{C})$ and $KR^{-s}(\mathbb{S}^{D+1,d}) \simeq KR^{-j-2}(\mathbb{S}^{D,d})$.

Proof. That the invariant takes values in the group is the content of Theorem VI.15. It remains to establish that the pairing is indeed the morphism to the KR group. This can be seen in several ways. The first is to realize that the pairing is given by an index, which has been computed in this fashion in Ref. 17. The second is to realize the pairing through a topological index using odd Chern characters and Pfaffians. Then the corresponding computations following Ref. 74 can be found in Refs. 4 and 50. □

Remark VII.8. Going through the computations in the Appendixes of Ref. 4 one can trace that the parameter is indeed shifted from j to $s = j + 1$ by using various suspensions, on operators and spaces, in the computation of the invariants. A key ingredient are then the sewing matrices which are identified with Chern–Simons terms.

C. Poincaré duality

If there is a Poincaré duality map $PD : KR^i(X) \to KR_{\dim(X)-i}(X)$, the fundamental class can be understood as $PD(1)$, and capping with the fundamental class is then the push-forward to a point (aka. integral) $\pi : X \to pt$.

$$\pi_* : KR^{-s}(X) \to KO^{\delta - s}(pt), [x] \mapsto [x] \cap PD(1) \tag{95}$$

The existence of such classes is in general a condition rather than a fact.[9,11]

Remark VII.9. The push-forward factors as $\mathbb{T}^d \to \mathbb{S}^{1,d} \to pt$. This explains the summation over the fixed points, if one views $\mathbb{S}^{1,d} = \Sigma^d_{odd}(\mathbb{S}^0, id)$ as the odd suspension of the even S^0.

Example VII.10. When $d = 2$, η is the isomorphism evaluating KQ-theory in the classical case of $j = 2$, that is the Kane–Mele invariant:

$$\eta : \widetilde{KQ}(\mathbb{T}^2) = \widetilde{KR}^{-4}(\mathbb{T}^2) \xrightarrow{\simeq} KO^{-2}(x_0)$$

When $d = 3$, η is the surjective map

$$\eta : KQ^{-1}(\mathbb{T}^3) = KR^{-5}(\mathbb{T}^3) \to KO^{-2}(x_0)$$

yielding a $\mathbb{Z}_2$ invariant for the shifted case $j = 3$.

This morphism can be understood as an intersection through assembly maps, if they exist. They are conjectured to exist by the Baum–Connes conjecture,[49] which is proven in various situations. The conjecture holds for the Abelian free group $\Gamma = \mathbb{Z}^d$, i.e., the translational symmetry group, and we call it the Baum–Connes isomorphism. In Ref. 2, Kitaev utilized it[76] to compute the KR groups. In Ref. 2 the assembly map is used to understand and calculate the KR-theory of $\mathbb{T}^d$. In this subsection, we briefly review the Baum–Connes isomorphism for $\Gamma = \mathbb{Z}^d$, which is useful for a version of the bulk-boundary correspondence.

Definition VII.11. Let Γ be a discrete countable group, the assembly map μ is a morphism from the equivariant K-homology of the classifying space of proper actions $E\Gamma$ to the K-theory of the reduced group C^*-algebra of Γ, i.e.,

$$\mu(\Gamma) : K_i^{\Gamma}(E\Gamma) \to K_i(C_\lambda^*(\Gamma, \mathbb{C})) \tag{96}$$

The classical complex Baum–Connes conjecture states that the assembly index map μ is an isomorphism. If Γ is torsion free, then the left hand side is reduced to the K-homology of the ordinary classifying space $B\Gamma$, i.e., $K_i^{\Gamma}(E\Gamma) = K_i(B\Gamma)$.

Definition VII.12. In the real case, the assembly map is similarly defined as

$$\mu_{\mathbb{R}}(\Gamma) : KR_j^{\Gamma}(E\Gamma) \to KR_j(C_\lambda^*(\Gamma, \mathbb{R})) \tag{97}$$

The real Baum–Connes conjecture follows from the complex Baum–Connes conjecture, so $\mu_{\mathbb{R}}(\mathbb{Z}^d)$ is an isomorphism. By the real assembly map $\mu_{\mathbb{R}}(\mathbb{Z}^d)$, one has the Baum–Connes isomorphism, sometimes also called the dual Dirac isomorphism, since $\mathbb{T}^d$ is the classifying space for $\mathbb{Z}^d$ with the universal cover $\mathbb{R}^d$,

$$\beta : KR_i(\mathbb{T}^d) = KR_i^{\mathbb{Z}^d}(\mathbb{R}^d) \simeq KR_i(C^*(\mathbb{Z}^d, \mathbb{R})) = KR_i(C(\mathbb{T}^d, \tau)) = KR^{-i}(\mathbb{T}^d) \tag{98}$$

This allows one to interpret the AZ-Hamiltonians as cycles. Dualizing with the isomorphism β (93) becomes $KR_s(\mathbb{T}^d) \times KR_{-\delta}(\mathbb{T}^d) \to KO^{\delta-s}(pt)$ which factors through the cycle-product, which is geometrically speaking the intersection with the fundamental class

$$KR^{-s}(\mathbb{T}^d) \times KR_{-\delta}(\mathbb{T}^d) \to KR_s(X) \times KR_{-\delta}(\mathbb{T}^d) \to KR_{s-\delta}(\mathbb{T}^d) \to KO_{s-\delta}(pt) = KO^{\delta-s}(pt). \tag{99}$$

The Baum–Connes isomorphism can be realized by an invertible real KKR-class β in $KKR(C_{\mathbb{R}}(\mathbb{T}^d), C(\mathbb{T}^d, \tau))$ connecting the KR-homology of $C_{\mathbb{R}}(\mathbb{T}^d)$ and the KR-theory of $C(\mathbb{T}^d, \tau)$, via the product map,[47]

$$KR_i(\mathbb{T}^d) \times KKR(C_{\mathbb{R}}(\mathbb{T}^d), C(\mathbb{T}^d, \tau)) \xrightarrow{\simeq} KR_i(C(\mathbb{T}^d, \tau)) \tag{100}$$

Let α be the inverse of β, that is, $\alpha \in KKR(C(\mathbb{T}^d, \tau), C_{\mathbb{R}}(\mathbb{T}^d))$ such that $\alpha \circ \beta = \mathrm{id}$, so α realizes the Dirac isomorphism

$$KR^{-i}(\mathbb{T}^d, \tau) \times KKR(C(\mathbb{T}^d, \tau), C_{\mathbb{R}}(\mathbb{T}^d)) \xrightarrow{\simeq} KR_i(\mathbb{T}^d)$$

Remark VII.13. By the above, the evaluation morphism $\pi_* : KR^{-s}(\mathbb{T}^d) \to KO^{\delta-s}(pt)$ is linked to the KKR-class α. As a generalization, an evaluation in KR-theory is given by a KKR-cycle in $KKR^d(X, X^\tau)$ for $d = \dim(X)$ realizing the topological index map in KK-theory,

$$KR^{-d-2}(X, \tau) \times KKR^d(X, X^\tau) \to KO^{-2}(X^\tau) \xrightarrow{\Sigma} KO^{-2}(x_0) \tag{101}$$

Here $\sum = \pi_*$ for X^τ finitely many points.

Dually the theory can be modeled by K-cycles or K-homology, such an idea has been carried out for example in Ref. 77. The evaluation in KR-homology then has the form,

$$KKR(X^\tau, X) \times KR_2(X) \to KR_2(X^\tau) \xrightarrow{\simeq} KR^{-2}(X^\tau) \xrightarrow{\Sigma} KR^{-2}(pt) \tag{102}$$

where the isomorphism is the Poincaré duality. This "effective bulk-boundary" correspondence on the level of K-homology is viewed as a generalized analytical index map.

In sum, the evaluation provides a new perspective to view the mod 2 index theorem in KK-theory,

$$\begin{tikzcd} KKR(X^\tau, X) \times KR_2(X) \arrow[r, "ind_a"] & KO^{-2}(pt) \arrow[d, "="] \\ KQ^{2-d}(X) \times KKR^d(X, X^\tau) \arrow[r, "ind_t"] & KO^{-2}(pt) \end{tikzcd} \tag{103}$$

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Ralph M. Kaufmann: Writing – original draft (equal). **Dan Li**: Writing – original draft (equal). **Birgit Wehefritz–Kaufmann**: Writing – original draft (equal).

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Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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