Symmetries, dimensions and topological insulators: the mechanism behind the face of the Bott clock

Michael Stone, Ching-Kai Chiu and Abhishek Roy

Department of Physics, University of Illinois, 1110 W Green St., Urbana IL 61801, USA
E-mail: m-stone5@illinois.edu, chiu7@illinois.edu and aroy2@uiuc.edu

Received 6 June 2010, in final form 18 October 2010
Published 21 December 2010
Online at stacks.iop.org/JPhysA/44/045001

Abstract
We provide an account of some of the mathematics of Bott periodicity and the Atiyah, Bott, Shapiro construction. We apply these ideas to understanding the twisted bundles of electron bands that underlie the properties of topological insulators, spin Hall systems and other topologically interesting materials.

PACS numbers: 73.43.−f, 74.20.Rp, 74.45.+c, 72.25.Dc

1. Introduction
Topological insulators and superconductors are many-fermion systems possessing an unusual band structure that leads to a bulk band gap, but topologically protected gapless extended surface modes. The existence of such materials was predicted theoretically [1–6], and several examples have now been confirmed experimentally [7–11]. Part of the topological protection arises from generic symmetries of the underlying one-particle Hamiltonians. These symmetries include time reversal and, in the case of superconductors, the particle–hole symmetry of the Bogoliubov–de Gennes (BdG) Hamiltonian.

There is a subtle interplay between the possibility of a topologically non-trivial band structure, the symmetries and the dimensions of the system [12–15]. This interplay is displayed in table 1. In this table, the first two columns contain the names associated with the symmetry class in the Dyson scheme [16], as completed to include superconductivity by Altland and Zirnbauer [17, 18]. The next three columns display the symmetries possessed by the Hamiltonians in this class. A minus sign indicates that the symmetry operation involves the electron spin and so squares to minus the identity. The last four columns indicate whether a non-trivial topological phase is possible in $d$ dimensions. A ‘0’ means that no non-trivial topology can exist, whilst a $\mathbb{Z}$ indicates that there are infinitely many possible phases that are classified by an integer. The most interesting case is $\mathbb{Z}_2$, which indicates that there are two possibilities—trivial or non-trivial—and that coupling two non-trivial phases together results in a trivial phase. The data in this table were obtained in [12, 13], but it was Kitaev
Table 1. The Dyson–Altland–Zirnbauer Hamiltonian classes, their symmetries and possible topological phases (after table 4 in [14]).

| Cartan | Dyson name         | TRS | PHS | SLS | $d=0$ | $d=1$ | $d=2$ | $d=3$ |
|--------|--------------------|-----|-----|-----|-------|-------|-------|-------|
| AIII   | Chiral unitary     | 0   | 0   | 1   | 0     | Z     | 0     | Z     |
| A      | Unitary            | 0   | 0   | 0   | 0     | Z     | 0     | Z     |
| D      | BdG               | 0   | +1  | 0   | 0     | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | Z     |
| DIII   | BdG               | -1  | +1  | 1   | 0     | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | Z     |
| AII    | Symplectic         | -1  | 0   | 0   | 0     | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | Z     |
| CII    | Chiral symplectic  | -1  | -1  | 1   | 0     | $\mathbb{Z}$ | 0     | $\mathbb{Z}_2$ |
| C      | BdG               | 0   | -1  | 0   | 0     | 0     | $\mathbb{Z}$ | 0     |
| CI     | BdG               | +1  | -1  | 1   | 0     | 0     | 0     | Z     |
| AI     | Orthogonal         | +1  | 0   | 0   | $\mathbb{Z}$ | 0     | 0     | 0     |
| BDI    | Chiral orthogonal  | +1  | +1  | 1   | $\mathbb{Z}_2$ | Z     | 0     | 0     |

who first pointed out [19] the striking pattern of correlations between the symmetry, topology and dimension. The correlations only become manifest after the AIII and A classes are treated separately, and the remaining eight classes are displayed in a particular order. Kitaev explained that the pattern arises from the interplay between topological K-theory and the two- and eight-fold Bott periodicity [20, 21] of the homotopy groups of $\text{U}(n)$ and $\text{O}(n)$ respectively.

The topological K-theory is a tool for classifying vector bundles. Now a precise classification of vector bundles requires homotopy. In band theory, for example, we have at each point $k$ in the Brillouin zone a Hamiltonian $H(k)$, and associated with it the subspace of negative-energy eigenstates that is to be filled by electrons. If, as we explore the Brillouin zone, this subspace twists in a manner that cannot be continuously undone, then the bundle of vector spaces is homotopically non-trivial. The non-triviality will be reflected in physical effects such as a quantum Hall effect, the absence of localized Wannier functions and the guaranteed existence of gapless surface states. In some cases homotopic non-triviality can be detected by computing integral invariants such as Chern numbers—but such homological invariants are only available in even dimensions, and for certain symmetry classes. In particular, the $\mathbb{Z}_2$ homotopy classes cannot be detected in this way. Because homotopy theory is harder and demands more technical machinery than homology, a complete classification of which vector bundles can be homotopically deformed into one another is difficult. This difficulty is compounded in the case of band theory because the ground-state bundles are only allowed to be deformed by additions to the Hamiltonian of terms that respect its symmetries—time reversal, sublattice or BdG particle–hole.

K-theory simplifies the classification of vector bundles by relaxing the notion of equivalence. The resulting lack of precision might seem like a bad thing, but it is not. Our desire is only to capture the features that are essential for the physics. For example, if we have a material whose Fermi sea has a single filled band with the Chern number $n$, it has the same Hall conductance as a solid possessing $n$-filled bands each with Chern number unity. The corresponding vector bundles have different ranks (dimensions of the vector spaces) and so cannot be continuously deformed into each other. In the reduced K-theory of bundles over a common base space $X$, denoted $\tilde{K}(X)$, bundles of different ranks are counted as equivalent if we can deform them into each other after adding suitable trivial bundles. In the one-band versus $n$-bands example, once we add a rank $n-1$ trivial bundle (for example $n-1$ previously ignored localized atomic core states) to the Chern number $n$ band, it can be continuously
deformed into the other bundle. The bundles are therefore equivalent both in $\tilde{K}(X)$ and in their physical properties.

Despite its simplifications, the full machinery of K-theory remains intimidatingly abstract. Nonetheless the basic mechanism that underlies the period-2 or period-8 pattern of correlations can be understood with relatively unsophisticated mathematical tools—representation theory and the basics of homotopy as described in [22], or perhaps [23]. The aim of this paper is to explain how this mechanism works, and fill in the details omitted in [19].

We begin in the next section by explaining why the symmetric spaces that underlie the Altland–Zirnbauer classification naturally occur in a certain order. We then explain why the symmetric space that classifies the ground-state bundles is one step further round the periodic Bott clock from the symmetric space whose tangent space contains the Hamiltonians. Section 3 reverses the discussion of Altland and Zirnbauer and derives the symmetry class of the Hamiltonian from the corresponding symmetric space. Section 4 is a slight digression that prepares some ingredients that are needed to accommodate the fact that time reversal reverses the direction of the Bloch momentum. Section five discusses the Atiyah–Bott–Shapiro [25] theory of real representations of Clifford algebras and in section 6 uses it to construct Hamiltonians in any symmetry class and with any possible topologically twisted ground state.

One thing that we do not do in this paper is discuss the complications that arise because the Brillouin zone is a torus. We restrict ourselves to constructing bundles over spheres. This is sufficient for the case of ‘strong’ topological insulators, but it does not capture the possibility of ‘weak’ (lower dimensional) insulators.

2. The Bott sequence of symmetric spaces

We begin with a somewhat backward account of the Altland–Zirnbauer tenfold-way classification of quantum Hamiltonians. Altland and Zirnbauer proceed [17, 18] by considering families of $N$-by-$N$ matrices representing single-electron Hamiltonians with given discrete symmetries—sublattice, time reversal or BdG particle–hole symmetry—each with and without spin. They show that for each symmetry class there is a corresponding Lie algebra $g$ of $N$-by-$N$ matrices, and a decomposition of this algebra as $g = m \oplus h$, where

$$[h, h] \in h, \quad [h, m] \in m, \quad [m, m] \in h.$$  \hspace{1cm} (1)

If a Hamiltonian $H$ possesses the properties defining the symmetry class, then the matrix $iH$ lies in the set $m$. Conversely any matrix in $m$ is a possible $iH$ in the symmetry class. Associated with the algebras $g$ and $h$ are compact Lie groups $G$ and $H \subset G$. From them we obtain a homogeneous space $G/H$ that is naturally a Riemannian manifold. Its points correspond to the set of evolution operators $U(t) = \exp(itH)$ where $t \in (-\infty, \infty)$ and $H$ runs over all Hamiltonians in the family. The commutation relations of the algebras ensure that for any point in $G/H$ there exists an isometry that reverses the directions of geodesics though the point. These isometries make $G/H$ into a symmetric space and Élie Cartan classified all possible symmetric spaces in the 1920s [24]. Cartan observed that there are precisely ten families of compact symmetric spaces in which the matrices in $g$ can have arbitrary large dimension $N$. Altland and Zirnbauer thus established a one-to-one correspondence between these ‘large’ families of compact symmetric spaces and the Hamiltonian symmetry classes. Because they make use of all ten families, their correspondence provides an exhaustive classification.

We proceed in the reverse direction. We begin with the symmetric spaces and from them extract the Altland–Zirnbauer Hamiltonian families. Only then do we identify their symmetry classes. The advantage of the backward approach is that we discover that the
symmetric spaces arise in a natural order. They are the sequence of order-parameter spaces that arise as we progressively break a large continuous symmetry by introducing more and more symmetry-breaking operators. As a bonus, the matrices representing the symmetry-breaking operators will later serve as the building blocks of model Hamiltonians that yield all possible topologically non-trivial band structures. After two or eight steps the sequence of spaces repeats itself. This is Bott periodicity.

The periods of two and eight are associated with two distinct super-families in the Altland–Zirnbauer classification, a set of two associated with the unitary group and a set of eight associated with the real orthogonal group. We will focus on the latter as that is the most intricate. The discussion is clear if we follow Dyson \[16\] and work as much as possible with matrices with real entries. In this we again depart from Altland and Zirnbauer who mostly use complex matrices.

The large continuous symmetry we begin with is the group $O(N)$. Here $N$ itself should be large. The mathematics literature usually takes a formal limit $N \to \infty$, but we only require that $N$ be large enough that low-dimensional exceptions can be disregarded. For example, the homotopy groups $\pi_n(O(N))$ become independent of $N$ once $n \leq N + 1$. (Similarly $\pi_n(U(N))$ is independent of $N$ once $n \leq 2N + 1$.)

To recover all eight symmetric spaces, $N$ needs to be a multiple of 16, so we consider the action of $O(16r)$ on a vector space $V$ over $\mathbb{R}$ of dimension $16r$. The symmetry breaking operators will be a set $\{J_i: i = 1, \ldots, k\}$ of mutually anti-commuting orthogonal complex structures acting on this space. This language means that the $J_i$ are orthogonal matrices that square to $-1$ and obey

$$J_i J_j + J_j J_i = -2 \delta_{ij} 1.$$  \hspace{1cm} (2)

They therefore constitute a representation of the Clifford algebra $\text{Cl}_{k,0}$. We usually think of representations of Clifford algebras as being Dirac gamma matrices. We will, however, reserve the symbols $\gamma_i$ for irreducible representations of the algebra. The $J_i$ will usually be highly reducible.

Because they are orthogonal matrices, we have that $J_i^2 = J_i^{-1} = -J_i$ and it is sometimes convenient to regard the skew-symmetric $J_i$ as being elements of $\mathfrak{o}(16r)$, the Lie algebra of $O(16r)$.

The subgroup of $O(16r)$ that commutes with $J_i$,

$$O^T J_i O = J_i,$$ \hspace{1cm} (3)

is $O(16r) \cap \text{Sp}(16r; \mathbb{R}) \simeq U(8r)$. If we think of $J_i$ being a block diagonal matrix

$$J_i = \text{diag} \left[ \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \ldots, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right],$$ \hspace{1cm} (4)

then commuting with $J_i$ forces a $16r$-by-$16r$ orthogonal matrix to take the form of an $8r$-by-$8r$ matrix whose entries are two-by-two blocks in the form

$$a \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + b \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \to a + ib.$$ \hspace{1cm} (5)

As indicated, these entries can be regarded as complex numbers $a + ib$. The matrix $J_i$ itself then acts as $i \times$ the $8r$-by-$8r$ identity matrix on an $8r$-dimensional complex vector space. It is because $J_i$ assembles a complex space out of a real space that it is called a complex structure.

In a similar manner, the subgroup of $U(8r)$ that commutes with both $J_1$ and $J_2$ is the unitary symplectic group $U(8r) \cap \text{Sp}(8r; \mathbb{C}) \equiv \text{Sp}(4r) \simeq U(4r, \mathbb{H})$. To display the last isomorphism with the quaternionic unitary group $U(4r, \mathbb{H})$ we gather the $16r$ real vector components into sets of four, and from each quartet construct a quaternion $x = x_0 + x_1 i + j(x_2 + i x_3)$. The
unit quaternions $i, j, k$ then act on $x$ from the left as multiplication into the column vector $(x_0, x_1, x_2, x_3)^T$ of the 4-by-4 matrices

$$
\begin{align*}
    i &= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \\
    j &= \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \\
    k &= \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}.
\end{align*}
$$

(6)

Here $1$ and $i$ are shorthand for the 2-by-2 sub-blocks:

$$
\begin{align*}
    1 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\
    i &= \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.
\end{align*}
$$

(7)

All three of the 4-by-4 real matrices $i, j, k$, are skew symmetric. The quaternionic-conjugate transpose of a matrix with quaternion entries therefore coincides with the ordinary transpose of the corresponding four times larger real matrix. The mutually anticommuting complex transpose of a matrix with quaternion entries therefore coincides with the ordinary transpose.

Now consider the subgroups that survive the introduction of yet more $J_i$'s. We closely follow [21], and readers who are prepared to take the results on trust may skip over some tedious enumeration to the resulting pattern of symmetry breaking displayed in equation (10).

After introducing $J_3$ we consider the operator $K = J_1 J_2 J_3$. This operator commutes with both $J_1$ and $J_2$ and obeys $K^2 = 1$. Therefore, $K$ possesses two quaternionic eigenspaces $V_\pm$ in which it takes the value $\pm 1$ respectively. Let the dimensions of these quaternionic spaces be $n_1$ and $n_2$, so that $n_1 + n_2 = 4r$. The subgroup of $\text{Sp}(4r)$ commuting with $J_1, J_2, J_3$, and so preserving this structure is $\text{Sp}(n_1) \times \text{Sp}(n_2)$. If we stop at this point, these dimensions can be any pair such that $n_1 + n_2 = 4r$, but in order to be able to continue and define a $J_4$ we will see that we need to take $n_1 = n_2 = 2r$.

Next introduce $J_4$ and let $L = J_3 J_4$. We have that $LK = -KL$, $L^2 = 1$ and $L$ commutes with $J_1$ and $J_2$. $L$ therefore preserves the quaternionic structure and is a quaternionic isometry from $V_+$ to $V_-$. It is therefore an element of $U(2r, \mathbb{H}) \cong \text{Sp}(2r)$ (and could not exist unless $n_1 = n_2$). Conversely, such an isometry can be used to define $L$ and hence $J_4 = J_3^{-1} L$. The group preserving this structure is the diagonal subgroup $\text{Sp}(2r)$ of $\text{Sp}(2r, \mathbb{H})$.

Now introduce $J_5$ and construct $M = J_1 J_4 J_5$ which has $M^2 = 1$ and commutes with $K$ and $J_1$. $M$ therefore acts within the $V_+$ (or $V_-$) eigenspace of $K$ and divides it into two mutually orthogonal eigenspaces $W_\pm$ with $W_- = J_2 W_+$. Conversely such a decomposition uniquely determines $J_5$. Since $J_2$ interchanges the first and second blocks in $x = (x_0 + x_1 i) + j(x_2 + x_3 i)$, the quaternionic isomorphisms that respect this decomposition must mix only $x_0$ with $x_1$ and $x_2$ with $x_3$ and so the quaternionic matrix entries can contain only 1 and $i$. This subgroup can therefore be identified with $U(2r)$.

Now introduce $J_6$ and set $N = J_2 J_4 J_6$ which commutes with $K$ and $M$, and therefore acts within either of $W_\pm$ and splits it into two mutually orthogonal eigenspaces $X_\pm$ such that $X_- = J_1 X_+$. Since $J_1$ acts as the 2-by-2 $i$, the subgroup preserving this structure
cannot have matrix entries with the quaternionic 4-by-4 matrix $i$, and it can be identified with $O(2r) \subseteq U(2r)$.

Now introduce $J_i$ and set $P = J_1 J_2 J_3$ which commutes with $K$, $M$ and $N$ and splits $X_i$ into $\pm 1$ subspaces $Y_i$. These may have differing dimensions, but in order to have the possibility of introducing $J_4$ we must take the dimensions to be equal. The group preserving this decomposition is therefore $O(r) \times O(r)$.

Finally we introduce $J_8$. Now the orthogonal transformation $Q = J_7 J_8$ commutes with $K, M$ and $N$ but anticommutes with $P$. It is therefore an isometry mapping $Y_{\pm} \leftrightarrow Y_{\mp}$. In order to preserve this structure we must take the diagonal subgroup $O(r)$ of $O(r) \times O(r)$.

The progressive symmetry breaking has led to the nested sequence of groups
\[
\cdots O(16r) \supset U(8r) \supset Sp(4r) \supset Sp(2r) \times Sp(2r) \supset Sp(2r) \supset O(2r) \supset O(r)
\]
\[
\times O(r) \supset O(r) \cdots
\]
(10)
The sequence can be extended to the left and to the right when $r$ is a suitably large power of 2. The pattern repeats with period 8. In each cycle $r$ increases or decreases by a factor of 16.

When complex numbers are allowed, the corresponding sequence of groups is simpler. We can now multiply the $J_i$ by $i$ so that $K_i = i J_i$ obeys $K_i^2 = 1$ and splits $C^{2r}$ into two spaces that may have arbitrary dimensions. To keep going, however, we must take the dimensions to be equal. Thus, we get
\[
\cdots U(2r) \supset U(r) \times U(r) \supset U(r) \cdots.
\]
(11)

We now motivate the construction of the symmetric spaces from the sequences of groups. Suppose we already possess a set $\{J_1, \ldots, J_d\}$ and wish to add a $J_{d+1}$ that anticommutes with them. Then the set of choices for $J_{d+1}$ is parametrized by a symmetric space. To see this, we first argue that the choices are parameterized by a homogeneous space and then prove that the homogeneous space obeys the stronger condition of being symmetric. Let the subgroup of $G_0 \equiv O(16r)$ that commutes with $J_1, \ldots, J_d$ be $G_i$ and its Lie algebra $g_i$. Then if $J_{d+1}$ squares to $-1$ and anticommutes with $J_1, \ldots, J_d$, so does $g^{-1} J_{d+1} g$ for any $g \in G_i$. The subgroup of $G_i$ that continues to commute with the new $J_{d+1}$ is $G_{d+1}$ and so it is reasonable to suppose that the range of choices for $J_{d+1}$ is the orbit of $J_{d+1} g$ under the action of conjugation by $G_i$—i.e. the coset, or homogeneous space $G_i / G_{d+1}$. These cosets, together with the two families of cosets that arise in the complex case, are displayed in tables 2 and 3.

We say ‘reasonable to suppose’ because it is not immediately clear that the orbit $g^{-1} J_{d+1} g$ contains all candidate $J_{d+1}$’s. It is easy to see that the orbit captures the connected part
of the space of choices. The disconnected parts—which are the parts of interest for Bott periodicity—need a bit more work, but the claim is correct. For example, the \(\mathbb{Z}_2\) appearing as \(\pi_0(R_2)\) arises from the two disconnected parts of the choice space for \(J_1\) in which the Pfaffian \(\text{Pf}(J_1)\) takes the value \(\pm 1\). Since

\[
\text{Pf}(MT AM) = \text{Pf}(A)\text{det}(M),
\]

(12)
each disconnected part is accessible from the another via conjugation by an orthogonal matrix \(g\) with \(\text{det}g = -1\). The \(\times \mathbb{Z}\) factors in the tables represent the choices of dimensions in \(O(n_1) \times O(n_2)\) and \(Sp(n_1) \times Sp(n_2)\). They make \(\pi_0\) of these spaces equal to \(\mathbb{Z}\).

Now we show that spaces \(G_i/G_{i+1}\) are in fact symmetric spaces. If \(a \in g_i = \text{Lie}(G_i)\) then so is \(J_1 a J_1^{-1}\). Thus, \(\text{Ad}(J_1) : g_i \to g_i\) is an involutive (squares to the identity) automorphism of \(g_i\). Let the eigenspaces of this map with eigenvalues \(\pm 1\) be \(h_i\) and \(m_i\). Then \(g_i = h_i \oplus m_i\) as a vector space, and the automorphism property requires that

\[
[h_i, h_i] \in h_i, \quad [h_i, m_i] \in m_i, \quad [m_i, m_i] \in h_i.
\]

(13)

Since \(h_i\) is precisely \(g_{i+1}\), this confirms that the homogeneous space \(G_i/G_{i+1}\) is indeed a symmetric space. Its connected part is \(\text{Exp}(m_1)\). Recall that matrices \(m \in m_i\) are the evolution generators \(iH\) in the Altland–Zirnbauer families. They commute with \(J_1, \ldots, J_i\), and anticommute with \(J_{i+1}\).

Each symmetric space plays two distinct roles. The first is that its tangent space contains the Hamiltonians of the corresponding symmetry class. The second is that entire symmetric space is the classification space for the vector bundle of ground states for the preceding symmetry class. A rank \(N\) vector bundle over a base space \(X\) can be thought of as an assignment of an \(N\)-dimensional subspace of some infinite-dimensional Hilbert space \(\mathcal{H}\) to each point \(x\) of the base space. Two bundles are deformable into each other only when the corresponding maps lie in the same homotopy class, denoted by \([X, R]\), of maps from \(X\) into the class \(R\) of subspaces of \(\mathcal{H}\) that are permitted by the bundle symmetries. To be precise, the large-enough-\(N\) version of the symmetric space \(G_{i-2}/G_{i-1}\) becomes the classification spaces known as \(R_i\). The \(R_i\) spaces have homotopy groups that are independent of \(N\) and the bundle classification we seek requires us to know all the homotopy groups of the \(R_i\) not just the \(\pi_0(R_i)\) that are displayed in table 2. We therefore sketch the argument that leads to the key result \(\pi_n(R_i) \simeq \pi_{n+1}(R_{i-1})\). From this we can obtain all the \(\pi_n(R_i)\), and as a corollary deduce Bott periodicity: that \(\pi_{n+k}(O(N)) \simeq \pi_n(O(N))\) once \(N\) is large enough.

We first show that each symmetric space \(R_{i+2} \equiv G_i/G_{i+1}\) in the Bott sequence of spaces is naturally embedded (as a totally geodesic submanifold) in the preceding one. To see this let \(A_i = J_i^{-1} J_{i+1}\). Then \(A_i\) is a skew symmetric orthogonal matrix that squares to \(-I\). It anticommutes with \(J_i\) but commutes with \(J_1, \ldots, J_{i-1}\). Thus \(A_i \in m_{i-1}\). Now \(J_{i+1} = J_i A_i\)

(14)

and

\[
\gamma(t) = J_i \exp[\pi A_i t] = J_i \cos \pi t + J_{i+1} \sin \pi t
\]

(15)
is a geodesic in $G_{i-1}/G_i$ that interpolates between $J_i = γ(0)$ and $-J_i = γ(1)$, and has $J_{i+1} = γ(1/2)$. The set of these geodesics is therefore parametrized by $G_{i}/G_{i+1}$. This is just as the set of geodesics from the north pole to the south pole of the sphere is parametrized by points on the equator of the sphere. Milnor [21] shows that these geodesics capture the topology of the loop space $Ω[G_{i-1}/G_i]$ in that the homotopy groups of $Ω[G_{i-1}/G_i]$ coincide with those of $G_{i}/G_{i+1}$ once $N$ is large enough. Then the standard isomorphism $π_n(ΩX) ≃ π_n(X)$ gives us $π_n(R_m) ≃ π_{n+1}(R_{m-1})$. Alternatively we can regard the space swept out by the geodesics as homeomorphic to the reduced suspension $Σ[G_{i}/G_{i+1}]$ of $G_{i}/G_{i+1}$. Bott then shows [20] that this suspension captures enough of $G_{i-1}/G_i$ that we obtain the same isomorphism. The two approaches are related because of the natural identification [23]

$$\text{Map}_*(ΣX, Y) = \text{Map}_*(X, \Omega Y)$$

between basepoint-preserving maps from the reduced suspension of $X$ to $Y$ and from $X$ to the space of based loops in $Y$.

We need the homotopy groups because, as we said earlier, the $R_i$ serve as classification spaces in the sense of bundle theory. In particular $R_0 ≡ BO \times Z$ is the classifying space for real vector bundles. Any rank-$N$ real vector bundle can be obtained as the pullback of the tautological bundle over some real Grassmanian $Gr_n(\mathbb{R}^{N m}) ≃ O(N + m)/O(N) \times O(m)$ consisting of $N$-dimensional subspaces of $\mathbb{R}^{N m}$. Here tautological means that the fibre over the point $p ∈ Gr_N(\mathbb{R}^{N m})$ is the corresponding $n$-dimensional subspace $p \subset \mathbb{R}^{N m}$. For $m$ sufficiently large, the homotopy equivalence classes of the vector bundles correspond one-to-one with the homotopy classes of the maps from $X$ to $Gr_N(\mathbb{R}^{N m})$. The 'large enough $m$' limit of $Gr_n(\mathbb{R}^{N m})$ is denoted by $BO(N)$ and rank-$N$ real bundles are classified by the homotopy classes $[X, BO(n)]$ of a continuous map from $X$ to $BO(N)$. In $K$-theory we relax the notion of bundle equivalence and identify bundles that become equivalent when trivial bundles (flat bands) of any rank are added to both or either of them. In this case we forget $N ∈ Z$ and $BO(N)$ becomes $BO$. We then have $K\bar{O}(X) = [X, BO]$, the homotopy classes of maps from $X$ to $BO$. We cannot forget the $Z$ factors when commuting homotopy, however. In particular, $π_k(BO) = Z \times BO$. Similarly for complex bundles, $π_k(BU) = Z \times BU$.

In the application to the band theory of solids, we want a tighter classification than that given by maps into $BO$. We are interested in the bundle of negative energy eigenstates of a family of Hamiltonians $H(x)$ in a given Altland–Zirnbauer class. So we allow only smooth deformations of the Hamiltonian that remain in that class. For the topological effects it is only the eigenstates that matter, and not their energy. So, following Kitaev, we flatten the spectrum and seek $Q_i ∈ m_i$ that has eigenvalues $±i$ (recall that Zirnbauer’s generators are $i$ times the Hamiltonian). The $Q_i$ are then in one-to-one correspondence with the negative-energy spaces of the original Hamiltonians. If our family of Hamiltonians lying in $m_i$ is parametrized by $x$ in a space $X$ (a Brillouin zone say), then the bundle of ground states over $X$ will be trivial if and only if the homotopy class of maps from $X$ into whatever classifying space parametrizes the possible $Q_i$ contains the constant map.

To find this classifying space, observe that the matrices $A_{i+1}$ that we met earlier all lie in $m_i$ and square to $-1$. They therefore can be used as a $Q_i$. The converse is also true. If $Q_i ∈ m_i$, and $Q_i Q_i = -1$, then $J_i Q_i$ anticommutes with $J_1, \ldots, J_{i-1}$ and so is a candidate $J_{i+2}$. The set of possible $Q_i$ is therefore parametrized by the set of choices $G_{i+1}/G_{i+2}$ for $J_{i+2}$. That is by $R_{i+2}$. We conclude that the classifying space for the class of Hamiltonians in $m_i$, whose evolution operators lie in $R_{i+2}$ is $R_{i+3}$ — the next space along in the Bott clock. The set of distinct ground-state bundles over $X$ is therefore given by the homotopy classes $[X, R_{i+3}]$ of continuous maps from $X$ to $R_{i+3}$. In particular, when $X$ is the sphere $S^2$ these classes are given
by \( \pi_d(R_{i+3}) \). Because \( \pi_d(R_m) \cong \pi_{n+1}(R_m-1) \), this homotopy group has the same number of distinct elements as \( \pi_0(R_{i+3+d}) \).

Unfortunately, in the case of most interest, when \( X \) is a Brillouin zone, the above count is not quite correct. It would lead to the stripes of \( \mathbb{Z} \)'s and \( \mathbb{Z}_2 \)'s in table 1 sloping the wrong way. The correct result is \( \pi_0(R_{i+3-d}) \). The change of sign of \( d \) arises because the antilinear symmetries time reversal and particle-hole (BdG) conjugation have the effect of inverting the Bloch wavevector \( k \) to \(-k\) modulo reciprocal lattice vectors. The resulting bundles are therefore more intricate than those classified by simple homotopy. Their classification is the subject of KR theory [26], and we will delay describing what happens until section 6.

In [19] Kitaev uses the notation \( \tilde{KO}^{-q}(X) \). Topologists define \( \tilde{K}^{-1}(X) = K(\Sigma X) \) by analogy with the cohomology theory where \( H^n(X) = H^{n+1}(\Sigma X) \). In this language

\[
\tilde{K}O^{-q}(X) = [\Sigma^q X, BO] = [X, \Omega^q BO] = [X, R_q].
\]

When \( X \) is \( S^d \), we have

\[
\tilde{K}O^{-q}(S^d) = [S^d, R_q] = \pi_0(R_{q+d})
\]

so \( q \) should be \( i + 3 \) for the Altland–Zirnbauer Hamiltonians in \( m_i \).

3. The discrete symmetries

The Altland–Zirnbauer classes are usually and most simply characterized by the presence or absence of three discrete symmetries [13]. These are a sublattice symmetry (SLS) generated by a linear map \( P \) that anticommutes with the Hamiltonian \( H \):

\[
P H = -H P,
\]

and two antilinear maps. The first, \( C \), implements BdG particle–hole symmetry (PHS). The second, \( T \), implements time-reversal symmetry (TRS). The antilinear maps give

\[
C H C^{-1} = -H, \quad C^2 = \pm \mathbb{I}; \quad T H T^{-1} = H, \quad T^2 = \pm \mathbb{I}.
\]

In any given basis we can represent \( C \) and \( T \) by complex matrices \( C \) and \( T \) such that

\[
C H C^{-1} = -H, \quad C^* C = \pm \mathbb{I}, \quad T H T^{-1} = H, \quad T^* T = \pm \mathbb{I}.
\]

In a vector space \( V \) over \( \mathbb{C} \), however, the operation of complex conjugation is not a basis-independent notion. To describe it in a basis-independent manner we need to introduce a real structure. This is a map \( \psi \) that is antilinear

\[
\psi(\lambda v) = \lambda^* \psi(v)
\]

and obeys \( \psi^2 = \mathbb{I} \). We can then decompose \( V = W \oplus \mathbb{R} iW \) where

\[
W = \{ v \in V : \psi(v) = v \}, \quad iW = \{ v \in V : \psi(v) = -v \}.
\]

In effect \( \psi \) selects privileged basis vectors \( e_n \) that are counted as real. They span \( W \). The set \( i e_n \) spans \( iW \). A complex vector \( v = (u_n + iv_n) e_n \) is decomposed into a real vector \( u_n e_n + v_n (i e_n) \) of twice the dimension. To recover the original complex space from this twice-as-big real space, we need a complex structure \( J \) such that the antilinearity of \( \psi \) corresponds to \( \psi J = -J \psi \).

If an operator commutes with a real structure \( \psi \), then there exists a basis (the \( e_n \) from above) in which the matrix representing the operator becomes real.

Now we find the symmetries possessed by the Hamiltonians corresponding to each symmetric space.
D ≡ O(16r). The coset generators \( m \in m_{-1} \) are real skew-symmetric matrices. These are not diagonalizable within the reals. We need to double the Hilbert space to \( \mathbb{R}^{32r} \) and tensor with \( i^2 = -\sigma_2 \) so that the Hamiltonian becomes \( H = -i\sigma_2 \otimes m \). Then taking \( \varphi = \sigma_3 \otimes 1 \) to be the real structure that defines complex conjugation, we have \( \varphi H = -H \varphi \). This \( \varphi \) therefore defines a particle–hole symmetry that squares to +1. We should not count the eigenvectors \( v \) and \( iv \equiv (-i\sigma_2 \otimes 1)v \) as being distinct. (We can regard the \( \mathbb{R}^{32r} \) space and the operators ‘ \( i \) ’ and \( \varphi \) as being inherited from the previous cycle of the Bott clock.)

DIII ≡ O(16r)/U(8r). The \( m \in m_0 \)'s are real skew-symmetric matrices that anticommute with \( J_1 \). We can keep \( C = \varphi \) as a particle–hole symmetry and take \( T = \varphi \otimes J_1 \) as a time reversal that commutes with \( H = -i\sigma_2 \otimes M \) and squares to −1. The product of \( C \) and \( T \) is \( J_1 \), and this a linear (commutes with −i\( \sigma_2 \otimes 1 \)) \('P\)'-type symmetry that anticommutes with \( H \).

AII ≡ U(8r)/Sp(4r). The generators \( m \in m_1 \) are real skew matrices that commute with \( J_1 \) and anticommute with \( J_2 \). They can be regarded as skew–quaternion–Hermitian matrices with complex entries. We no longer need to set \( i \rightarrow -i\sigma_2 \otimes 1 \) as the matrices no longer have elements coupling between the artificial copies. We instead use \( J_1 \) as the surrogate for ‘\( i \).’ Now \( H = J_1m \) is real symmetric, and commutes with \( T = J_2 \). This \( T \) acts as a time reversal operator squaring to −1.

CII ≡ Sp(4r)/Sp(2r) \times Sp(2r). The matrices \( m \in m_2 \) commute with \( J_1 \) and \( J_2 \) but anticommute with \( J_3 \). Again \( H = J_1m \). We can set \( T = J_3 \) as this commutes with \( H \) and squares to −1. \( P = J_2J_3 \) anticommutes with \( H \) but commutes with \( J_1 \) (and so is a linear map) while \( C = J_2 \) anticommutes with \( H \), is antilinear and squares to −1.

CI ≡ Sp(2r)/U(2r). The \( m \in m_3 \) anticommute with \( J_3 \). Now \( J_3J_5 \) commutes with \( J_1J_2J_3 \), and so is an allowed operator. It anticommutes with \( H = J_1m \) and commutes with \( J_1 \). It is therefore a ‘\( P\)'-type linear map. The map \( T = J_3J_4J_5 \) is antilinear (anticommutes with \( J_1 \)), commutes with \( H \) and \( T^2 = +1 \). We can take \( C = J_2 \) again.

AI ≡ U(2r)/O(2r). The \( m \in m_4 \) anticommute with \( J_4 \), and we may restrict ourselves to the subspace on which \( K = J_1J_2J_3 \) takes a definite value, say +1. The Hamiltonian \( J_1m \) commutes with \( J_4 \)—but \( J_4 \) does not commute with \( J_1J_2J_3 \) and so is not allowed as an operator on our subspace. Indeed no product involving \( J_4 \) is allowed. But \( C = J_2 \) commutes with \( J_1J_2J_3 \) and still anticommutes with \( H \). Thus we still have a particle–hole symmetry squaring to −1. The old time reversal \( J_3 \) now anticommutes with \( H \) and looks like another particle–hole symmetry but is not really an independent one as in this subspace \( J_3 = J_2J_4 \) and \( J_1 \) is simply multiplication by ‘\( i \).’

BDI ≡ O(2r)/O(r) \times O(r). The \( m \in m_6 \) anticommute with \( J_5 \), and we may restrict ourselves to the eigenspaces of \( K = J_1J_2J_3 \), \( M = J_1J_4J_5 \). The \( m \) also commute with the antilinear operator \( N = J_2J_4J_6 \) which we can regard as our real structure \( \varphi \). We therefore set \( C = \varphi = N \). With \( H = J_1m \) we have that \( T = J_2J_4J_7 \) commutes with \( H \) and squares to +1. We can also take \( P = J_1J_4J_7 \) as a ‘\( P\)'-type linear map anticommuting with \( H \).

D ≡ O(r)/O(r) \times O(r). Now the \( m \in m_7 \) anticommute with \( J_5 \), and, except for the factor ‘\( i \)’ \( J_1 \), we should stay in the space where \( K = J_1J_2J_3 \), \( M = J_1J_4J_5 \) and \( P = J_1J_4J_7 \) take the value +1. With \( H = J_1m \) we have that \( C = \varphi = N \) anticommutes with \( H \), and brings us full circle.

We have ended up with the symmetries displayed in table 4.
4. Backwards and forwards

As mentioned in section 3, the case of most interest, the Brillouin zone, requires us to take into account the \( k \) to \(-k\) effect of antilinear symmetries. In this short section we make a slight digression from the main story in order to introduce the ingredients we need to cope with this effect.

We consider mutually anticommuting real matrices \( \tilde{J}_i, i = 1, \ldots, k \), that now square to \(+1\). These obey

\[
\tilde{J}_i J_j + J_i \tilde{J}_j = 2 \delta_{ij},
\]

and so form representations of the Clifford algebra \( Cl_{0,k} \).

Again we seek the subgroups of \( O(16r) \) that continue to commute with the \( \tilde{J}_i \) as we enlarge the set. An analysis similar to the one in the previous section gives

\[
\cdots O(16r) \supset O(8r) \times O(8r) \supset O(8r) \supset U(4r) \supset \text{Sp}(2r) \supset \text{Sp}(r) \times \text{Sp}(r) \supset \text{Sp}(r) \supset U(r) \cdots.
\]

The sequence of groups is ‘backwards’, compared to the previous one, but the sequence of symmetric spaces

\[
R_0 = O(16r)/O(8r) \times O(8r), \quad R_1 = [O(8r) \times O(8r)]/O(8r) \simeq O(8r), \quad R_2 = O(8r)/U(4r),
R_3 = U(4r)/\text{Sp}(2r), \quad R_4 = \text{Sp}(2r)/\text{Sp}(r) \times \text{Sp}(r), \quad R_5 = [\text{Sp}(r) \times \text{Sp}(r)]/\text{Sp}(r) \simeq \text{Sp}(r),
R_6 = \text{Sp}(r)/U(r), \quad R_7 = U(r)/O(r)
\]

parametrizing the choice space for \( \tilde{J}_{d+1} \) is in the same direction as before. It is, however, offset by 2—i.e. the set of choices for \( \tilde{J}_{d+1} \) is \( R_d \). This offset arises because, once we have chosen \( \tilde{J}_1 \) and \( \tilde{J}_2 \) to bring us back to an orthogonal group, the choice of a higher \( \tilde{J} \) is the same as choosing \( \tilde{J}_1 \tilde{J}_2 \), and these square to \(-1\). The shift is reflected in the Clifford algebra isomorphism \( Cl_{p,0} \otimes \text{Cl}_{0,2} \simeq \text{Cl}_{0,p+2} \) given by

\[
\tilde{e}_i \leftrightarrow e_i \otimes \tilde{e}_2, \quad i = 1, \ldots, p, \quad \tilde{e}_1^2 = \tilde{e}_2^2 = 1, \quad (\tilde{e}_1 \tilde{e}_2)^2 = -1,
\]

\[
\tilde{e}_{p+1} \leftrightarrow \text{id} \otimes \tilde{e}_1,
\]

\[
\tilde{e}_{p+2} \leftrightarrow \text{id} \otimes e_2.
\]

Now suppose we have both \( J_1 \) and \( \tilde{J}_1 \). Then \( \tilde{J}_1 \) decomposes \( \mathbb{R}^{16r} \) into \( \mathbb{R}^{8r} \times \mathbb{R}^{8r} \) and \( O(16r) \) into \( O(8r) \times O(8r) \), and then \( J_1 \) breaks us down to the diagonal \( O(8r) \). If we are given \( J_1 \) first,
and then $J_1$, we have $O(16r) \rightarrow U(8r) \rightarrow O(8r)$, so we get to the same place independent of the order. This observation reflects the Clifford algebra isomorphism $\text{Cl}_{p,q} \otimes Cl_{1,1} \cong \text{Cl}_{p+1,q+1}$. (In [19] Kitaev says that the positive Clifford generators effectively 'cancel' the negative ones.) If we are given $q$ positive Clifford generators and $p$ negative ones, and seek the degree of freedom to choose another positive one, then that degree of freedom is given by $R_{q-p}$. In other words, we end up with the group labelled by $q-p \mod 8$ in the table below, and degree of freedom is given by the coset of that group by the one to its right:

| 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 0 |
|---|---|---|---|---|---|---|---|---|
| $R_0$ | $R_1$ | $R_2$ | $R_3$ | $R_4$ | $R_5$ | $R_6$ | $R_7$ |

On the other hand, if we have $p$ negative generators and $q$ positive ones, the degree of freedom for the choice of the next negative one is $R_{p-q+2}$.

5. Real representations

Much of the insight into topologically non-trivial band theory has relied on illustrative model Hamiltonians. These Hamiltonians are usually constructed from sets of gamma matrices, and the time-reversal and charge-conjugation properties of the gamma matrices play a key role. We therefore explore the representation theory of the irreducible $\gamma$-matrices that compose the generally reducible $J_i$ and $\tilde{J}_i$ from the previous sections. These matrices form representations of the Clifford algebras $\text{Cl}_{p,q}$ with $p$ generators $e_i$ obeying $e_i^2 = -1$ and $q$ generators $\tilde{e}_i$ obeying $\tilde{e}_i^2 = 1$. The $\text{Cl}_{p,q}$ are real algebras in that they consist of linear combinations of products of the generators with only real number coefficients. (If we were to allow complex coefficients, then the distinction between $p$ and $q$ disappears.) Although they are real algebras, most physics discussions of their representation theory—see for example [27]—consider representations over complex vector spaces. This greatly obscures the connection between the algebra and the topology. Atiyah, Bott and Shapiro showed [25] that the connection becomes much clearer when we consider irreducible representations (irreps) of $\text{Cl}_{p,q}$ over $\mathbb{R}$. In other words, $\gamma_i$'s that are $d_{p,q}$-by-$d_{p,q}$ real matrices.

The real representation theory of $\text{Cl}_{p,q}$ is sharply different from the complex representation theory. In the complex case it is well known that the irreps have dimension $2^\lfloor (p+q)/2 \rfloor$. They are unique when $p+q$ is even and there are two inequivalent irreps when $p+q$ is odd. We might think that we can always get a real irrep from a complex one by simply using the correspondence (5) in reverse. If, however, the matrices all commute with a real structure then this process yields a reducible representation. Similarly some irreps that are inequivalent over the complex numbers become equivalent when expanded to become real. Consider the simple example $\text{Cl}_{1,0}$. Over the complex numbers the two irreps $e_1 \mapsto i$ and $e_1 \mapsto -i$ are inequivalent, but when expanded to

$$e_1 \mapsto \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad e_1 \mapsto \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

we have

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^{-1} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

so they are now equivalent.

Consider first the Clifford algebra $\text{Cl}_k \equiv \text{Cl}_{k,0}$ generated by $k$ mutually anticommuting elements $e_i$ that square to $-1$. We find the results displayed in table 5.
Table 5. The dimension and number of the real irreps of $\text{Cl}_k$. Observe that $N(\text{Cl}_k)/i^*N(\text{Cl}_{k+1})$ coincides with $\pi_0(\mathbb{R}^{k+1})$.

| $k$ | $\text{Cl}_k$ | $d_k$ | $N(\text{Cl}_k)$ | $N(\text{Cl}_k)/i^*N(\text{Cl}_{k+1})$ |
|-----|---------------|-------|------------------|----------------------------------|
| 1   | $\mathbb{C}$  | 2     | $\mathbb{Z}$     | $\mathbb{Z}_2$                   |
| 2   | $\mathbb{H}$  | 4     | $\mathbb{Z}$     | 0                                |
| 3   | $\mathbb{H} \oplus \mathbb{H}$ | 4 | $\mathbb{Z} \oplus \mathbb{Z}$ | $\mathbb{Z}$ |
| 4   | $\mathbb{H}(2)$ | 8 | $\mathbb{Z}$     | 0                                |
| 5   | $\mathbb{C}(4)$ | 8 | $\mathbb{Z}$     | 0                                |
| 6   | $\mathbb{R}(8)$ | 8 | $\mathbb{Z}$     | 0                                |
| 7   | $\mathbb{R}(8) \oplus \mathbb{R}(8)$ | 8 | $\mathbb{Z} \oplus \mathbb{Z}$ | $\mathbb{Z}$ |
| 8   | $\mathbb{R}(16)$ | 16 | $\mathbb{Z}$     | $\mathbb{Z}_2$                   |

The dimensions $d_k$ of the irreps are found by characterizing the Clifford algebra as a matrix algebra over $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$ and multiplying the size of the matrices by 1, 2 or 4, respectively. This algebra is displayed in the second column where, for example, $\mathbb{H}(2)$ means the algebra of 2-by-2 matrices with quaternionic entries. After the fact, we may realize that the dimensions could have been read off from table 2 by noting that the product of $d_k$ with the real, complex or quaternionic dimensions of the commuting groups—$8r$, $4r$, $2r+2r$, $2r$, $2r$, $1r+1r$, $r$—remains constant at 16$r$.

To see why there are sometimes two inequivalent representations, consider the case $p = 3$, $q = 0$. The algebra is generated by $e_1$, $e_2$ and $e_3$ all of which square to $-1$. The product $\omega = e_1e_2e_3$ commutes with everything in the algebra, and $\omega^2 = 1$. In an irrep it can map to either $+I$ or $-I$. No change of basis can change the sign, so there must be two inequivalent irreps.

The most interesting features in table 5 are the last two columns. The symbol $N(\text{Cl}_k)$ denotes the additive free group generated by the real irreps of $\text{Cl}_k$. If an algebra $A$ has $d$ irreps $A_1, A_2, \ldots, A_d$, then $N(A)$ has elements

$$n = n_1A_1 \oplus n_2A_2 \oplus \cdots \oplus n_dA_d$$

where the coefficients $n_i \in \mathbb{Z}$ and

$$(n_1, n_2, \ldots, n_d) \in \mathbb{Z} \oplus \mathbb{Z} \oplus \cdots \oplus \mathbb{Z}$$

with $d$ copies.

When all the coefficients $n_i$ are positive, we can think of these elements as being direct sums of irreps. It is convenient to permit the coefficients to be negative, however, so that $N(\text{Cl}_k)$ becomes an additive group. We do this because group-theory language enables us to describe how the representation theory evolves as we add or remove generators from the algebra. In particular, the natural inclusion $i : \text{Cl}_k \to \text{Cl}_{k+1}$ induces a map $i^* : N(\text{Cl}_{k+1}) \to N(\text{Cl}_k)$ that consists of restricting each irrep of $\text{Cl}_{k+1}$ to $\text{Cl}_k$. In other words, we simply omit $\gamma_{k+1}$ and decompose the resulting (usually reducible) representation of $\text{Cl}_k$ into its irreps. Atiyah, Bott and Shapiro [25] then consider the quotient group $N(\text{Cl}_k)/i^*N(\text{Cl}_{k+1})$. In this quotient group a (generally reducible) representation maps to zero if it can be obtained by restricting a representation of $\text{Cl}_{k+1}$ to $\text{Cl}_k$.

The origin of the $\mathbb{Z}_2$ groups in $N(\text{Cl}_k)/i^*N(\text{Cl}_{k+1})$ is easy to understand. Each time the dimension of the gamma matrices doubles, restriction to the smaller set of gamma matrices leads to a reducible representation that decomposes into two copies of the unique irrep of the smaller set. Thus an even number of copies of this irrep maps to zero in
Table 6. The dimension and number of the real irreducible representations of $\text{Cl}_{p,q}$. The subscript 2 denotes that there are two inequivalent representations with this dimension.

| $\text{Cl}_{p,q}$ | $q = 0$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|-------------------|---------|---|---|---|---|---|---|---|---|
| $p = 0$           | 1       | 2 | 2 | 4 | 4 | 2 | 8 | 16| 16|
| 1                 | 2       | 2 | 4 | 4 | 4 | 8 | 16| 16| 32|
| 2                 | 4       | 4 | 4 | 4 | 2 | 8 | 16| 32|   |
| 3                 | 4       | 8 | 8 | 8 | 8 | 8 | 16|   |   |
| 4                 | 8       | 8 | 16| 16| 16| 32|   |   |   |
| 5                 | 8       | 16| 16| 16| 32|   |   |   |   |
| 6                 | 8       | 16| 32|   |   |   |   |   |   |
| 7                 | 8       | 16|   |   |   |   |   |   |   |
| 8                 | 16      |   |   |   |   |   |   |   |   |

$N(\text{Cl}_k)/i^*N(\text{Cl}_{k+1}) \cong \mathbb{Z}_2$, while an odd number of copies maps to the non-trivial element $1 \in \mathbb{Z}_2$.

The $\mathbb{Z}$ groups arise in the cases when $\text{Cl}_k$ has two inequivalent irreps and $N(\text{Cl}_k) = \mathbb{Z} \oplus \mathbb{Z}$. The restriction of the unique irrep of $\text{Cl}_{k+1}$ then supplies a reducible representation of $\text{Cl}_k$ that contains one copy of each of its inequivalent irreps. In $N(\text{Cl}_k)/i^*N(\text{Cl}_{k+1})$ we must therefore identify $(n_1, n_2) \sim (n_1 + m, n_2 + m)$ for any integer $m$. The (Grothendiek) map

$$(n_1, n_2) \mapsto n_1 - n_2 \quad (30)$$

is then a group isomorphism taking each equivalence class to an integer. Consequently a representation that contains an equal number of the two inequivalent irreps maps to zero in $N(\text{Cl}_k)/i^*N(\text{Cl}_{k+1})$, while one with unequal numbers $n_1, n_2$ provides the element $n_1 - n_2 \in \mathbb{Z}$.

Observe from the table that, despite their very different origin, $N(\text{Cl}_k)/i^*N(\text{Cl}_{k+1})$ coincides with $\pi_0(R_{k+1})$. This is not by chance. The real representation theory of the Clifford algebra somehow captures the topology of the classifying spaces. The way this works—essentially the Atiyah–Bott–Shapiro construction—will be the subject of the next section.

For $\text{Cl}_{p,q}$ with $p$ negative ($e^2 = -1$) and $q$ positive ($\tilde{e}^2 = 1$) generators, the dimension $d_{p,q}$ of the irreducible real matrices is displayed in table 6. The entries in this table can be extended down and to the right by noting that one step down and one step to the right doubles the size of the real matrices—i.e. $d_{p,q+1} = 2d_{p,q}$. This last fact follows from the isomorphism $\text{Cl}_{p,q} \otimes \text{Cl}_{1,1} \cong \text{Cl}_{p+1,q+1}$ given by

$$e_i \leftrightarrow e_i \otimes \tilde{e} e, \quad i = 1, \ldots, p + q,$$
$$\tilde{e}_{p+q+1} \leftrightarrow \text{id} \otimes \tilde{e},$$
$$e_{p+q+2} \leftrightarrow \text{id} \otimes e,$$

and the associated real-representation extension

$$\gamma_i \mapsto \gamma_i \otimes \sigma_1, \quad i = 1, \ldots, p + q,$$
$$\tilde{\gamma}_{p+q+1} \mapsto \text{id} \otimes \sigma_3,$$
$$\gamma_{p+q+2} \mapsto \text{id} \otimes (-i\sigma_2).$$

We also have $d_{p+8,q} = d_{p,q+8} = 16d_{p,q}$.

Knowing the dimensions and number of the irreps we can now read off the groups $N(\text{Cl}_{p,q})/i^*N(\text{Cl}_{p+1,q})$. These are displayed in table 7. Again observe that $N(\text{Cl}_{p,q})/i^*N(\text{Cl}_{p+1,q})$ always coincides with $\pi_0(R_{p-q+1})$. 

14
Table 7. The quotient groups $N(C_{p,q})/i N(C_{p+1,q})$. The table extends with period eight in both $p$ and $q$. Observe that $N(C_{p,q})/i N(C_{p+1,q})$ coincides with $\pi_0(R_{p-q+1})$.

| $q$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|-----|---|---|---|---|---|---|---|---|
| $p = 0$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ |
| 1 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $\mathbb{Z}$ | 0 |
| 2 | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 | $\mathbb{Z}$ |
| 3 | $\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 | 0 |
| 4 | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 | 0 |
| 5 | 0 | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ | 0 |
| 6 | 0 | 0 | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ | $\mathbb{Z}$ |
| 7 | $\mathbb{Z}$ | 0 | 0 | 0 | $\mathbb{Z}$ | 0 | $\mathbb{Z}_2$ | $\mathbb{Z}_2$ |

6. Constructing representative Hamiltonians

We now reach the payoff for our labours in the previous sections. We use a simplified version of the Atiyah–Bott–Shapiro (ABS) construction [25, 26] to generate model Hamiltonians in any given Altland–Zirnbauer symmetry class, either over the $d$-sphere parametrized by a unit vector $x$ or over the $d$-sphere equipped with an involution that mimics the $k \rightarrow -k$ inversion in the Brillouin zone. By applying what we know about the real representations of real Clifford algebras we show that the ABS construction can provide Hamiltonians whose bundle of negative energy states lies in any of the topological classes.

We wish to construct operators $\tilde{Q}(x)$ and $\tilde{Q}(k)$ that square to $\mathbb{I}$ (so that $P(x) = (\mathbb{I} - \tilde{Q}(x))/2$ is the projection operator onto the negative eigenspace of $\tilde{Q}(x)$) and have the appropriate discrete symmetries

$$B_\eta \tilde{Q}^*(x) B_\eta^{-1} = \eta \tilde{Q}(x)$$

or

$$B_\eta \tilde{Q}^*(k) B_\eta^{-1} = \eta \tilde{Q}(-k),$$

where $\eta = \pm 1$ and $B^* B = \pm \mathbb{I}$. We first construct Hamiltonians with $x \in S^d$. To do this we assemble a set of $d+1$ matrices $\Gamma_n$ lying in the desired $\mathfrak{m}_n$ by setting $\Gamma_n = J_{i+1} J_{i+1+n}$, $n = 1, \ldots, d+1$. We know from section 3 that when multiplied by a suitable operator ‘$i$’ they possess the required discrete symmetries. The $\Gamma_n$ also obey the Clifford algebra

$$\Gamma_n \Gamma_m + \Gamma_m \Gamma_n = -2 \delta_{nm} \mathbb{I},$$

so the normalized linear combination

$$\tilde{Q}(x) = i \sum_{n=1}^{d+1} x_n \Gamma_n, \quad \|x\| = 1,$$

squares to the identity and so gives a map from $S^d$ to the classifying space $R_{i+3}$ (the space of choices for $J_{i+2}$ —any normalized linear combination of the $J_{i+1}^{-1} \Gamma_n$ provides a candidate for $J_{i+2}$).

Now any bundle over a retractable space, such as a disc, is trivial. Conversely a trivial bundle over a space $X$ can be extended to the one over the retractable cone $CX$ over $X$. Consequently the bundle of negative energy states will be trivial or not depending on whether $\tilde{Q}(x)$ can be smoothly extended from $S^d$, considered as the equator of $S^{d+1}$, to the upper

1 The cone $CX$ over $X$ is the retractable space $(X \times I)/(X \times \{0\})$ where $I = [0, 1]$. 

15
hemisphere of $S^{d+1}$ considered as the cone over $S_d$—taking care, of course, to preserve the discrete symmetries characterizing $\tilde{Q}$. Thus, whether the bundle of negative energy states is trivial or not depends on whether the representation in which our $J_i$ (and hence the $\Gamma_n$) live extends to the one with an additional matrix $J_{\Gamma_3 \gamma_1}$. In other words, whether it is trivial or not in $N(Cl_{d+3})/i^* N(Cl_{d+3}) \simeq \pi_d(R_{d+3}) \simeq \pi_0(R_{d+3})$. That the equivalence classes of bundles are in one-to-one correspondence with the elements of $\pi_d(R_{d+3}) \simeq \pi_0(R_{d+3})$ is exactly the classification we obtained from the purely topological considerations in section 2. The construction in equation (34) is thus able to generate bundles in any equivalence class and provides a one-to-one mapping between the topological $K(S^d)$ and the purely algebraic $N(Cl_{d+3})/i^* N(Cl_{d+3})$. This mapping is the ABS construction.

A comment about the minimal size of the matrix Hamiltonians in each class is in order. When, in section 3, we discussed the symmetries of the Hamiltonians, the reader will have noted that we restricted ourselves to eigenspaces of various operators that commuted with all Hamiltonians in each class. The Hamiltonians we have just constructed therefore generate multiple copies of the ground state bundles. In other words, the minimum sizes of our $\Gamma_n$ and $\Gamma_n \tilde{J}$ are not the dimensions appearing in table 7, but are those numbers divided by an appropriate power of 2. This power of 2 is the same for all representations in a given row, however, and so it does not affect the topological properties of the bundle. If we were to use complex matrices, the necessary power of 2 would vary with $d$, and this is why the dimensions of the complex representations fail to reveal the pattern of topological information.

In the case of topological insulators, the base space $X$ is a Brillouin zone and therefore a $d$-dimensional torus. We wish to obtain ground state bundles over $X$ of the Bloch Hamiltonians $H(k) \equiv \exp(-i k \cdot r) H \exp(i k \cdot r)$. The antilinear maps $T$ and $C$ act as

$$TH(k)T^{-1} = H(-k), \quad C H(k) C^{-1} = -H(-k). \quad (35)$$

Consequently, in addition to ordinary bundles over $X$, we need to study bundles that are compatible with the involution that takes $k$ to $-k$ (modulo reciprocal lattice vectors). This is the subject of KR-theory [26]. We will not consider the complications due to the fact that $X$ is torus, but instead model the Brillouin zone with its $k \rightarrow -k$ involution by replacing the $d + 1$ coordinates $x_n$ with one coordinate $M$, and $d$ coordinates $k_n$, $n = 2, \ldots, d + 1$. We can take these coordinates to obey

$$|k|^2 + M^2 = 1, \quad (36)$$

so the $k$-space has the topology of a sphere with the north pole $(k = 0, M = 1)$ representing the time-reversal-invariant $\Gamma$-point in the Brillouin zone, and with the south pole $(k = 0, M = -1)$ being another fixed point at infinity.

We also replace the $\Gamma_n$ that go with the $k_n$ by $\Gamma_n = J_{\Gamma_1} \Gamma_n J_{\Gamma_1}$. These $\Gamma_n$ are real symmetric matrices obeying

$$\Gamma_n \Gamma_m + \Gamma_m \Gamma_n = 2 \delta_{nm} \mathbb{I}, \quad 1 < n, m \leq d + 1$$

$$\Gamma_n \Gamma_1 + \Gamma_1 \Gamma_n = 0. \quad (37)$$

The $\tilde{\Gamma}_n$ have the same anticommutation relations with the $J_i$ that are used to construct $C$ and $T$, but because they do not get multiplied by ‘i’ in constructing a Hamiltonian, they transform under these symmetries with an extra minus sign. Thus

$$\tilde{Q}(M, k) = i MT \Gamma_1 + \sum_{n=2}^{d+1} k_n \Gamma_n \quad (38)$$

is a matrix that possesses the same $C$ and $T$ symmetries as $i \Gamma_1$. Because the $d$ positive generators take us backwards in the Bott clock, we anticipate that the topological classification is given
by $\pi_0(R_{+3-d})$ instead of $\pi_0(R_{+3+d})$, but it is not exactly obvious how to see this from the homotopy perspective. The algebraic construction makes it clear however. The bundle of negative energy states of $Q(M, k)$ will be trivial if and only if we can extend our Hamiltonian to one higher dimension. Because we do not wish to impose any relation between the upper and lower hemisphere of the $S^{d+1}$, the extra dimension should be of the non-inverting $x$ type. The extensibility of the bundle is therefore determined by an element of

$$N(Cl_{i+2,d})/i^* N(Cl_{i+3,d}) = \pi_0(R_{i+3-d}).$$

(39)

in agreement with [19] and table 1.

There is a physical interpretation of the connection between this bundle extensibility and topological triviality. Consider a Hamiltonian with $d$ ‘momentum-like’ terms and a single ‘mass-like’ term. Now allow the mass term to depend on the position and to change sign on a domain wall. We will then find gapless states bound to the interface between the positive and negative mass domains. If we can add another ‘mass-like’ term that respects the Hamiltonian symmetries, then these surface states will become gapped. Therefore the gapless surface states are not protected by the symmetry precisely when the bundle can be extended to a retractable disc and so is homotopically trivial.

7. Conclusions

We have explained the principle features of table 1 by relating them to the topology of the Bott sequence of Cartan symmetric spaces and to the real representation theory of Clifford algebras. Of course, most of the mathematics we have described are not new, being in [20, 21, 25, 26]. We hope, however, that we have done a service in explaining that the deep ideas in these papers have their origin in relatively simple facts from group theory and linear algebra.

There are a number of issues that we have not discussed. First, we have given a simple algebraic explanation of the $d \rightarrow -d$ sign change effected by the $k \rightarrow -k$ inversion of the Block momentum. We have not found a comparably simple homotopic explanation of this sign change. Such an explanation is desirable given its significance. Second, the spaces $K(X)$ have more than just the additive properties that arise from taking direct sums of fibres. They also have a ring structure that comes from taking tensor products. The tensor product of two representations of a Clifford algebra is not a representation, however. To generate the ring structure one needs to consider graded representations and graded tensor products [25]. It remains to be seen if these concepts have a natural interpretation in the present context.

It would also be interesting to explore how the groups $N(Cl_{p,q})/i^* N(Cl_{p+1,q})$ are related to the pattern of dimensional reduction in [12]. These authors make use of complex gamma matrices, but whenever they commute with a suitable complex structure our real matrices can be rewritten as complex matrices of half the size. They cannot be so reduced when they commute with a real structure, but in that case the complex matrices become real when written in a suitable basis. Our arguments could, therefore, be recast into the language of complex gamma matrices, but at the cost of complicating the discussion.

We should add that the ABS construction has been used previously in condensed matter physics to characterize the stability of gapless Fermi surfaces [28]. Our application is to gapped systems.
Acknowledgments

This work was supported by the National Science Foundation under grant NSF DMR 09-03291. MS would like to thank Matthew Ando and Sheldon Katz for explaining K theory, and Taylor Hughes for not only patiently explaining the physics of topological insulators but also for help with the present exposition.

References

[1] Kane C and Mele E J 2005 Phys. Rev. Lett. 95 146802
Kane C and Mele E J 2005 Phys. Rev. Lett. 95 226801
[2] Bernevig B A and Zhang S-C 2006 Phys. Rev. Lett. 96 106802
[3] Moore J E and Balents L 2007 Phys. Rev. B 75 121306
[4] Fu L, Kane C L and Mele E J 2007 Phys. Rev. Lett. 98 106803
[5] Roy R 2009 Phys. Rev. B 79 195321
[6] Roy R 2009 Phys. Rev. B 79 195322
[7] Hsieh D, Qian D, Wray L, Xia Y, Hor Y S, Cava R J and Hasan M Z 2008 Nature 452 970974
[8] Hsieh D et al 2009 Science. 323 919–22
[9] Xia Y, Qian D, Hsieh D, Wray L, Pal A, Lin H, Bansil A, Grauer D, Hor Y S and Cava R J 2009 M. Z. Hasan. Nature Phys. 5 398–402
[10] König M, Wiedmann S, Brüne C, Roth A, Buhmann H, Molenkamp L W, Qi X-L and Zhang S-C 2007 Science 318 766–70
[11] Chen Y L et al 2009 Science 325 178–81
[12] Qi X-L, Hughes T and Zhang S-C 2008 Phys. Rev. B 78 195424
[13] Schnyder A P, Ryu S, Furusaki A and Ludwig A W W 2008 Phys. Rev. B 78 195125
[14] Schnyder A P, Ryu S, Furusaki A and Ludwig A W W 2009 AIP Conf. Proc. 1134 10
[15] Schnyder A P, Ryu S, Furusaki A and Ludwig A W W 2009 arXiv:0912.2157
[16] Dyson F J 1962 J. Math. Phys. 3 1199–215
[17] Zirnbauer M 1996 J. Math. Phys. 37 4986–5018
[18] Allard A and Zirnbauer M 1997 Phys. Rev. B 55 1142–61
[19] Kitaev A 2008 Advances in Theoretical Physics: Landau Memorial Conference (Chernogolovka, Russia, 22–26 June 2008) (AIP Conf. Proc. vol 1134) ed V Labeved and M Feigel’sman pp 22–30 (arXiv:0901.2686)
[20] Bott R 1959 Ann. Math. 70 313–37
[21] Milnor J 1963 Morse Theory (Annals of Mathematics Studies AM-51) (Princeton, NJ: Princeton University Press)
[22] Mermin N D 1979 Rev. Mod. Phys. 51 591–648
[23] Crossley M D 2000 Essential Topology (Berlin: Springer)
[24] Cartan E 1926 Bulletin de la Société Mathématique de France 54 214–6
Cartan E 1927 Bulletin de la Société Mathématique de France 55 114–34
[25] Atiyah M F, Bott R and Shapiro A 1964 Topology 3 3–38 (Suppl.)
[26] Atiyah M F 1966 Q. J. Math. Oxford (2) 17 367–86
[27] Polchinski J 2001 String Theory vol 2 (Cambridge: Cambridge University Press) appendix B
[28] Hořava P 2005 Phys. Rev. Lett. 95 016405