Bundle gerbes for topological insulators*

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Abstract

Bundle gerbes are simple examples of higher geometric structures that show their utility in dealing with topological subtleties of physical theories. I will review a recent construction of torsion topological invariants for condensed matter systems via equivariant bundle gerbes. The construction covers static and periodically driven systems with time reversal invariance in 2 and 3 space dimensions. It involves refinements of geometry of gerbes that will be discussed in the first lecture, the second one being devoted to the applications to topological insulators.

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I. LECTURE 1. WESS-ZUMINO AMPLITUDES AND BUNDLE GERBES

A. Introduction

These lectures are devoted to the application of techniques related to gerbes to the construction of torsion invariants of low-dimensional topological insulators. In recent times, the subject of topological insulators has been an important point of junction between condensed matter theory and mathematics. The interaction started from the realizations of the role that the 1st Chern number plays in the integer quantum Hall effect \[1\] and the relations of the later to the index theorem. It gained a new momentum with the introduction of \(K\)-theoretic invariants to classify time-reversal topological insulators \[3, 4\]. In these lectures I shall present a geometric picture of the simplest of those \(K\)-theoretic invariants, the 2- and 3-dimensional Kane-Mele \(Z_2\)-valued index and its generalization to the so called Floquet topological insulators that we proposed in \[5, 6\]. The geometric picture is centered on the concept of Wess-Zumino amplitudes and their refinements and on the underlying geometry of bundle gerbes and equivariant structures on them. These concepts will be the topic of the first lecture preparing the ground for the second one where I shall describe how they are applied to construct indices classifying time-reversal invariant topological insulators.

B. 2d Wess-Zumino amplitudes and their square root

Let us start by recalling what are the Wess-Zumino amplitudes \[3, 8\]. Let \(M\) be a manifold and \(H\) a closed real \((k + 1)\)-form on \(M\) whose periods, i.e. integrals over singular \((k + 1)\)-cycles, are in \(2\pi\mathbb{Z}\). Mathematically, the Wess-Zumino (WZ) amplitude is a Cheeger-Simons differential character, i.e. a homomorphism

\[
Z_k(M) \rightarrow \mathbb{R}/(2\pi\mathbb{Z}) \quad (I.1)
\]

from the group of singular \(k\)-cycles in \(M\) to \(U(1)\) that takes on boundaries \(\partial c_{k+1}\) the values \(\int_{c_{k+1}} H\mod 2\pi\mathbb{Z}\). The differential characters (with arbitrary \((k + 1)\)-forms \(H\)) form an Abelian group \(\widehat{H}^{k+1}(M)\). We shall consider here the case with \(k = 2\) where \(H\) is a 3-form and we shall use physicist’s notation writing

\[
e^{iS_{WZ}(\phi)} \in U(1) \quad (I.2)
\]

for the values of the differential character on a singular 2-cycle \(c_{\phi}\) determined by a smooth map \(\phi: \Sigma \rightarrow M\) from a closed oriented 2-surface \(\Sigma\) to \(M\). It follows then from the definition that if there exist an oriented 3d-manifold \(\Sigma\) such that \(\partial \Sigma = \Sigma\) and a smooth map \(\phi: \Sigma \rightarrow M\) extending \(\phi\), i.e. such that \(\check{\phi}|_{\partial \Sigma} = \phi\), then

\[
e^{iS_{WZ}(\phi)} = \exp \left[ i \int_{\Sigma} \phi^* H \right]. \quad (I.3)
\]

Differential characters corresponding to a given 3-form \(H\) differ by elements \(\chi \in Hom(H_2(M), U(1)) \cong H^2(M, U(1))\), or more exactly, by multiplication by \(\chi([c_{\phi}])\), where \([c_{\phi}]\) denotes the homology class of the 2-cycle \(c_{\phi}\).

We shall be interested in the case where \(M = U(N)\) and \(H\) is the closed bi-invariant 3-form,

\[
H = \frac{1}{{12\pi}} \text{tr}(g^{-1}dg)^3, \quad (I.4)
\]

that is normalized so that its set of periods is \(2\pi\mathbb{Z}\). Since \(H_2(U(N)) = 0\), the WZ amplitudes are uniquely fixed by the rule \([1.3]\) as every \(\phi\) extends to \(\check{\phi}\) in this case.

The main idea pursued in this lectures is that the presence of time reversal symmetry imposes the consideration of square roots of WZ amplitudes. In quantum mechanics the time reversal is realized by an anti-unitary operator in the space of states. In particular, in the space of states \(\mathbb{C}^N \cong \mathbb{C}^{\otimes 2j}\) with \(N = 2j + 1\) carrying the representation of spin \(j = 0, \frac{1}{2}, 1, \ldots\), the time reversal is realized by the anti-unitary operator \(\theta = e^{\pi i S_y} C\), where \(C\) is the complex conjugation and \(S_y\) is the \(y\)-component of the spin operator \(\hat{S}\). In this case \(\theta^2 = (-1)^{2j}I\). We shall be mostly interested in the case when \(\theta^2 = -I\) corresponding to half-integer spins, e.g. to \(j = \frac{1}{2}\) as for electrons. The adjoint action of \(\theta\) induces an involution \(\Theta : U(N) \rightarrow U(N)\),

\[
\Theta(V) = \theta V \theta^{-1}, \quad (I.5)
\]
which preserves the bi-invariant 3-form $H$ on $U(N)$. Suppose now that we equip the closed oriented surface $\Sigma$ with a nontrivial orientation-preserving involution $\vartheta$ with discrete non-empty set of fixed points. The typical example will be the action induced on the torus $\mathbb{T}^2 = \mathbb{R}^2/(2\pi\mathbb{Z})^2$ by the map $k \mapsto -k$ on $\mathbb{R}^2$. Other examples may be given by the map $(z, y) \mapsto (z, -y)$ on the hyperelliptic curve $y^2 = p(z)$, where $p$ is a polynomial. Let $\phi : \Sigma \to U(N)$ be an equivariant map, i.e. such that

$$\phi \circ \vartheta = \Theta \circ \phi.$$  \hfill (I.6)

Suppose that there exists an oriented 3d manifold $\overset{\sim}{\Sigma}$ equipped with an orientation-preserving involution $\overset{\sim}{\vartheta}$ such that $\partial \overset{\sim}{\Sigma} = \Sigma$ and $\partial |_{\partial \overset{\sim}{\Sigma}} = \vartheta$ and an extension $\overset{\sim}{\phi} : \overset{\sim}{\Sigma} \to U(N)$ of $\phi$ such that

$$\overset{\sim}{\phi} \circ \overset{\sim}{\vartheta} = \Theta \circ \overset{\sim}{\phi}.$$  \hfill (I.7)

Let us set

$$\sqrt{e^{iSWZ(\phi)}} = \exp \left[ \frac{i}{7} \int_{\overset{\sim}{\Sigma}} \overset{\sim}{\phi}^* H \right].$$  \hfill (I.8)

Does this provide a correct definition of the square root of the WZ amplitude of equivariant maps $\phi : \Sigma \to U(N)$?

**Proposition 1.** Assume that $\theta^2 = -I$. Let $\Sigma = \mathbb{T}^2$, $\vartheta = -k$, and let $\phi : \Sigma \to U(N)$ satisfy (I.6). Applying at most an $SL(2, \mathbb{Z})$ change of variables on $\Sigma$, we may assume that $\det(\phi)$ does not wind around the first circle of $\mathbb{T}^2 = S^1 \times S^1$. Let $\overset{\sim}{\Sigma} = D \times S^1$, where $D$ is a unit disk in $\mathbb{C}$, with $\overset{\sim}{\vartheta}(z, \lambda) = (\bar{z}, \lambda)$. Then there exists an extension of $\overset{\sim}{\phi} : \overset{\sim}{\Sigma} \to U(N)$ of $\phi$ satisfying (I.7) and the right hand side of (I.8) does not depend on its choice so that $\sqrt{e^{iSWZ(\phi)}}$ given by (I.8) is well defined.

**Remarks.** 1. The essence of the last statement is that the imposition of condition (I.7) on $\overset{\sim}{\phi}$ makes $\int_{\overset{\sim}{\Sigma}} \overset{\sim}{\phi}^* H$ well defined modulo $4\pi$ rather than only modulo $2\pi$ which would be the case without that restriction. The assumption $\theta^2 = -I$ is essential for both assertions of Proposition 1.

2. The proof of that proposition is rather laborious. It is a simple extension of the one given in [6] where it was assumed that $\det(\phi)$ has no windings.

The applications of the above construction will be discussed in Lecture 2. Let us only mention here that, when applied to the map $\phi : \mathbb{T}^2 \to U(N)$, $\phi(k) = I - 2P(k)$, where $P(k) = \theta P(-k)\theta^{-1}$ is the family of projectors on the valence band states of a time-reversal invariant 2d insulator, it gives

$$\sqrt{e^{iSWZ(\phi)}} = (-1)^{KM},$$  \hfill (I.9)

where $KM \in \mathbb{Z}_2$ is the Kane-Mele invariant [3, 26] of such insulators.

Although the nonlocal expressions (I.3) for $e^{iSWZ(\phi)}$ and (I.8) for $\sqrt{e^{iSWZ(\phi)}}$ in terms of 3d integrals define well those quantities in the cases described above, we shall also need local expressions for them in terms of 2d integrals with corrections. Such expressions may be conveniently described using the holonomy of bundle gerbes and its appropriate refinement. The local expressions are essential for the construction of a 3d index that will be presented in Sec. [12] below. Such index will be our main tool for building topological invariants of insulators.

### C. Bundle gerbes with connection

Bundle gerbes were introduced by Murray in [10] as a geometric example of more abstract gerbes considered in [11] and [12]. I shall follow closely the original definition of [10].

Let $\pi : Y \to M$ be a surjective submersion and

$$Y^{[n]} = Y \times_M Y \times_M \cdots \times_M Y = \{(y_1, \ldots, y_n) \in Y^n \mid \pi(y_1) = \cdots = \pi(y_n)\}.$$  \hfill (I.10)

By $p_{i_1 \cdots i_m} : Y^{[n]} \to Y^{[m]}$ we shall denote the maps $(y_1, \ldots, y_n) \mapsto (y_{i_1}, \ldots, y_{i_m})$.

**Definition [10].** A bundle gerbe with connection $G$ over $M$ is a quadruple $(Y, B, L, t)$, where $\pi : Y \to M$ is a surjective submersion, $B$ is a 2-form on $Y$ (called curving), $L$ is a Hermitian line bundle with unitary
connection\(^1\) over \(Y \[^2\]\) with (real) curvature 2-form \(p_1^*B - p_0^*B\), \(t\) is a line-bundle isomorphism over \(Y \[^3\]\)

\[
t : p_{12}^*\mathcal{L} \otimes p_{23}^*\mathcal{L} \rightarrow p_{13}^*\mathcal{L}
\]

acting fiberwise\(^2\) as

\[
\mathcal{L}_{y_1,y_2} \otimes \mathcal{L}_{y_2,y_3} \xrightarrow{\mathcal{L} \otimes 1} \mathcal{L}_{y_1,y_3}
\]

for \((y_1,y_2,y_3) \in Y \[^3\]\) and defining an (associative) groupoid multiplication on \(\mathcal{L} \subset Y\). In particular, \(t\) provides canonical isomorphisms \(\mathcal{L}_{y,y} \cong \mathbb{C}\) and \(\mathcal{L}_{y_1,y_2}^{-1} \cong \mathcal{L}_{y_2,y_1}\), where \(\mathcal{L}_{y_1,y_2}^{-1}\) denotes the line dual to \(\mathcal{L}_{y_1,y_2}\).

The condition on the curving 2-form implies that \(p_1^*dB = p_0^*dB\) so that \(dB = \pi^*H\) for some closed 3-form \(H\) on \(M\) called the curvature of gerbe \(\mathcal{G}\).

Gerbes over \(M\) form a 2-category with objects, 1-isomorphisms between objects and 2-isomorphisms between 1-isomorphisms\(^3\). We shall only need 1-isomorphisms \(\eta : \mathcal{G} \rightarrow \mathcal{G}'\) between gerbes \(\mathcal{G} = (Y,B,\mathcal{L},t)\) and \(\mathcal{G}' = (Y,B',\mathcal{L}',t')\) with the same \(Y\). They may be given by a line bundle \(\mathcal{N}\) over \(Y\) with curvature \(B' - B\), and by an isomorphism \(\nu\) of line bundles over \(Y\)

\[
\nu : \mathcal{L} \otimes p_2^*\mathcal{N} \rightarrow p_1^*\mathcal{N} \otimes \mathcal{L}'
\]

interwining the groupoid multiplications \(t\) and \(t'\). In particular, \(\nu\) establishes an isomorphism

\[
\mathcal{L}_{y_1,y_2} \otimes \mathcal{L}_{y_2,y_3}^{-1} \cong \mathcal{N}_{y_1} \otimes \mathcal{N}_{y_2}^{-1}.
\]

1-isomorphic gerbes have the same curvature. A 2-isomorphism \(\mu : \eta_1 \Rightarrow \eta_2\) between 1-isomorphisms \(\eta^\alpha : \mathcal{G} \rightarrow \mathcal{G}'\), \(\alpha = 1,2\), \(\eta^\alpha = (\mathcal{N}^\alpha, \nu^\alpha)\) is an isomorphism \(m : \mathcal{N}^1 \rightarrow \mathcal{N}^2\) of line bundles over \(Y\) that makes commutative the diagram

\[
\begin{array}{ccc}
\mathcal{L} \otimes p_2^*\mathcal{N}^1 & \xrightarrow{\nu} & p_1^*\mathcal{N}^1 \otimes \mathcal{L}' \\
\Id_{\mathcal{L}} \otimes p_2^*m & & p_1^*m \otimes \Id_{\mathcal{L}'} \\
\mathcal{L} \otimes p_2^*\mathcal{N}^2 & \xrightarrow{\nu} & p_1^*\mathcal{N}^2 \otimes \mathcal{L}'
\end{array}
\]

Gerbes \(\mathcal{G}\), 1-isomorphisms \(\eta\) between them and 2-isomorphisms \(\mu\) can be multiplied and composed in natural ways and pulled back by maps \(T : M' \rightarrow M\). The 1-isomorphism classes of gerbes over \(M\) form an Abelian group \(\mathcal{G}(M)\).

**Remark.** If \(\eta : \mathcal{G} \rightarrow \mathcal{G},\ \eta = (\mathcal{N}, \nu)\), is a 1-isomorphism of the same gerbe over \(M\) then line bundle isomorphism \(\nu\) allows to view \(\mathcal{N}\) as a pullback of a flat bundle \(N\) over \(M\). The identity 1-isomorphism \(\Id_{\mathcal{G}}\) with trivial bundle \(\mathcal{N}\) and identity isomorphism \(\nu\) is an example of such a 1-isomorphism. There exists a 2-isomorphism \(\mu : \eta \Rightarrow \Id_{\mathcal{G}}\) if and only if the flat line bundle \(N\) corresponding to \(\mathcal{N}\) is trivializable, with the trivialization defining the isomorphism \(m\) corresponding to \(\mu\).

### D. Bundle gerbe holonomy

Group \(\mathcal{G}(\Sigma)\) of 1-isomorphism classes of gerbes over a closed oriented surface \(\Sigma\) is isomorphic to \(U(1)\). If \(\mathcal{G} = (Y,B,\mathcal{L},t)\) is a gerbe over \(M\) and \(\phi : \Sigma \rightarrow M\) then the phase in \(U(1)\) associated to the 1-isomorphism class of gerbe \(\phi^*\mathcal{G}\) over \(\Sigma\) is called the holonomy of \(\mathcal{G}\) along \(\phi\) and is denoted \(\text{Hol}_{\mathcal{G}}(\phi)\). We shall need an explicit representation of such a phase.

Let us choose a triangulation of \(\Sigma\) composed of triangles \(c\), edges \(b\) and vertices \(v\). We suppose that it is sufficiently fine so that there exist maps \(s_c : c \rightarrow Y\) such that

\[
\pi \circ s_c = \phi|_c,
\]

\(^1\) All line bundles considered here are assumed to be equipped with such structures and their isomorphisms to preserve them, unless stated otherwise.

\(^2\) We denote by \(\mathcal{L}_{y_1,y_2}\) the fiber of \(\mathcal{L}\) over \((y_1,y_2) \in Y \[^2\] \).
For each edge we shall also choose a a map $s_b : b \mapsto Y$ such that $\pi \circ s_b = \phi|_b$ and for each vertex $v$ a point $s_v \in Y$ such that $\pi(s_v) = \phi(v)$. Then the holonomy of $G$ along $\phi$ may be given by the expression

$$\text{Hol}_G(\phi) = e^{i \sum_c \int_c^\pi \phi_{|b} \otimes \text{hol}_L(s_c|b, s_b)},$$

where we use a slightly abusive notation in which $\text{hol}_L(\ell)$ stands for the parallel transport of in line bundle $L$ along curve $\ell$ in $Y$ which is a linear map from the fiber of $L$ over the initial point of $\ell$ to the one over the final point. It follows that the expression on the right hand side of (I.17) is an element of the line

$$\otimes_{v \in b \subset \partial \Sigma} L_{s_c(v), s_b(v)}^\pm \cong C\,.$$

where the minus power (the dual line) is chosen if $v$ has a negative orientation, i.e. is the initial point of the edge $b$ with orientation inherited from $c$. The groupoid structure on $L$ defined by the isomorphism $t_{\ell}$ of (I.60) makes the line (I.18) canonically isomorphic to $C$. Indeed, for a fixed vertex $v_0$ as in Fig. 2

$$\text{Hol}_G(\phi) \in \otimes_{v \in b \subset \partial \Sigma} L_{s_c(v), s_b(v)}^\pm \cong C\,.$$

A cyclic permutation of terms does not change the isomorphism with $C$ because of the associativity of the groupoid multiplication in $L$. Hence, the right hand side of (I.17) may be canonically viewed as a complex number that, in fact, belongs to $U(1)$. The holonomy of gerbe with curvature $H$ is a differential character that we shall use to define the WZ amplitude corresponding to the closed 3-form $H$ setting

$$e^{i S_{\text{WZ}}(\phi)} = \text{Hol}_G(\phi)\,.$$

For the later use, let us notice that if we used the same formula (I.17) for a surface $\Sigma$ with boundary $\partial \Sigma \cong S^1$ then we would obtain

$$\text{Hol}_G(\phi) \in \otimes_{v \in b \subset \partial \Sigma} L_{s_c(v), s_b(v)}^\pm \cong L_{\phi|_{\partial \Sigma}}^\partial\,.$$

where $L^\partial$ is the transgression line bundle over loop space $LM$ canonically induced by gerbe $G$ over $M$.  

\[ \text{FIG. 1: Triangulation of $\Sigma$ for gerbe holonomy calculation} \]

\[ \text{FIG. 2: Triangulation of $\Sigma$ around vertex $v_0$} \]
E. Gerbes equivariant under involution

Equivariance of gerbes has been studied by several authors, see \[13,20\]. We shall discuss here a simple version of such equivariance under an action of \(\mathbb{Z}_2\) group.

Let \(\Theta : M \to M\) be an involution and let \(\mathcal{G} = (Y,B,L,t)\) be a bundle gerbe over \(M\) with curvature \(H\). We shall assume that \(\Theta\) may be lifted to an involution \(\Theta : Y \to Y\) covering \(\Theta\), i.e. such that the diagram

\[
\begin{array}{ccc}
Y & \xrightarrow{\Theta} & Y \\
\pi \downarrow & & \downarrow \pi \\
M & \xrightarrow{\Theta} & M
\end{array}
\]

is commutative. We would like to compare gerbe \(\mathcal{G}\) to its pullback \(\Theta^*\mathcal{G}\) that can be realized as the quadruple \((Y,\Theta_Y B, (\Theta_Y^2)^*L, (\Theta_Y^3)^*t)\).

**Definition.** \(\Theta\)-equivariant structure on \(\mathcal{G}\) is a pair \((\eta,\mu)\) where \(\eta = (N,\nu)\) is a 1-isomorphism \(\eta : \mathcal{G} \to \Theta^*\mathcal{G}\) and \(\mu : \Theta^*\eta \circ \eta = \text{Id}_{\mathcal{G}}\) is a 2-isomorphism between 1-isomorphisms of \(\mathcal{G}\). Besides, as 2-isomorphisms between 1-isomorphisms \(\eta \circ \Theta^*\eta \circ \eta : \mathcal{G} \to \Theta^*\mathcal{G}\) and \(\eta : \mathcal{G} \to \Theta^*\mathcal{G}\),

\[
\Theta^*\mu \circ \text{Id}_{\eta} = \text{Id}_{\eta} \circ \mu.
\]

**Remarks.**
1. The existence of a 1-isomorphism \(\eta : \mathcal{G} \to \Theta^*\mathcal{G}\) implies that \(H = \Theta^*H\).
2. The composition \(\Theta^*\eta \circ \eta = (Q,\rho)\) with \(Q = \Theta_Y N \otimes N\) is a 1-isomorphism of gerbe \(\mathcal{G}\) and, consequently, \(Q = \pi^*Q\), where \(Q\) is a flat line bundle over \(M\). Line bundle \(Q\) comes with an involutive isomorphism \(\Theta_Q\)switching the tensor factors that covers \(\Theta\). The 2-isomorphism \(\mu\) is given by a trivialization of \(Q\) defined by a flat normalized section \(S : M \to Q, |S| = 1\). Relation \((1.23)\) translates to the condition

\[
\Theta_Q \circ S = S \circ \Theta.
\]

F. Square root of gerbe holonomy

Under special conditions that will be specified below, a \(\Theta\)-equivariant structure \((\eta,\mu)\) on a gerbe \(\mathcal{G} = (Y,B,L,t)\) over \(M\) permits to determine a square root of the holonomy \(\text{Hol}_\mathcal{G}(\phi)\) of maps \(\phi : \Sigma \to M\) that satisfy the equivariance condition \((1.16)\) for an orientation-preserving involution \(\vartheta : \Sigma \to \Sigma\) with discrete fixed points.

Let us choose a fundamental domain in \(\Sigma\) for \(\vartheta\) whose closure \(F\) is a (piecewise) smooth submanifold with boundary of \(\Sigma\), see Fig.3 for examples of possible choices of \(F\) for \(\Sigma = \mathbb{T}^2\). We shall triangulate \(F \subset \Sigma\) in a way that is \(\vartheta\)-symmetric when restricted to \(\partial F\) (\(\vartheta\) preserves \(\partial F\) reversing its orientation). Assuming that the triangulation of \(F\) is sufficiently fine so that the maps \(s_c\) satisfying \((1.10)\) exist, we shall first consider

\[
\text{Hol}_\mathcal{G}(\phi|_F) \in \bigotimes_{v \in \partial F, (\vartheta)} L^\pm_{s_c, s_c(v)}
\]

according to \((1.21)\). Let us now choose a fundamental domain for \(\vartheta\) acting in \(\partial F\) and let \(\ell\) be its closure. Connected components of \(\ell\) are either curves beginning and ending at fixed points of \(\vartheta\) or closed loops, see FIG. 3: Two examples of fundamental domain \(F\) for \(\Sigma = \mathbb{T}^2\).
Fig. 3. The maps $s_b : b \to Y$ such that $\pi \circ s_b = \phi|_b$ may be chosen so that for $b \subset \ell$,
\[
s_{\partial Y} \circ \phi = \Theta_Y \circ s_b.
\]
Similarly, we may choose $s_v \in Y$ for vertices $v$ in the interior of $\ell$ so that
\[
s_{\partial(v)} = \Theta_Y(s_v).
\]
In this case,
\[
\otimes_{v \in b \subset \partial F} L_{s_v,s_b(v)}^{\pm 1} \cong \left( \otimes_{v \in b \subset \ell} \left( \mathcal{L}_{s_v,s_b(v)} \otimes L_{\Theta_Y(s_v),\Theta_Y(s_b(v))}^{-1} \right) \right) \otimes \left( \otimes_{v \in \partial \ell} L_{\Theta_Y(s_v),s_v}^{\pm 1} \right)
\]
\[
\cong \left( \otimes_{v \in b \subset \ell} \left( N_{s_v} \otimes N_{s_b(v)}^{-1} \right) \right) \otimes \left( \otimes_{v \in \partial \ell} \left( L_{\Theta_Y(s_v),s_v} \right) \right)
\]
\[
\cong \left( \otimes_{v \in b \subset \ell} N_{s_b(v)}^{\pm 1} \right) \otimes \left( \otimes_{v \in \partial \ell} \left( L_{\Theta_Y(s_v),s_v} \otimes N_{s_v}^{-1} \right) \right),
\]
where the second line is obtain using the line bundle isomorphism $\nu$ of the 1-isomorphism $\eta : \mathcal{G} \to \Theta^* \mathcal{G}$, see relation (I.14).

In the next step, let us set, abusing again notations,
\[
\text{hol}_Y(\phi|_F) = \otimes_{b \subset \ell} \text{hol}_Y(s_b) \in \otimes_{v \in b \subset \ell} N_{s_b(v)}^{\pm 1},
\]
where $\text{hol}_Y(s_b)$ stands for the parallel transport in line bundle $N$ along $s_b$. We infer that
\[
\text{Hol}_Y(\phi|_F) \otimes \text{hol}_Y(\phi|_F) \in \otimes_{v \in \partial \ell} \left( \mathcal{L}_{\Theta_Y(s_v),s_v} \otimes N_{s_v} \right)^{\pm 1}
\]
The latter expression will eventually give the value of the square root of $\text{Hol}_Y(\phi)$ after the identification of lines $\mathcal{L}_{\Theta_Y(s_v),s_v} \otimes N_{s_v}$ with $\mathbb{C}$ that we shall discuss now.

Let us first note that $\phi(\partial \ell) \subset M'$, where
\[
M' = \left\{ x \in M \mid \Theta(x) = x \right\}
\]
is the fixed point set of $\Theta$ that, for simplicity, we shall assume to be a submanifold of $M$. We shall denote by $Y' \subset Y$ the preimage by $\pi$ of $M'$. Note that $s_v \in Y'$ for $v \in \partial \ell$. Let $r : Y' \to Y'$ be defined by $r(y') = (\Theta_Y(y'),y')$. Consider the line bundle
\[
N' = r^* \mathcal{L} \otimes N|_{Y'},
\]
over $Y'$ with fibers
\[
N_{y'} = \mathcal{L}_{\Theta_Y(y'),y'} \otimes N_{y'}.
\]
Note that $N'$ is flat. Besides, it has a natural structure of a pullback of a flat line bundle $N'$ over $M'$ given by the identification of its fibers over points $y'_1$ and $y'_2$ with $\pi(y'_1) = \pi(y'_2)$:
\[
\begin{align*}
N'_{y'_1} & = \mathcal{L}_{\Theta_Y(y'_1),y'_1} \otimes N_{y'_1} \\
& \cong \mathcal{L}_{\Theta_Y(y'_1),y'_1} \otimes L_{y'_2,y'_1}^{\pm 1} \otimes N_{y'_1} \\
& \cong \mathcal{L}_{\Theta_Y(y'_1),y'_1} \otimes \mathcal{L}_{\Theta_Y(y'_2),y'_2} \otimes N_{y'_1} \\
& \cong \mathcal{L}_{\Theta_Y(y'_1),y'_1} \otimes \mathcal{L}_{\Theta_Y(y'_2),y'_2} \otimes N_{y'_2} \\
N'_{y'_2} & = \mathcal{L}_{\Theta_Y(y'_2),y'_2} \otimes N_{y'_2}.
\end{align*}
\]
$N'$ together with this structure represents the 1-isomorphism $\eta|_{M'} : \mathcal{G}' \to \mathcal{G}'$, where $\mathcal{G}' = \mathcal{G}|_{M'}$. In particular, the above identification defines a line bundle isomorphism $\nu' : N' \to \Theta^*_Y N'$. Now
\[
N' \otimes N' \cong \Theta^*_Y N' \otimes N' \cong (\Theta^*_Y N \otimes N)|_{M'} \cong Q|_{M'} \cong \mathbb{C},
\]
where $Q$ is the flat line bundle over $Y$ corresponding to the 1-isomorphism $\Theta^*_Y \eta \circ \eta : \mathcal{G} \to \mathcal{G}$. Recall that $Q \cong \pi^* Q$ where $Q$ is a flat line bundle over $M$ provided with a flat section $S$ as a part of the $\Theta$-equivariant structure on gerbe $\mathcal{G}$. Thus section $S' = S|_{M'}$ may be viewed as providing a trivialization of the flat line bundle $N' \otimes N'$. If $M'$ is simply connected then there also exists section $\sqrt{S'}$ trivializing flat line $N'$ such that $\sqrt{S'} \otimes \sqrt{S'} = S'$ (all flat line bundles on simply connected manifolds are trivializable). Besides, $\sqrt{S'}$ is determined modulo a locally constant function taking values in $\{ \pm 1 \}$. In particular, if $M'$ is simply
connected, the trivialization $\sqrt{S'}$ of $N'$ is defined up to a global sign. From (1.30) it follows that if $M'$ is connected and simply connected then

$$\text{Hol}_G(\phi|F) \otimes \text{hol}_{N'}(\phi|\ell) \in \bigotimes_{v \in \partial \ell} N'_{\phi(v)} \cong \mathbb{C}$$  \hspace{1cm} (1.36)$$

and the last isomorphism using section $\sqrt{S'}$ of $N'$ is independent of the choice of that section (the global sign change cancels between the terms coming from the two ends of connected components of $\ell$).

**Proposition 2.** For $M'$ connected and simply connected, the latter isomorphism associates to $\text{Hol}_G(\phi|F) \otimes \text{hol}_{N'}(\phi|\ell)$ a phase in $U(1)$ that does not depend on the choices of $F$, $\ell$, the triangulation of $F$, the lifts $s_c$, $s_b$ and $s_v$ and of the sign of $\sqrt{S'}$.

**Remark.** The independence of the phase assigned to $\text{Hol}_G(\phi|F) \otimes \text{hol}_{N'}(\phi|\ell)$ on the choices of $s_c$, $s_b$ and $s_v$ is proven by a direct check, that on the triangulation by passing to a finer one with respect to two arbitrary triangulations, on the choice of $\ell$ by replacing one of its connected components by its $\bar{\theta}$ image and on $F$ by replacing one of its triangles by its $\bar{\theta}$ image. Multiplying the expressions corresponding to fundamental domains $F$ and $\bar{\theta}F$ one restores $\text{Hol}_G(\phi)$ proving that the phase in question squares to $\text{Hol}_G(\phi)$.

**Definition.** Under the assumptions of Proposition 2, we define $\sqrt{\text{Hol}_G(\phi)}$ by the relation

$$\text{Hol}_G(\phi|F) \otimes \text{hol}_{N'}(\phi|\ell) \sim \sqrt{\text{Hol}_G(\phi)} \otimes \sqrt{S'}(\phi(v))^{\pm 1}.$$  \hspace{1cm} (1.37)$$

Recalling that $\text{Hol}_G(\phi)$ was used to define the WZ amplitudes, see (1.20), we obtain this way a local definition of $\sqrt{e^{S_{WZ}(\phi)}}$.

**G. 3d index with values $\pm 1$**

Let, as above, $G$ be a gerbe on $M$ with curvature $H = \Theta^*H$ and let $(\eta, \mu)$ be a $\Theta$-equivariant structure on $G$. Let $R$ be an oriented 3d-manifold with an orientation-reversing involution $\rho$ with discrete fixed points and let $\Phi : R \rightarrow M$ satisfy the equivariance condition

$$\Phi \circ \rho = \Theta \circ \Phi.$$  \hspace{1cm} (1.38)$$

Let $F_R \subset R$ be the closure of a fundamental domain for $\rho$ with smooth boundary $\partial F_R$ preserved by $\rho$. Define

$$K(\Phi) = \frac{\int_{F_R} \Phi^* H}{e^{\frac{1}{2} \int_{F_R} \Phi^* H} \sqrt{e^{S_{WZ}(\phi|\partial F_R)}}}.$$  \hspace{1cm} (1.39)$$

**Proposition 3.** Under the same assumption as in Proposition 2, $K(\Phi)$ is independent of the choice of the fundamental domain $F_R$ and takes values $\pm 1$.

That $K(\Phi)^2 = 1$ follows from the definition of the WZ amplitudes. The proof of independence of the choice of $F_R$ is done by local changes of $F_R$ and the use of the local construction of $\sqrt{e^{S_{WZ}(\phi|\partial F_R)}}$ described in Sec.12 above. I do not know how to establish such independence without that construction (e.g. employing the definition of the square root of the WZ amplitude from Sec.13). It is at this point that the bundle gerbe theory shows its utility. Below, we shall consider index $K(\Phi)$ for $R = \mathbb{T}^3$ with $\rho$ induced by the map $k \mapsto -k$ in $\mathbb{R}^3$. In particular, for the map $\mathbb{T}^3 \ni k \mapsto \Phi(k) = I - 2P(k)$, where $P(k) = \Theta P(-k)\Theta^{-1}$ are projectors on the valence band states of a 3d time-reversal invariant insulator, we shall obtain the relation:

$$K(\Phi) = (-1)^{KM'},$$  \hspace{1cm} (1.40)$$

where $KM' \in \mathbb{Z}_2$ is the strong Kane-Mele invariant of such insulators [33].
We shall define the curving 2-form
\[ B \]
the homotopy
\[ Poincare \ \text{Lemma}: \]
should explain the origin of the notation. Note that
\[ H \]
−
\[ V \]
sub-interval of the unit circle joining \( e \)
are two projections from \( Y \) holding for \( \varepsilon \)
\[ G \]
\( Y \) is then an open subset of \( (-2\pi,0) \times U(N) \) and the projection \( \pi \) on the second component is clearly a surjective submersion. Then
\[ Y^\varepsilon = \{ (\varepsilon_1, \ldots, \varepsilon_n) \in (-2\pi,0)^n \times U(N) \mid e^{-i\varepsilon_i} \notin \text{spec}(V), \; i = 1, \ldots, n \}. \] (I.42)
Consider a smooth map from \( Y \) to the Lie algebra \( u(N) \) of Hermitian \( N \times N \) matrices,
\[ Y \ni (\varepsilon, V) \rightarrow i \ln_{-\varepsilon}(V) = H_{\varepsilon}^{\text{eff}}(V) \in u(N), \] (I.43)
where \( \ln_{\phi}(re^{i\varphi}) = \ln r + i\varphi \) for \( \phi - 2\pi < \varphi < \phi \) is a particular branch of the logarithmic function. More explicitly, if
\[ V = \sum_n \lambda_n |\psi_n\rangle \langle \psi_n| \] (I.44)
is the spectral decomposition of \( V \) then
\[ H_{\varepsilon}^{\text{eff}}(V) = i \sum_n \ln_{-\varepsilon}(\lambda_n) |\psi_n\rangle \langle \psi_n|. \] (I.45)
\( H_{\varepsilon}^{\text{eff}}(V) \) is a Hermitian matrix with the spectrum inside the interval \( (\varepsilon, \varepsilon + 2\pi) \), as is easy to see from the definition of \( \ln_{-\varepsilon} \). Moreover,
\[ V = e^{-iH_{\varepsilon}^{\text{eff}}(V)}, \] (I.46)
so that \( V \) may be considered as the time-one evolution operator corresponding to Hamiltonian \( H_{\varepsilon}^{\text{eff}} \), which should explain the origin of the notation. Note that \( H_{\varepsilon}^{\text{eff}}(V) \) is locally constant in \( \varepsilon \) for fixed \( V \). Let \( h \) be the homotopy
\[ [0,1] \times Y \ni (t, \varepsilon, V) \rightarrow h^t(\varepsilon, e^{-itH_{\varepsilon}^{\text{eff}}(V)}) \in Y. \] (I.47)
We shall define the curving 2-form \( B \) on \( Y \) such that \( dB = \pi^* H \) using this homotopy as in the proof of the Poincare Lemma:
\[ B = \int_0^1 (i\partial_t h^* \pi^* H) dt. \] (I.48)
Let us consider the closed 2-form \( F \) on \( Y^{[2]} \),
\[ F = p^*_2 B - p^*_1 B, \quad \text{where} \quad p_i(\varepsilon_1, \varepsilon_2, V) = (\varepsilon_i, V), \quad i = 1, 2 \] (I.49)
are two projections from \( Y^{[2]} \) to \( Y \). A direct calculation based on the relation
\[ H_{\varepsilon_2}^{\text{eff}}(V) = H_{\varepsilon_1}^{\text{eff}}(V) + 2\pi P_{\varepsilon_1, \varepsilon_2}(V), \] (I.50)
holding for \( \varepsilon_1 \leq \varepsilon_2 \), where \( P_{\varepsilon_1, \varepsilon_2}(V) \) is the spectral projector of \( V \) on the part of the spectrum in the sub-interval of the unit circle joining \( e^{-i\varepsilon_1} \) to \( e^{-i\varepsilon_2} \) clockwise if \( \varepsilon_1 < \varepsilon_2 \) and \( P_{\varepsilon, \varepsilon} = 0 \), gives:
\[ F(\varepsilon_1, \varepsilon_2, V) = i \text{tr} P_{\varepsilon_1, \varepsilon_2}(V)(dP_{\varepsilon_1, \varepsilon_2}(V))^\wedge 2 - \frac{1}{4} d \left( \text{tr} H_{\varepsilon_1}^{\text{eff}}(V) dP_{\varepsilon_1, \varepsilon_2}(V) \right). \] (I.51)
for $\epsilon_1 \leq \epsilon_2$. We need to construct a line bundle $\mathcal{L}$ over $Y^{[2]}$ with curvature $F$. Let us decompose:

\[ Y^{[2]}_+ = Y^{[2]}_+ \cup Y^{[2]}_0 \cup Y^{[2]}_0, \]

\[ Y^{[2]}_+ = \{(\epsilon_1, \epsilon_2, V) \in Y^{[2]} \mid \epsilon_1 < \epsilon_2, P_{\epsilon_1, \epsilon_2} \neq 0\}, \]

\[ Y^{[2]}_0 = \{(\epsilon_1, \epsilon_2, V) \in Y^{[2]} \mid \epsilon_2 \leq \epsilon_1, P_{\epsilon_2, \epsilon_1} = 0 \text{ or } \epsilon_1 \geq \epsilon_2, P_{\epsilon_1, \epsilon_2} = 0\}, \]

are disjoint open subsets of $Y^{[2]}$. Let $\sigma$ denote the map $(\epsilon_1, \epsilon_2, V) \mapsto (\epsilon_2, \epsilon_1, V)$ intertwining $Y^{[2]}_+$. There is a tautological vector bundle $\mathcal{E}$ (with dimension only locally constant, in general) over $Y^{[2]}_+$ whose fiber over $(\epsilon_1, \epsilon_2, V)$ is $P_{\epsilon_1, \epsilon_2}(V) \mathbb{C}^N$. We set

\[ \mathcal{L}|_{Y^{[2]}_+} = \text{det}(\mathcal{E}) \equiv \wedge^{\text{max}} \mathcal{E} \quad \text{and} \quad \mathcal{L}|_{Y^{[2]}_0} = (\sigma^* \mathcal{L}|_{Y^{[2]}_+})^{-1}, \quad \mathcal{L}|_{Y^{[2]}_0} = Y^{[2]} \otimes \mathbb{C}. \]

Vector bundle $\mathcal{E}$ has a Hermitian structure inherited from the scalar product in $\mathbb{C}^N$ and a unitary connection such that for its local section $S$,

\[ \nabla S(\epsilon_1, \epsilon_2, V) = P_{\epsilon_1, \epsilon_2}(V) dS(\epsilon_1, \epsilon_2, V), \]

Line bundle $\mathcal{L}|_{Y^{[2]}_0}$ inherits both these structures from $\mathcal{E}$. In particular, the induced connection on $\mathcal{L}$, that we shall denote by $\nabla^B$, is often called the Berry connection and has the (real) curvature 2-form

\[ F^B(\epsilon_1, \epsilon_2, V) = i \text{tr} P_{\epsilon_1, \epsilon_2}(V)(dP_{\epsilon_1, \epsilon_2}(V))^\wedge. \]

We shall correct connection $\nabla^B$ on $\mathcal{L}|_{Y^{[2]}_+}$ adding to it a 1-form $-iA$ on $Y^{[2]}_+$, where

\[ A(\epsilon_1, \epsilon_2, V) = \frac{i}{4} \text{tr} H^B_{\epsilon_1}(V)(dP_{\epsilon_1, \epsilon_2}(V)). \]

The corrected connection $\nabla^B - iA$ is then equal to the 2-form $F$ of line bundle $\mathcal{L}|_{Y^{[2]}_+}$ and the latter will be corrected by adding to it the form $i \sigma^* A$. Finally, the trivial line bundle $\mathcal{L}|_{Y^{[2]}_0}$ will be considered with the Hermitian structure inherited from $\mathbb{C}$ and with the trivial flat connection.

We have to define isomorphisms

\[ t : p_1^{*2} \mathcal{L} \otimes p_2^{*2} \mathcal{L} \rightarrow p_1^{*3} \mathcal{L} \]

of line bundles over $Y^{[3]}$, where $p_{ab}(\epsilon_1, \epsilon_2, \epsilon_3, V) = (\epsilon_a, \epsilon_b, V)$. There will be several cases of which nontrivial are only the ones when $-2\pi < \epsilon_a < \epsilon_b < \epsilon_c < 0$ for some permutation of $(\epsilon_1, \epsilon_2, \epsilon_3)$ and $P_{\epsilon_a, \epsilon_c}(V) \neq 0 \neq P_{\epsilon_b, \epsilon_c}(V)$. Let $(u_1, \ldots, u_k)$ be an orthonormal basis of the range of $P_{\epsilon_a, \epsilon_c}(V)$ and $(u_{k+1}, \ldots, u_{k+l})$ an orthonormal basis of the range of $P_{\epsilon_b, \epsilon_c}(V)$. Then $(u_1, \ldots, u_{k+l})$ is an orthonormal basis of the range of $P_{\epsilon_a, \epsilon_c}(V)$. We shall denote by $(u_1 \wedge \cdots \wedge u_k)^{-1}$ the element of the dual line $\left(\wedge^{\text{max}} P_{\epsilon_a, \epsilon_c}(V) \mathbb{C}^N\right)^{-1}$ that pairs to 1 with $u_1 \wedge \cdots \wedge u_k$, etc., and set

\[
\begin{align*}
    t((u_1 \wedge \cdots \wedge u_k) \otimes (u_{k+1} \wedge \cdots \wedge u_{k+l})) &= u_1 \wedge \cdots \wedge u_{k+l} & \text{for } \epsilon_1 < \epsilon_2 < \epsilon_3, \\
    t((u_{k+1} \wedge \cdots \wedge u_{k+l})^{-1} \otimes (u_1 \wedge \cdots \wedge u_k)^{-1}) &= (u_1 \wedge \cdots \wedge u_k)^{-1} & \text{for } \epsilon_3 < \epsilon_2 < \epsilon_1, \\
    t((u_1 \wedge \cdots \wedge u_k) \otimes (u_{k+1} \wedge \cdots \wedge u_{k+l})^{-1}) &= u_1 \wedge \cdots \wedge u_k & \text{for } \epsilon_1 < \epsilon_2 < \epsilon_3, \\
    t((u_{k+1} \wedge \cdots \wedge u_{k+l})^{-1} \otimes (u_1 \wedge \cdots \wedge u_k)^{-1}) &= (u_1 \wedge \cdots \wedge u_k)^{-1} & \text{for } \epsilon_3 < \epsilon_2 < \epsilon_1, \\
    t((u_1 \wedge \cdots \wedge u_k) \otimes (u_{k+1} \wedge \cdots \wedge u_{k+l})) &= u_{k+1} \wedge \cdots \wedge u_{k+l} & \text{for } \epsilon_2 < \epsilon_3 < \epsilon_1, \\
    t((u_{k+1} \wedge \cdots \wedge u_{k+l})^{-1} \otimes (u_1 \wedge \cdots \wedge u_k)) &= (u_1 \wedge \cdots \wedge u_k) & \text{for } \epsilon_3 < \epsilon_2 < \epsilon_1.
\end{align*}
\]

It is easy to see that the isomorphism $t$ defined this way intertwines the Hermitian structures and the Berry connections. The following lemma shows that it intertwines also the connections modified by the addition of 1-forms $t^*iA$:

**Lemma.** For $(\epsilon_1, \epsilon_2, \epsilon_3, V) \in Y^{[3]}$ and $-2\pi < \epsilon_a < \epsilon_b < \epsilon_c < 0$,

\[ A(\epsilon_a, \epsilon_b, V) + A(\epsilon_b, \epsilon_c, V) = A(\epsilon_a, \epsilon_c, V). \]

It is easy, although somewhat tedious, to check that the isomorphism $t$ is associative. Such check completes the construction of a basic gerbe $\mathcal{G} = (Y, B, \mathcal{L}, t)$ over $U(N)$. 

I. Towards time-reversal equivariant basic gerbe over $U(N)$

Recall that $\Theta$ acts on $U(N)$ for $N$ even by conjugation with the anti-unitary map $\theta$ of $\mathbb{C}^N$ such that $\theta^2 = -I$. We would like to construct a $\Theta$-equivariant structure on the basic gerbe $\mathcal{G}$ over $U(N)$. In the first step, we need to obtain a 1-isomorphism $\eta : \mathcal{G} \to \Theta^*\mathcal{G}$. Define the involution $\Theta_Y : Y \to Y$ covering $\Theta$ by

$$\Theta_Y(\epsilon, V) = (-\epsilon - 2\pi, \Theta(V)).$$

(I.68)

The pullback gerbe $\Theta^*\mathcal{G}$ is represented by the quadruple $(Y, \Theta_Y^*\mathcal{G}, (\Theta_Y^*)^*\mathcal{L}, (\Theta_Y^*)^*t)$. If the spectral decomposition of $V$ is given by (1.44) then

$$\Theta(V) = \sum_n \overline{\lambda_n} \theta |\psi_n\rangle \langle \psi_n| \theta^{-1}$$

(I.69)

is the spectral decomposition of $\Theta(V)$. In particular, the spectrum of fixed points of $\Theta$ is symmetric under $\lambda \mapsto \bar{\lambda}$. Relation $\ln \epsilon_{\lambda} = -\ln \epsilon_{\lambda + 2\pi}$ implies that:

$$\theta H^\text{eff}_\epsilon(V) \theta^{-1} = \sum_n \ln \epsilon_{\lambda_n} \theta |\psi_n\rangle \langle \psi_n| \theta^{-1} = -\sum_n \ln \epsilon_{\lambda_n} \theta |\psi_n\rangle \langle \psi_n| \theta^{-1} = -H^\text{eff}_{-\epsilon-2\pi}(\Theta(V)).$$

(I.70)

Using this identity, it is straightforward to check that $\Theta_Y^*\mathcal{G} = B$.

Now, it is easy to see that line bundles $\mathcal{L}$ and $(\Theta_Y^*)^*\mathcal{L}$ over $Y^2$ are isomorphic. Since

$$\Theta_Y^2(\epsilon_1, \epsilon_2, V) = (-\epsilon_1 - 2\pi, -\epsilon_2 - 2\pi, \Theta(V)),$$

it follows that $\Theta_Y^2$ intertwines the subsets $Y^2$ and leaves $Y_0^2$ invariant. If $(\epsilon_1, \epsilon_2, V) \in Y^2_0$ and $(u_1, \ldots, u_k)$ is an orthonormal basis of the range of $P_{\epsilon_1, \epsilon_2}(V)$ then $(\theta u_1, \ldots, \theta u_k)$ is an orthonormal basis of the range of $P_{-\epsilon_2, -\epsilon_1}(\Theta(V))$. Similarly, if $(\epsilon_1, \epsilon_2, V) \in Y^2_0$ and $(u_1, \ldots, u_k)$ is an orthonormal bases of the range of $P_{\epsilon_2, \epsilon_1}(V)$ then $(\theta u_1, \ldots, \theta u_k)$ is an orthonormal basis of $P_{-\epsilon_2, -\epsilon_1}(\Theta(V))$.

The line bundle isomorphism $\nu : \mathcal{L} \to (\Theta_Y^2)^*\mathcal{L}$ (linear on fibers) defined by

$$\nu(u_1 \wedge \cdots \wedge u_k) = (\theta u_k \wedge \cdots \wedge \theta u_1)^{-1} \quad \text{for} \quad (\epsilon_1, \epsilon_2, V) \in Y^2_0,$$

(I.72)

$$\nu(u_1 \wedge \cdots \wedge u_k)^{-1} = (\theta u_k \wedge \cdots \wedge \theta u_1) \quad \text{for} \quad (\epsilon_1, \epsilon_2, V) \in Y^2_0,$$

(I.73)

and by identifying the trivial bundles over $Y^2_0$, intertwines the Hermitian structures and the Berry connections. It also intertwines the corrected connections as follows from the the relation

$$(\Theta_Y^2)^*(-\sigma^*A) = A$$

(I.74)

that holds on $Y^2$. It is straightforward to check that $\nu$ intertwines the groupoid multiplications $t$ and $(\Theta_Y^2)^*t$ (the change of the order of vectors in $Y^2$ and $Y^2_0$ is essential here). We infer that isomorphism $\nu$ together with a trivial bundle $N$ over $Y$ defines a 1-isomorphism $\eta : \mathcal{G} \to \Theta^*\mathcal{G}$.

Let us observe that

$$(\Theta_Y^2)^*\nu \circ \nu = (-1)^{\kappa} \text{Id}_\mathcal{L},$$

(I.75)

where $\kappa(\epsilon_1, \epsilon_2, V)$ is equal to the dimension of the range of $P_{\epsilon_1, \epsilon_2}(V)$ on $Y_0^2$ and of $P_{\epsilon_2, \epsilon_1}(V)$ on $Y_0^2$ and vanishes on $Y^2_0$. The sign in (1.75) is induced by the action of $\theta^2 = -I$. As discussed in Sec. I.E, 1-isomorphism $\Theta^*\eta \circ \eta : \mathcal{G} \to \mathcal{G}$ corresponds to a flat line bundle $Q$ over $U(N)$. We may take

$$Q = (Y \times \mathbb{C})/\sim$$

(I.76)

where $\sim$ is the equivalence relation

$$(\epsilon_1, V, z_1) \sim (\epsilon_2, V, z_2) \quad \text{if} \quad z_2 = (-1)^{k(\epsilon_1, \epsilon_2, V)} z_1.$$

Elements of $Q$ will be denoted $[\epsilon, V, z]$. Projection $\pi_Q : Q \to U(N)$ forgets $\epsilon$ and $z$. Line bundle $Q$ comes with the involution $\Theta_Q$,

$$\Theta_Q([\epsilon, V, z]) = ([\epsilon - 2\pi, \Theta(V), z])_\sim,$$

(I.78)
that is linear on the fibers and covers involution $\Theta$.

Now, 1-isomorphism $\Theta^*\eta \circ \eta$ is 2-isomorphic to a trivial one if and only if the flat line bundle $Q$ is trivializable. This holds if and only if the holonomy of $Q$ along the loop

$$[0, 2\pi] \ni \varphi \mapsto V(\varphi) = \text{diag}(e^{i\varphi}, 1, \ldots, 1)$$

in $U(N)$ is equal to 1. Indeed, the above loop is a generator of $\pi_1(U(N)) \cong \mathbb{Z}$ (the latter isomorphism is given by the winding number of the determinant). Consider

$$W(\varphi) = \begin{cases} [-\frac{4\pi}{\varphi}, V(\varphi), 1] & \text{if } \varphi \in [0, \pi], \\ [-\frac{4\pi}{\varphi}, V(\varphi), -1] & \text{if } \varphi \in [\pi, 2\pi]. \end{cases}$$

$$[0, 2\pi] \ni \varphi \mapsto W(\varphi)$$

is a horizontal lift to $Q$ of the loop $V(\varphi)$. Since $W(2\pi) = -W(0)$, it follows that the holonomy of $Q$ along the loop (I.70) is equal to $-1$ so that $Q$ is not trivializable. Consequently, 1-isomorphism $\Theta^*\eta \circ \eta : \mathcal{G} \to \mathcal{G}$ is not 2-isomorphic to the identity 1-isomorphism. A choice of a different 1-isomorphism $\eta : \mathcal{G} \to \mathcal{G}$ would change the flat line bundle $Q$ by a tensor factor $\Theta^*Q \otimes \hat{Q}$ for some flat bundle $\hat{Q}$ over $U(N)$ and would not change the holonomy along loop (I.79). We conclude that there is no $\Theta$-equivariant structure on the basic gerbe $\mathcal{G}$ on $U(N)$! Note however that the holonomy of flat line bundle $Q$ squares to 1.

**Remark.** In the case when $\theta^2 = I$, the same construction gives 1-isomorphism $\Theta^*\eta \circ \eta$ coinciding with $\text{Id}_\mathcal{G}$ so that the $\Theta$-equivariant structure on $U(N)$ does exist in that case.

**J. Lift to the double cover of $U(N)$**

A possible way out from the difficulty encountered in the previous section is to pass to the double cover $\tilde{U}(N)$ of group $U(N)$,

$$\tilde{U}(N) = \{(V, \omega) \in U(N) \times U(1) \mid \omega^2 = \det(V)\}$$

with covering map $\tilde{\pi} : \tilde{U}(N) \to U(N)$ forgetting $\omega$. Let us denote by $\hat{\Theta}$ the involution

$$(V, \omega) \mapsto (\Theta(V), \omega^{-1})$$

of $\tilde{U}(N)$, by $\hat{Q}$ the pullback $\tilde{\pi}^*Q$ of line bundle $Q$ of (I.76) to $\tilde{U}(N)$ and by $\hat{\Theta}_Q$ the pullback $\tilde{\pi}^*\Theta_Q$ of the involution $\Theta_Q$ of (I.78) that is explicitly given by the relation

$$\hat{\Theta}_Q((V, \omega), [\epsilon, V, z]) = ((\Theta(V), \omega^{-1}), [-\epsilon - 2\pi, \Theta(V), z]).$$

$\hat{\Theta}_Q$ is an involution of $\hat{Q}$ linear on fibers that covers $\hat{\Theta}$.

Unlike $Q$, the flat line bundle $\hat{Q}$ possesses global section $\hat{S}$ given by the formula

$$\hat{S}(V, \omega) = ((V, \omega), [\epsilon, V, \omega \det(e^{\mp H^\text{eff}}(V))]).$$

An easy check based on relation (I.50) shows that the equivalence class on the right hand side is well defined. Since $\langle \omega \det(e^{\mp H^\text{eff}}(V)) \rangle^2 = 1$, it follows that section $\hat{S}$ is flat and normalized. Besides

$$\hat{\Theta}_Q \circ \hat{S}(V, \omega) = ((\Theta(V), \omega^{-1}), [-\epsilon - 2\pi, \Theta(V), \omega \det(e^{\mp H^\text{eff}}(V))])$$

$$\quad = ((\Theta(V), \omega^{-1}), [-\epsilon - 2\pi, \Theta(V), \omega^{-1} \det(e^{\mp H^\text{eff}}(V))])$$

$$\quad = ((\Theta(V), \omega^{-1}), [-\epsilon - 2\pi, \Theta(V), \omega^{-1} \det(e^{\mp H^\text{eff}}(\Theta(V))]) = S(\Theta(V), \omega^{-1}),$$

where the last but one equality is a consequence of (I.70).

It follows that, although there is no $\Theta$-equivariant structure on the basic gerbe $\mathcal{G}$ over $U(N)$, there is a $\tilde{\Theta}$-equivariant structure on the pullback gerbe $\tilde{\mathcal{G}} = \tilde{\pi}^*\mathcal{G}$ over $\tilde{U}(N)$. Indeed, $\tilde{\eta} = \tilde{\pi}^*\eta$ provides a 1-isomorphism $\tilde{\eta} : \tilde{\mathcal{G}} \to \tilde{\pi}^*\Theta^*\mathcal{G} = \tilde{\Theta}^*\mathcal{G}$ and the trivializing section $\tilde{S}$ of the flat line bundle $\hat{Q}$ defines a 2-isomorphisms $\hat{\mu} : \tilde{\Theta}^*\hat{\eta} \circ \hat{\Theta}_Q \Rightarrow \text{Id}_{\hat{Q}}$. Relation (I.85) assures that condition (I.23) holds for $\hat{\mu}$.
The set $U(N)'$ of $\Theta$-invariant points of $U(N)$ is a closed subgroup conjugate to group $Sp(N)$, which is connected and simply connected. In particular, $\det(V) = 1$ for $V \in U(N)'$. This implies that the subset $\bar{U}(N)'$ of $\tilde{\Theta}$-invariant points in $\tilde{U}(N)$ coincides with the subgroup $U(N)' \times \{ \pm 1 \}$ that is simply connected but has two connected components that we shall accordingly denote $\bar{U}(N)'_\pm \cong U(N)'$. It follows that the restriction of section $\bar{\rho}' = \bar{\rho}|_{\bar{U}(N)'}$ to $\bar{U}(N)'_\pm$ may be identified with the sections $\bar{\rho}'_\pm$ of bundle $Q' = Q|_{U(N)'}$ defined by

$$U(N)' \ni V \mapsto [\epsilon, V, \pm \det(e^{\frac{1}{2} H_{\rho}'})]_\pm.$$  \hfill (I.86)

Suppose now that $\phi : \Sigma \mapsto U(N)$ is an equivariant map, i.e. that relation (I.6) holds for it. For $\Sigma$ which is a 2-torus or a hyperelliptic curve with involutions $\vartheta$ described before, one may choose a base of 1-homology of $\Sigma$ composed of loops that are invariant under $\vartheta$, up to the orientation change, and each containing two fixed points of $\vartheta$, see Fig.\textit{4}.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig4.png}
\caption{Closed surface $\Sigma$ of genus $g = 3$ with fundamental domain $F$ for orientation preserving involution $\vartheta$ with $8 = 2g + 2$ fixed points marked as black dots}
\end{figure}

Determinant of field $\phi$ satisfies the relation

$$\det(\phi(\vartheta x)) = \det(\Theta \circ \phi(x)) = \det(\phi(x))^{-1}$$  \hfill (I.87)

and $\det(\phi(x)) = 1$ at fixed points of $\vartheta$. It follows that $\det \circ \phi$ has even winding numbers around the homology 1-cycles of $\Sigma$. As the result, $\phi$ may be lifted to a map $\hat{\phi} : \Sigma \to \tilde{U}(N)$. The lift is unique up to a multiplication by $(I, -1) \in \tilde{U}(N)$. Besides, it is still equivariant:

$$\hat{\vartheta} \circ \hat{\phi} = \hat{\Theta} \circ \hat{\phi}$$  \hfill (I.88)

because this property holds at fixed points of $\vartheta$. We may then define

$$\sqrt{\det(\phi)} = \sqrt{\det(\phi)} = \sqrt{\text{Hol}_\vartheta(\hat{\phi})},$$  \hfill (I.89)

where the right hand side is determined using the $\hat{\Theta}$-equivariant structure on $\tilde{U}(N)$, see Sec.\textit{4}. Some care is needed, however.

First, the subset $\tilde{U}(N)'$ of fixed points of $\hat{\Theta}$, although simply connected, is disconnected. As the result, we may multiply the trivializing section $\sqrt{S}$ of line bundle $\tilde{N}'$ (that is the pullback to $\tilde{U}(N)'$ of line bundle $N'$ over $U(N)'$ by $\pm 1$ chosen differently on two components of $\tilde{U}(N)'$). For vertices $\nu$ at the two ends of a connected component of $\ell \subset \partial F$, see Fig.\textit{4} the lifted field $\hat{\rho}$ takes values in the same component of $\tilde{U}(N)'$ if $\det \circ \phi$ winds an even number of times around zero along that component and in different components if it winds an odd number of times. Hence, the changes of sign in section $\sqrt{S}$ described above result in the multiplication of $\sqrt{\text{Hol}_\vartheta(\hat{\phi})}$ defined by (I.37) by $(-1)^w$ where $w$ is the total winding number of $\det \circ \phi$ along $\ell$. Note, however, that $2w$ is the total winding number of $\det \circ \phi$ along the boundary $\partial F$ of the fundamental domain $F \subset \Sigma$ and the latter is necessarily equal to zero. We infer that even if the fixed point set $\tilde{U}(N)'$ is not connected, $\sqrt{\text{Hol}_\vartheta(\hat{\phi})}$ defined by (I.37) does not depend on the choice of section $\sqrt{S}$.

Second, we should show that $\sqrt{\text{Hol}_\vartheta(\hat{\phi})}$ does not depend on the choice of the lift $\hat{\phi}$ of $\phi$ to $\tilde{U}(N)$. Indeed, $\sqrt{\text{Hol}_\vartheta(\hat{\phi})}$ calculated for a different lift is equal to the one for the original lift but obtained using
the \( \hat{\Theta} \)-equivariant structure of \( \hat{G} \) with 2-isomorphism \( \hat{\mu} \) corresponding to section \( -\hat{S} \) of line bundle \( \hat{Q} \) and to section \( i\sqrt{S'} \) of line bundle \( \hat{N}' \). Such modification does not change the phase associated to the left hand side of (1.37) as the additional factors in \( \sqrt{S'(\phi(v))^\pm 1} \) from the ends of each connected component of \( \ell \) cancel each other (note that this would be also the case if we multiplied \( \hat{S} \) by any phase). As the result, square root of the WZ amplitudes of equivariant maps \( \phi \) is uniquely defined by formula (1.89) for the special type of surfaces with involution \( (\Sigma, \vartheta) \) considered above.

**Remark.** The construction described above would not work for surfaces with involution like in Fig. 4 but with an additional handle inside \( F' \) and its \( \vartheta \)-image.

We shall need a more explicit description of section \( \sqrt{S'} \) trivializing the flat line bundle \( \hat{N}' \). Let us look first at the line bundle \( \mathcal{N}' \) over \( U(N)' \) whose pullback to \( Y' \) may be identified with the bundle \( \mathcal{N}' = U(N)' \). We shall suppose below that \( -\epsilon - 2\pi < \epsilon \). Then

\[
\mathcal{N}'_{(\epsilon, V)} = \mathcal{L}_{(-\epsilon - 2\pi, \epsilon, V)} \otimes \mathcal{N}_{(\epsilon, V')} = \wedge^{\max} P_{-\epsilon - 2\pi, V}(V) \mathbb{C}^N
\]

(1.90)

for \( V \in U(N)' \) and the bundle isomorphism \( \nu' : \mathcal{N}' \to \Theta^*_Y \mathcal{N}' \) is given by

\[
\mathcal{N}'_{(\epsilon, V)} \ni (u_1 \wedge \cdots \wedge u_m) \mapsto (\theta u_m \wedge \cdots \wedge \theta u_1)^{-1} \in \mathcal{N}'_{(-\epsilon - 2\pi, V)},
\]

(1.91)

where \( (u_1, \ldots, u_m) \) is an orthonormal basis of the range of \( P_{-\epsilon - 2\pi, V}(V) \) (\( m \) is necessarily even). The map (1.39) takes the form

\[
\mathcal{N}'_{(\epsilon, V)} \otimes \mathcal{N}'_{(\epsilon, V')} \ni (u_1 \wedge \cdots \wedge u_m) \otimes (u_1' \wedge \cdots \wedge u_m') \mapsto (\theta u_m \wedge \cdots \wedge \theta u_1)^{-1} \otimes (u_1' \wedge \cdots \wedge u_m')
\]

\[
\mapsto (-1)^{m/2} \det\langle u_i|\theta u_j\rangle^{-1}.
\]

(1.92)

and induces the line bundle isomorphism \( \mathcal{N}' \otimes \mathcal{N}' \to Q' \). The restriction of the section \( \sqrt{S'} \) of line bundle \( \hat{N}' \) to \( \hat{U}(N)' \) may be identified with the section \( \sqrt{S'_\pm} \) of line bundle \( N' \) obtained from the assignment

\[
U(N)' \ni V \mapsto \sigma \text{pf}(\langle u_i|\theta u_j\rangle) u_1 \wedge \cdots \wedge u_m \in \mathcal{N}'_{(\epsilon, V)}
\]

(1.93)

where \( \sigma^2 = \pm 1 \) for \( \sqrt{S'_\pm} \) and \( \text{pf}(\cdot) \) stands for the Pfaffian of an antisymmetric matrix. It is somewhat tedious but straightforward to check that, indeed, (1.93) defines a section \( \sqrt{S'_\pm} \) of \( N' \). Besides, under the line bundle isomorphism \( \mathcal{N}' \otimes \mathcal{N}' \to Q' \) induced by (1.92)

\[
\sqrt{S'_\pm}(V) \otimes \sqrt{S'_\pm}(V) \mapsto [\epsilon, V, \pm(-1)^{m/2}], = S'_\pm(V),
\]

(1.94)

where the last equality follows from (1.86) and the relation \( \det(\text{e}^{4\pi \text{det}(\mathcal{V}')} - (\pm 1)^{m/2} \text{hol}_{\mathcal{Q'}}(\phi(v)) \) holding for \( V \in U(N)' \) that is easy to check. Formula (1.92) provides an explicit description of the trivializations \( \sqrt{S'_\pm} \) of line bundle \( N' \) and, in the final count, of \( \sqrt{\text{Hol}_{\mathcal{Q'}}(\phi)} \) which ends up as given by the formula

\[
\sqrt{\text{Hol}_{\mathcal{Q'}}(\phi)} \otimes \text{hol}_{\mathcal{N}'}(\phi(v)) = \sqrt{\text{Hol}_{\mathcal{Q'}}(\phi)} \otimes_{\epsilon \in \theta\mathcal{E}} \sqrt{S'_\pm(\phi(v))^\pm 1},
\]

(1.95)

where the signs in \( \sqrt{S'_\pm} \) have to be chosen consistently with the winding of \( \det \phi \), as discussed above. This is the only modification with respect to formula (1.37).

It is not difficult to show by studying the evolution of the left hand side of (1.37) under smooth changes of \( \phi \) that, for \( \Sigma = \mathbb{T}^2 \) with \( \vartheta k = -k \), the square root of the WZ amplitude defined by (1.86) coincides with the one defined in Sec. I.B via a 3d integral.

In a similar way as for the square root of the WZ amplitude discussed above, one may define the 3d index \( K(\Phi) \) of an equivariant map to \( U(N) \) from a 3d torus with the orientation reversing involution induced by the map \( k \mapsto -k \). One just sets \( K(\Phi) = K(\Phi_+) \), where \( \Phi_+ \) is one of the two lifts of \( \Phi \) to \( \hat{U}(N) \). The independence on the choice of the lift follows from the similar property for the square root of WZ amplitudes on 2d tori, at least when the fundamental domain \( F_\mathcal{R} \) chosen for the calculation of \( K(\Phi_+) \) has the boundary composed of two 2-dimensional tori. We shall extensively use such 3d index in Lecture 2.

**Remark.** Although the time-reversal symmetry with \( \vartheta^2 = I \) gives rise to a \( \Theta \)-equivariant structure on the basic gerbe \( \mathcal{G} \) over \( U(N) \), the fixed point subgroup \( U(N)' \) is conjugate to group \( O(N) \) here and is neither connected nor simply connected. The square root of the WZ amplitudes of equivariant maps is not well defined in this case.
II. LECTURE 2. APPLICATIONS TO TOPOLOGICAL INSULATORS

A. Crystalline systems and Bloch theory

We shall be interested in properties of condensed matter systems with crystalline symmetry. The simplest models of such systems have the space of states

\[ \mathcal{H} = L^2(\mathcal{C}, \mathcal{V}), \]  

(II.1)

where \( \mathcal{C} \), a “crystal”, is an infinite discrete subset of \( d \)-dimensional Euclidean space \( \mathbb{E}^d \) symmetric under a group \( \Gamma \cong \mathbb{Z}^d \) of discrete translations (the “Bravais lattice”) and \( \mathcal{V} \) is a finite-dimensional Hilbert space of internal degrees of freedom (like spin).

\[ \Gamma = \left\{ \sum_{i=1}^{d} n_i a_i \mid n_i \in \mathbb{Z} \right\}, \]  

(II.2)

where \( a_i \) are \( d \) linearly independent vectors in \( \mathbb{R}^d \). The action of \( \Gamma \) on \( \mathcal{C} \) induces a representation of \( \Gamma \) in the space of states by the formula \( (U_a \psi)(x) = \psi(x - a) \) for \( x \in \mathcal{C} \) and \( a \in \Gamma \). The Fourier transform \( \psi \mapsto \hat{\psi} \) over \( \Gamma \),

\[ \hat{\psi}_k(x) = \sum_{a \in \Gamma} e^{-ik \cdot a} \psi(x - a) \]  

(II.3)

for \( k \in \mathbb{R}^d \), takes values in Bloch functions satisfying the twisted periodic conditions \( \hat{\psi}_k(x - a) = e^{ik \cdot a} \hat{\psi}_k(x) \). Note that \( \psi_k(x) = \psi_{k+b}(x) \) for \( b \in 2\pi \Gamma^* \cong \Gamma^* \), the “reciprocal lattice”. The inverse formula states that

\[ \psi(x) = \frac{1}{|BZ|} \int_{BZ} \hat{\psi}_k(x) \, dk, \]  

(II.4)

where \( BZ = \mathbb{R}^d / \Gamma^* \cong \mathbb{T}^d \) is the “Brillouin torus” and \( |BZ| \) denotes its Euclidean volume. The set of Bloch functions for fixed \( k \) forms a finite-dimensional Hilbert space \( \hat{\mathcal{H}}_k = \hat{\mathcal{H}}_{k+b} \) with the norm squared

\[ \| \hat{\psi}_k \|^2 = \sum_{x \in \mathcal{F}} |\hat{\psi}_k(x)|^2 \]  

(II.5)

where \( \mathcal{F} \subset \mathcal{C} \) is an arbitrary unit cell of the crystal having exactly 1 representative in each coset of \( \mathcal{C} / \Gamma \), see Fig.5. The Plancherel formula states that

\[ \sum_{x \in \mathcal{C}} |\psi(x)|^2 = \frac{1}{|BZ|} \int \| \hat{\psi}_k \|^2 \, dk. \]  

(II.6)
Restriction of Bloch functions to a fixed unit cell $\mathcal{F}$ provides an identification $\mathcal{H}_k \cong L^2(F, \mathcal{V}) \cong \mathbb{C}^N$, where $N = |\mathcal{F}| \times \dim(\mathcal{V})$. Hence the Fourier transform may be viewed as a unitary isomorphism

$$L^2(\mathcal{C}, \mathcal{V}) \cong L^2(BZ, \mathbb{C}^N)$$ \hspace{1cm} (II.7)

sending $\mathcal{V}$-valued functions $\psi(x)$ on $\mathcal{C}$ to $\mathbb{C}^N$-valued functions $\hat{\psi}(k)$ on $BZ$. Compactly supported functions on $\mathcal{C}$ correspond to analytic functions on $BZ$ and the action of $U(a)$ becomes the multiplication by $e^{ik\cdot a}$.

Time evolution of the crystalline system is governed by a Hamiltonian $H_c$

$$(H_c \psi)(x) = \sum_{y \in \mathcal{C}} h(x, y) \psi(y)$$ \hspace{1cm} (II.8)

where $h(x, y) \in \text{End}(\mathcal{V})$ are assumed to vanish for $|y - x| > r$ for some fixed range $r > 0$. We also assume that $h(x, y) = h(x + a, y + a)$ for $a \in \Gamma$ so that $[H_c, U(a)] = 0$. Under isomorphism (II.7), Hamiltonian $H_c$ becomes a family of Hermitian $N \times N$ matrices $\hat{H}(k)$ analytically depending on $k \in BZ$. Diagonalization of $\hat{H}(k)$ leads to energy bands $e_n(k)$ (that generically avoid crossing) such that

$$\hat{H}(k) \hat{\psi}_n(k) = e_n(k) \hat{\psi}_n(k).$$ \hspace{1cm} (II.9)

$E \in \text{spec}(H_c)$ if and only if $E = e_n(k)$ for some $n$ and $k$, see Fig. 6. We shall be interested in insulators

![Energy bands](image_url)

where Hamiltonian $H_c$ has a spectrum gap around the Fermi energy $\epsilon_F$. The bands with energies smaller than $\epsilon_F$ are called valence bands and the ones with energies bigger than $\epsilon_F$ are termed conduction bands. Below, we shall always assume that the Fermi energy $\epsilon_F = 0$. This may be achieved by subtracting non-zero $\epsilon_F$ from Hamiltonian $H_c$.

### B. Chern insulators and their homotopic invariant

Consider a crystalline insulator in two dimensions. The simplest topological invariant of $2d$ insulators is the 1$^{st}$ Chern number

$$c_1 = \frac{i}{2\pi} \int_{BZ} \text{tr} P(k) \left( dP(k) \right)^2,$$ \hspace{1cm} (II.10)

where $P(k)$ are the spectral projections of the Bloch Hamiltonians $\hat{H}(k)$ on the negative eigenvalues (i.e. on the valence band energies). Geometrically, $c_1$ is the 1$^{st}$ Chern number of the valence band sub-bundle $\mathcal{E}$ of the trivial bundle $BZ \times \mathbb{C}^N$ over the Brillouin torus whose fibers are spanned by the valence band eigenstates.

---

3 This eliminates external magnetic field so e.g. the Harper-Hofstadter model.

4 This is the energy such that the ground state of the second-quantized systems has all states with energy $< \epsilon_F$ occupied and all states with energy $> \epsilon_F$ empty.
of $\hat{H}(k)$. The 1st Chern number is equal to the integral of the trace of the curvature of the Berry connection $\nabla^B$ on the sub-bundle $E$ divided by $2\pi$. It is an integer that is constant under continuous deformations of Hamiltonian $H_c$ which do not close the spectral zero-energy gap.

A simple example is provided by Hamiltonians

$$\hat{H}(k) = \tilde{d}(k) \cdot \hat{\sigma}$$  \hspace{1cm} (II.11)

for $N = 2$, where $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices. Spectrum of $\hat{H}(k)$ is composed of $\pm |\tilde{d}(k)|$. In particular, for $|\tilde{d}(k)|$ not vanishing on $BZ$, the model describes an insulator. The 1st Chern number is in this case equal to the degree of the map

$$BZ \ni k \mapsto \frac{\tilde{d}(k)}{|\tilde{d}(k)|} \in S^2.$$  \hspace{1cm} (II.12)

One of the simplest models with nontrivial $c_1$ was proposed by Haldane [24]. It lives on the hexagonal crystal of Fig. 5 and has the tight binding Hamiltonian

$$H_c = t \sum_{n.n.} |x\rangle\langle y| \pm i t_2 \sin(\varphi) \sum_{n.n.n} |x\rangle\langle y| + M \sum_{x \in A} |x\rangle\langle x| - M \sum_{x \in B} |x\rangle\langle x|,$$  \hspace{1cm} (II.13)

where $n.n.$ denotes the nearest neighbors and $n.n.n.$ the next nearest neighbors $(x, y) \in C^2$, and $A$ and $B$ denote two orbits of $\Gamma$ in $C$. The signs in front of the $n.n.n.$ terms are chosen as plus if $x \in A$ and $y = x + a_1$, $y = x - a_1 + a_2$, and $y = x - a_2$, and if $x \in B$ and $y = x - a_1$, $y = x + a_1 - a_2$, and $y = x + a_2$. In the other half of cases the sign is chosen as minus. In the Fourier transformed picture, $H_c$ becomes a family of Hermitian matrices (II.11) with

$$d_x = t (1 + \cos(k \cdot a_1) + \cos(k \cdot k_2)), \quad d_y = t (\sin(k \cdot a_1) + \sin(k \cdot a_2)),$$  \hspace{1cm} (II.14)

$$d_z = M + 2t_2 \sin(\varphi) (\sin(k \cdot a_1) - \sin(k \cdot a_1 - k \cdot a_2) - \sin(k \cdot a_2)).$$  \hspace{1cm} (II.15)

The phase diagram of 1st Chern numbers is given in Fig. 7.

![FIG. 7: Phase diagram of the Haldane model (from [25])](image)

Numbers $c_1$ are obtained by counting with signs the points in $BZ$ where $\tilde{d}(k)$ lies along the positive $z$-axis. Such count may be viewed as a localization of the integral formula (II.10).

The 1st Chern number may be also obtained from a 3d integral. Let

$$\Phi(t, k) = e^{2\pi i P(k)} = e^{2\pi i P(k)} + I - P(k).$$  \hspace{1cm} (II.16)

Note that $\Phi(t, k)$ are unitary matrices and that $\Phi(0, k) = I = \Phi(1, k)$ so that $\Phi$ may be viewed as a map from a 2-sphere $S^2$ to the group $U(N)$ for which one may consider the homotopic invariant

$$\deg(\Phi) \equiv \frac{1}{2\pi} \int_{[0,1] \times BZ} \Phi^* H \in \mathbb{Z},$$  \hspace{1cm} (II.17)
where $H$ is the same bi-invariant 3-form on $U(N)$ as before (not to be confused with the crystalline Hamiltonian $H_c$). A small calculation performing the $t$-integral shows that

$$\text{deg}(\Phi) = \frac{i}{2\pi} \int_{BZ} \text{tr} P(k) \left( dP(k) \right)^{\wedge 2} = c_1.$$  \hspace{1cm} (II.18)

**Remark.** Formula (II.18) is a realization of the Bott isomorphism $\tilde{K}^0(BZ) \cong \tilde{K}^1(SBZ)$ between the $K$-theory groups, where $SM$ is the suspension of space $M$.

### C. Time reversal symmetry and the 2d Kane-Mele invariant

Consider now the time reversal anti-unitary operator $\theta$ acting on the space of internal degrees of freedom $\mathcal{V}$ such that $\theta^2 = \pm I$. It acts point-wise on the wave functions $\psi(x) \in L^2(C, \mathcal{V})$ and becomes under the Fourier transform (II.7) the operator

$$\hat{\psi} \mapsto \theta \hat{\psi} \circ \vartheta,$$

where $\theta$ is viewed now as the anti-unitary operator in $L^2(F, \mathcal{V}) \cong \mathbb{C}^N$ for $F$ a fixed unit cell in $C$ and where $\vartheta : BZ \to BZ$ is induced by $k \mapsto -k$. For time-reversal symmetric crystalline Hamiltonians $\theta H_c \theta^{-1} = H_c$,

$$\theta \hat{H}(k) \theta^{-1} = \hat{H}(-k).$$ \hspace{1cm} (II.20)

If $\hat{\psi}_n(k)$ is an eigenvector of $\hat{H}(k)$ then $\theta \hat{\psi}_n(k)$ is an eigenvector of $\hat{H}(-k)$ with the same eigenvalue. As the result, the band spectrum is symmetric under $k \mapsto -k + b$ for each $b$ in the reciprocal lattice $\Gamma^r$. Finally, if $\theta^2 = -I$ then vectors $\theta \hat{\psi}_n(k)$ and $\hat{\psi}_n(k)$ are orthogonal. Indeed,

$$\langle \psi | \theta \psi \rangle = \langle \theta^2 \psi | \theta \psi \rangle = -\langle \psi | \theta \psi \rangle = 0.$$ \hspace{1cm} (II.21)

Such pairs of eigenvectors vectors in $\mathbb{C}^N$ are called Kramers pairs. In particular, for time-reversal symmetric momenta $k = -k + b$ (the so called TRIM), the spectrum of $\hat{H}(k)$ has even degeneration and the typical picture of bands is as in Fig. 8. In particular, the dimension of the range of the projectors $P(k)$ on the valence band states is even.

![FIG. 8: Time reversal symmetric energy bands for $\theta^2 = -I$](image)

Symmetry (II.20) implies that

$$\theta P(k) \theta^{-1} = P(-k)$$ \hspace{1cm} (II.22)

and, consequently, that the corresponding Chern number vanishes. Indeed,

$$c_1 = \frac{i}{2\pi} \int_{BZ} \text{tr} \theta P(-k) \left( dP(-k) \right)^{\wedge 2} \theta^{-1} = \frac{i}{2\pi} \int_{BZ} \text{tr} P(-k) \left( dP(-k) \right)^{\wedge 2} = -c_1 = 0,$$  \hspace{1cm} (II.23)

since the 2-form $\text{tr} P(dP)^{\wedge 2}$ is purely imaginary. The vanishing of the 1st Chern number implies that the vector bundle $\mathcal{E}$ over $BZ$ formed by the valence band states is topologically trivial. In [3], Kane
and Mele observed, however, that, for \( \theta^2 = -I \), vector bundle \( E \) (of even rank \( m \)) may still exhibit nontrivial topological properties when considered together with the action of \( \theta \) mapping anti-unitarily fibers \( E_k \) to \( E_k^{-1} \). The nontrivial topological property is captured by an obstruction to the existence of a global frame of sections \( (\tilde{\psi}_1(k), \ldots, \tilde{\psi}_m(k)) \) of \( E \) (not necessarily composed of eigenfunctions of \( \hat{H}(k) \)) such that \( \tilde{\psi}_{2i}(k) = \theta \tilde{\psi}_{2i-1}(-k) \), i.e., formed by globally defined Kramers pairs. Kane and Mele showed that the obstruction is given by a \( \mathbb{Z}_2 \)-valued index, that we shall denote by \( KM \) and describe in the form established in [20].

One chooses an arbitrary global frame \( (\tilde{\psi}_1(k), \ldots, \tilde{\psi}_m(k)) \) trivializing bundle \( E \) and defines the “sewing” matrix

\[
w_{ij}(k) = \langle \tilde{\psi}_i(-k)|\theta \tilde{\psi}_j(k) \rangle. \tag{II.24}
\]

\( w(k) = (w_{ij}(k)) \) is a unitary \( m \times m \) matrix that satisfies \( w(-k) = -w(k)^T \). It follows that \( \det(w(k)) = \det(w(-k)) \) so that the determinant of \( w(k) \) does not wind around the cycles of \( BZ \) and, consequently, it has a globally defined square root determined up to an overall sign. Besides, at four TRIM \( k \in BZ \), \( w(k) \) is an antisymmetric matrix. The Kane-Mele index \( KM \) is given by:

\[
(-1)^{KM} \prod_{\text{TRIM } k} \frac{\sqrt{\det(w(k))}}{\text{pf}(w(k))} = e^{iS_{WZ}(w)}, \tag{II.25}
\]

where \( \text{pf} \) denotes the Pfaffian of an antisymmetric matrix. The first equality is the expression of ref. [20] whereas the second equality seems to be new and will be discussed elsewhere. It was observed already in the original paper [3] that \( KM \) lives in the Real \( K \)-theory group of the \( 2d \)-torus \( BZ \) equipped with involution \( \theta \) [24], namely in the reduced group \( \tilde{K}R^{-1}(BZ) \cong \mathbb{Z}_2 \). Index \( KM \) is invariant under deformations of the crystalline system preserving the time reversal symmetry and the gap.

Kane and Mele discussed in [3] a concrete model with a nontrivial value of \( KM \). The model was obtained by coupling two copies of the Haldane model corresponding to two components of spin = \( \frac{1}{2} \) by an additional interaction between two spin components (mimicking the spin-orbit interaction). A somewhat different version of a model with \( KM \neq 0 \) was proposed in [28]. The nontrivial topological phases with \( KM = -1 \) were soon realized experimentally [29]. Mathematical proofs that \( KM \) realizes the obstruction to the global choice of a frame of vector bundle \( E \) composed of Kramers pairs were given in [30, 31].

D. Kane-Mele invariant as the square root of a WZ amplitude

In ref. [6], we showed that the invariant \( KM \) may be represented as the square root of the WZ amplitude of the field

\[
BZ \ni k \mapsto \phi(k) = I - 2P(k) \in U(N) \tag{II.26}
\]

that satisfies the equivariance condition [1.6], see (I.22). Our formula (I.9) for \( KM \) seems to provide a realization unknown in mathematical literature of the Bott isomorphism in Real \( K \)-theory \( \tilde{K}R^{-4}(BZ) \cong \tilde{K}R^{-3}(SBZ) \). The proof given in [6] that \( \sqrt{\alpha_{SWZ}(\phi)} \) is equal to \((-1)^{KM}\) was based on the localization at TRIM of the nonlocal formula (I.8) for the square root of the WZ amplitude of \( \phi \). Although rather laborious, it involved interesting elements such as a new boundary gauge anomaly for WZ amplitudes. Here, we shall show that definition (I.89) and the local expression (I.95) provide a more direct way to establish relation (I.9) resembling the derivation of the Kane-Mele invariant in [26].

In order to calculate \( \sqrt{\alpha_{SWZ}(\phi)} = \sqrt{\text{Hol}_{\xi_{SWZ}(\phi)}} \) using (I.95), let us start by choosing as (the closure of) a fundamental domain \( F \subset BZ \) the “effective Brillouin zone”

\[
BZ_+ = \{ k \in BZ \mid 0 \leq k_1 \leq \pi \}, \tag{II.27}
\]

as on the left hand side of Fig. 3. Let \( \mathcal{G} = (Y, B, \mathcal{L}, t) \) be the basic gerbe on \( U(N) \) constructed in Sec. II. Consider map \( s : BZ_+ \to Y \) defined by

\[
s(k) = (\frac{3}{2}\pi, \phi(k)) \tag{II.28}
\]
which is well defined because $\text{spec}(\phi(k)) \subset \{\pm 1\}$. It satisfies the relation $\pi \circ s = \phi|_F$. In the calculation of $\text{Hol}_G(\phi|_F)$ as given by (II.17), we shall use $s_c = s|_c$ for all triangles of a triangulation of $BZ_+$. Similarly, we shall set $s_b = s|_b$ for all edges $b \subset F$ except those in $\ell$ for $\ell \subset \partial F$ chosen as on the left hand side of Fig. [3]. For those, we shall take $s_b = s|_b$, where $s_\ell : \ell \to Y$ is given by
\[ s_\ell(k) = (1/2\pi, \phi(k)) \in Y. \] (II.29)

This will ensure relation (II.26) for $b \subset \ell$. Finally, for $v \in \partial \ell$, we shall set $s_v = s_\ell(v) = (-1/2\pi, \phi(v)) \in Y$. With those choices, the expression for the gerbe holonomy of $\phi|_F$ simplifies to
\[\text{Hol}_G(\phi|_F) = e^{i \sum_{c \in F} \int_c s_c^* B \otimes \text{hol}_E(s_c|_b, s_b)} = e^{i \int_{\partial F} s^* B \text{hol}_E(s|_\ell, s_\ell)} \in \bigotimes_v \mathcal{L}(v, s_v). \] (II.30)

A direct calculation using the relation $H^\text{eff}_{-2\pi}(\phi(k)) = -\pi P(k)$ and the identity $(PdP)^2 = 0$ shows that
\[ s^* B = -\frac{i}{2} \text{tr } P(dP)^{\wedge 2}. \] (III.31)

Let $(\hat{\psi}_i(k)|_{m=1})$ be a global orthonormal frame of the valence vector bundle $\mathcal{E}$ whose existence is guaranteed by the vanishing of the $1^\text{st}$ Chern number of $\mathcal{E}$. One has the relations
\[ P(k) = \sum_{i=1}^m \hat{\psi}_i(k)(\hat{\psi}_i(k)|, \quad A^B(k) = i \sum_{i=1}^m (\hat{\psi}_i(k) d\hat{\psi}_i(k)), \] (II.32)

where $A^B$ is the Berry connection 1-form corresponding to the curvature 2-form $F^B = dA^B = i \text{tr } P(dP)^{\wedge 2}$. Hence, by the Stokes formula,
\[ \int_F s^* B = -\frac{i}{2} \int_F dA^B = -\frac{1}{2} \int_{\partial F} A^B = -\frac{1}{2} \int_{\ell} (A^B - \vartheta^* A^B), \] (II.33)

where we used the relation $\partial F = \ell \cup \vartheta(\ell)$. Now
\[ (\vartheta^* A^B)(k) = i \sum_{i=1}^m (\hat{\psi}_i(-k)|d\hat{\psi}_i(-k)) = i \sum_{i=1}^m (\vartheta d\hat{\psi}_i(-k)|\vartheta\hat{\psi}_i(-k)). \] (II.34)

Substituting to the right hand side the relation $\vartheta\hat{\psi}_i(-k) = -\sum_j w_{ij}(k) \hat{\psi}_j(k)$, where $w_{ij}(k) = -w_{ji}(-k)$ in the sewing matrix of (II.24), we infer that
\[ \vartheta^* A^B = -i \text{tr } w^{-1} dw - A^B \] (II.35)

and, consequently, that
\[ \int_F s^* B = -\int_{\ell} A^B - \frac{i}{2} \int_{\ell} \text{tr } w^{-1} dw. \] (II.36)

On the other hand, the map $(s|_\ell, s_\ell)$ from $\ell$ to $Y^{[2]}$ is given by $(s(k), s_\ell(k)) = (-\frac{3}{2} \pi, -\frac{1}{2} \pi, \phi(k))$. Since $P_{-\frac{3}{2} \pi, -\frac{1}{2} \pi}(\phi(k)) = P(k)$, it follows that $\mathcal{L}_{s(k), s_\ell(k)} = \wedge \max P(k) \mathbb{C}^N$ and the parallel lift of $(s|_\ell, s_\ell)$ to $\mathcal{L}$ is given by
\[ e^{i \int_0^{k_2} \left(A^B(a, k'_2) + A(-\frac{3}{2} \pi, -\frac{1}{2} \pi, \phi(a, k'_2))\right) \hat{\psi}_1(a, k_2) \wedge \cdots \wedge \hat{\psi}_m(a, k_2). \] (II.37)

for $k_2 \in [0, \pi]$ and $a = 0$ or $a = \pi$ corresponding to one of the two connected components of $\ell$. But
\[ A(-\frac{3}{2} \pi, -\frac{1}{2} \pi, \phi(a, k'_2)) = -\frac{1}{2} \text{tr } (H^\text{eff}_{-2\pi}(\phi(a, k'_2)) dP(a, k'_2)) \]
\[ = -\frac{1}{2} \text{tr } (P(a, k'_2)) dP(a, k'_2) = -\frac{1}{2} \text{tr } dP(a, k'_2) = 0. \] (II.38)

As the result, one obtains from (II.37) the following expression for the line bundle $\mathcal{L}$ holonomy term:
\[ \text{hol}_E(s|_\ell, s_\ell) = e^{i \int_0^{k_2} \left(A^B(v) \wedge \cdots \wedge \hat{\psi}_m(v)\right)^{\pm 1}. \] (II.39)
From (II.30), (II.36) and (II.39), one then infers that

\[ \text{Hol}_G(\phi|_F) = e^\frac{i}{2} \int_{v \in \delta} \text{tr} w^{-1} dw \otimes \left( \hat{\psi}_1(v) \wedge \cdots \wedge \hat{\psi}_m(v) \right)^{\pm 1} \in \otimes_{v \in \delta} \mathcal{N}^\pm_{Y(v(s), s)} \quad (\text{II.40)} \]

Now, the triviality of line bundle \( \mathcal{N} \), for the 1-isomorphism \( \eta = (\mathcal{N}, \nu) : G \to \Theta^*G \) constructed in Sec. I \( \) implies that

\[ \text{hol}_{\mathcal{N}}(\phi|_\ell) = 1 \in \otimes_{v \in \delta} \mathcal{N}_{s_v} \quad (\text{II.41)} \]

Hence

\[ \text{Hol}_G(\phi|_F) \otimes \text{hol}_{\mathcal{N}}(\phi|_\ell) = e^{-\frac{i}{2} \int_{v \in \delta} \text{tr} w^{-1} dw} \otimes \left( \hat{\psi}_1(v) \wedge \cdots \wedge \hat{\psi}_m(v) \right)^{\pm 1} \]

\[ = e^{\frac{i}{2} \int_{v \in \delta} \text{tr} w^{-1} dw} \left( \hat{\psi}_1(0, 0) \wedge \cdots \wedge \hat{\psi}_m(0, 0) \right)^{-1} \otimes \left( \hat{\psi}_1(\pi, \pi) \wedge \cdots \wedge \hat{\psi}_m(\pi, \pi) \right)^{-1} \otimes \left( \hat{\psi}_1(0, 0) \wedge \cdots \wedge \hat{\psi}_m(0, 0) \right) \quad (\text{II.42)} \]

Using the sections \( \sqrt{S_{\pm}} \) of the line bundle \( \mathcal{N} \) determined by assignment (I.93), and noting that when we lift \( \phi(k) = I - 2P(k) \) to a map \( \tilde{\phi}(k) \) with values in \( \tilde{U}(N) \) then at all TRIM \( \tilde{\phi}(k) \) is in the same component of \( \tilde{U}(N) \) \( \) because \( \det(\phi(k)) = 1 \) for all \( k \), the last expression may be rewritten as

\[ \text{Hol}_G(\phi|_F) \otimes \text{hol}_{\mathcal{N}}(\phi|_\ell) = e^{\frac{i}{2} \int_{v \in \delta} \text{tr} w^{-1} dw} \left( \text{pf}(w(\pi, 0)) \text{pf}(w(0, \pi)) \right) \]

\[ \cdot \sqrt{S_{\pm}^1(\phi(\pi, 0))^{-1} \otimes S_{\pm}^1(\phi(\pi, \pi)) \otimes S_{\pm}^1(\phi(0, 0))} \quad (\text{II.43)} \]

with the same sign in all \( \sqrt{S_{\pm}^1} \). This gives

\[ \sqrt{e^{i\text{Swz}(\phi)}} = e^{\frac{i}{2} \int_{v \in \delta} \text{tr} w^{-1} dw \frac{\text{pf}(w(\pi, 0)) \text{pf}(w(0, \pi))}{\text{pf}(w(\pi, \pi)) \text{pf}(w(0, 0))} } \]

\[ = \frac{\sqrt{\det(w(\pi, \pi)) \det(w(0, 0))}}{\sqrt{\det(w(\pi, 0)) \det(w(0, \pi))}} \frac{\text{pf}(w(\pi, 0)) \text{pf}(w(0, \pi))}{\text{pf}(w(\pi, \pi)) \text{pf}(w(0, 0))} \quad (\text{II.44)} \]

which is equivalent to expression (II.25) for \( (-1)^{KM} \) given in [20] (recall that \( \sqrt{\det(w(k))} \) is defined on \( BZ \) modulo a global sign).

Let us mention another possible representation of \( (-1)^{KM} \). To this end we observe that field \( \Phi \) of (II.16) may be considered as a map

\[ R \equiv \mathbb{R}/\mathbb{Z} \times BZ \ni (t, k) \mapsto \Phi(t, k) \in U(N) \quad (\text{II.45)} \]

satisfying equivariance condition (II.38) for the orientation reversing involution \( \rho(t, k) = (-t, -k) \). Indeed,

\[ \Phi(-t, -k) = e^{-2\pi i t P(-k)} = e^{-2\pi i k P(k)} = \theta e^{2\pi i k P(k)} \theta^{-1} = \theta \Phi(t, k) \theta^{-1} \quad (\text{II.46)} \]

Let us consider the 3d index defined in Sec. I \( G \)

\[ \mathcal{K}(\Phi) = \frac{e^{\frac{i}{2} \int_{F_R} \Phi^* H}}{\sqrt{e^{i\text{Swz}(\Phi|_{\partial F_R})}}} \quad (\text{II.47)} \]

for the fundamental domain \( F_R = [0, \frac{1}{2}] \times BZ \) of involution \( \rho \). Now, field \( \Phi \) also satisfies the relation

\[ \Phi(t, -k) = \theta \Phi(t, k) \theta^{-1} = \Theta \Phi^{-1}(t, k) \quad (\text{II.48)} \]

which implies that \( \Phi^* H(t, -k) = (\Phi^{-1})^* H(t, k) = -\Phi^* H(t, k) \) and, consequently, that the numerator in (II.47) vanishes. Hence

\[ \mathcal{K}(\Phi) = \frac{1}{\sqrt{e^{i\text{Swz}(\Phi|_{\partial F_R})}}} = \sqrt{e^{i\text{Swz}(\Phi|_{\partial F_R})}} = (-1)^{KM} \quad (\text{II.49)} \]
where the last but one equality follows from the fact that $K(\Phi) = \pm 1$. The gain from the representation (II.49) of the Kane-Mele invariant is that index $K(\Phi)$ may be computed by using other choices of the fundamental domain $F_R$, e.g. by taking $F_R = (\mathbb{R}/\mathbb{Z}) \times BZ_+$. The corresponding formula for $KM$ is close, at least in the spirit, to the $\mathbb{Z}_2$-valued index defined in [32], which was not shown previously to be equal to the Kane-Mele index.

E. 3d Kane-Mele invariants

In ref. [33], Fu, Kane and Mele extended their index to 3d time-reversal insulators. In its strong form which is related to a $K$-theory class in $\widetilde{KR}^{-4}(BZ)$ pulled back from $\widetilde{KR}^{-4}(S^3) \cong \mathbb{Z}^2$, where here $BZ$ is the 3d Brillouin torus $\cong \mathbb{R}^3/(2\pi\mathbb{Z})^3$ with the orientation-reversing involution $\rho$ induced by $k \mapsto -k$ in $\mathbb{R}^3$. The strong Kane-Mele index $KM^s$ is still defined by the first equality in (II.25) but the product is now over 3d TRIM which is $BZ$. On the other hand, there are 6 weak 2d indices $KM(i,a)$ for $i = 1, 2, 3$ and $a = 0, \pi$ obtained by restricting the products over TRIM to one of six $\rho$-invariant 2d sub-tori $T^2(i,a) \subset BZ$, see Fig.9. Clearly, the strong index $KM^s$ is equal to the sum or difference (mod 2) of two weak indices corresponding to each pair of 2d $\rho$-invariant sub-tori perpendicular to a coordinate axis:

$$KM^s = KM(i, \pi) - KM(i, 0)$$  \hspace{1cm} (II.50)

for each $i = 1, 2, 3$.

For the map

$$BZ \ni k \mapsto \Phi(k) = I - 2P(k) \in U(N),$$  \hspace{1cm} (II.51)

where $P(k)$ are the spectral projectors on the valance band states of the 3d time reversal invariant insulator, the equivariance

$$\Phi \circ \rho = \Theta \circ \Phi$$  \hspace{1cm} (II.52)

is assured by the relation $P(-k) = \theta P(k) \theta^{-1}$ following from the time-reversal invariance of the Hamiltonian. We may then consider the 3d index $K(\Phi)$ with values $\pm 1$ defined in Sec. [1G]. Taking for the the fundamental domain $F_R \subset BZ$ the 3d effective Brillouin zone $BZ_+$ corresponding to $k_1 \in [0, \pi]$, we obtain:

$$K(\Phi) = \frac{\int_{BZ_+} \Phi^* H}{\sqrt{e^{iSWZ(\Phi|_{T^2(1,\pi)})}} / \sqrt{e^{iSWZ(\Phi|_{T^2(1,0)})}}},$$  \hspace{1cm} (II.53)

where $T^2(1,a)$ for $a = 0, \pi$ are two boundary 2d sub-tori in $\partial BZ_+$, see Fig.9. We have the following

**Lemma.** $\int_{BZ_+} \Phi^* H = 0$.

**Proof.** Consider the mapping

$$BZ_+ \equiv [0, \frac{1}{2}] \times BZ_+ \ni (t,k) \mapsto \Phi(t,k) = e^{2\pi i t P(k)} \in U(N).$$  \hspace{1cm} (II.54)
Since $H$ is a closed 3-form, it follows from the Stokes Theorem that
\[ \int_{\partial \mathcal{B}Z_+} \Phi^* H = 0. \] (II.55)

On the other hand,
\[ \partial \mathcal{B}Z_+ = \{ \frac{1}{2} \} \times \mathcal{B}Z_+ - \{ 0 \} \times \mathcal{B}Z_+ - [0, \frac{1}{2}] \times \mathbb{T}^2(1, \pi) + [0, \frac{1}{2}] \times \mathbb{T}^2(1, 0), \] (II.56)

and the contribution to the integral over $\partial \mathcal{B}Z_+$ of the first piece is equal to $\int_{\mathcal{B}Z_+} \Phi^* H$ whereas the contributions of the other pieces vanish (on the second piece, $\Phi = I$ and for the third and the fourth piece, we use the same argument that proved the vanishing of the numerator in (II.47)). This establishes relation (II.55).

Using the last lemma, we infer that
\[ K(\Phi) = \sqrt{\frac{\text{e}^{i S_{\mathcal{W}Z}(\Phi|_{\mathcal{T}_1,0})}}{\text{e}^{i S_{\mathcal{W}Z}(\Phi|_{\mathcal{T}_1,\pi})}}}, \] (II.57)

By (1.9), the square-roots of the WZ amplitudes give the two weak $KM$ indices and we finally obtain the relation
\[ K(\Phi) = (-1)^{KM^*} \] (II.58)
announced in Sec. I G.

The index $(-1)^{KM^*}$ is equal to the Chern-Simons amplitude of the connection with covariant derivative $\nabla S(k) = P(k)dS(k)$ on the (topologically trivial) valence vector bundle $\mathcal{E}$, see [31] and references therein. This can be easily proven directly from the second equality in (II.25) and will be discussed elsewhere.

F. Floquet theory of periodically driven crystalline systems

There exist an interesting possibility that one can induce nontrivial topological properties of materials by external forcing, for example by irradiating a sample of the material with microwaves [35]. Although such a scenario for inducing topological phases has been realized up to now only in artificial systems made of arrays of coupled waveguides or of cold atoms in optical lattices, the idea has inspired a considerable theoretical activity.

Suppose that the Hamiltonian of a crystalline system acting in space of states $\mathcal{H} = L^2(\mathcal{C}, \mathcal{V})$ depends periodically on time, i.e.
\[ H_c(t + T) = H_c(t), \] (II.59)
for $H_c(t)$ of the form (II.8) with $h(t, x, y) = h(t + T, x, y) = h(t, x + a, y + a)$ for $a \in \Gamma$. Such Hamiltonians generate evolution operators $U_c(t)$ satisfying
\[ i\partial_t U_c(t) = H_c(t) U_c(t), \quad U_c(0) = I \] (II.60)
which are not periodic but satisfy the relation
\[ U_c(t + T) = U_c(t) U_c(T). \] (II.61)

In the Fourier picture, we obtain (analytic in $k$) families of periodic in time Hermitian $N \times N$ matrices $\hat{H}(t, k) = \hat{H}(t + T, k)$ and of unitary $N \times N$ matrices $\hat{U}(t, k)$ satisfying the relation
\[ \hat{U}(t + T, k) = \hat{U}(t, k) \hat{U}(T, k). \] (II.62)

The main idea of the Floquet theory of periodically driven systems is to replace the Bloch diagonalization of static Hamiltonians by the diagonalization of the evolution operators over one period of time. One just looks for the eigenvalues and eigenfunctions such that
\[ \hat{U}(T, k) \hat{\psi}_n(k) = e^{-iTr_k} \hat{\psi}_n(k). \] (II.63)
We parameterized the eigenvalues of unitary matrices $\hat{U}(T, k)$ by “quasi-energies” $\epsilon_n(k)$ defined modulo $\frac{2\pi}{T}$. They form a pattern of bands in $BZ \times \mathbb{R}$ that repeats itself with this period, see Fig. 10. Note that the time-dependent states $\hat{\psi}_n(t, k) = \hat{U}(t, k) \hat{\psi}_n(k)$ satisfy the relation

$$i\partial_t \hat{\psi}_n(t, k) = \hat{H}(t, k) \hat{\psi}_n(t, k), \quad \hat{\psi}_n(t + T, k) = e^{-iT\epsilon_n(k)} \hat{\psi}_n(t, k). \tag{II.64}$$

They are called Floquet states.

### G. Topological invariants of gapped Floquet 2d and 3d systems

Suppose that there is a gap in the quasi-energy spectrum of $\hat{U}(T, k)$ around $\epsilon$ with $-\frac{2\pi}{T} < \epsilon < 0$ for all $k \in BZ$. Like in (I.43), we may then define the effective Hamiltonians

$$H^\text{eff}_\epsilon(k) = \frac{i}{T} \ln_{-\epsilon T} \hat{U}(T, k) \tag{II.65}$$

that depend analytically on $k \in BZ$ and satisfy

$$\hat{U}(T, k) = e^{-iT H^\text{eff}_\epsilon(k)} \tag{II.66}$$

(the definitions coincide with the ones of Sec. I H if the period $T$ is set to 1). For two gap quasi-energies $-\frac{2\pi}{T} < \epsilon_1 \leq \epsilon_2 < 0$,

$$H^\text{eff}_{\epsilon_2}(k) - H^\text{eff}_{\epsilon_1}(k) = \frac{2\pi}{T} P_{\epsilon_1, \epsilon_2}(k), \tag{II.67}$$

where $P_{\epsilon_1, \epsilon_2}(k)$ is the spectral projection of $\hat{U}(T, k)$ on the part of the spectrum in the sub-interval of the circle joining $e^{-iT\epsilon_1}$ to $e^{-iT\epsilon_2}$ clockwise, see (I.50).

Effective Hamiltonian may be used to define the periodized evolution operators

$$V_\epsilon(t, k) = \hat{U}(t, k) e^{it H^\text{eff}_\epsilon(k)} \tag{II.68}$$

that satisfy the relations

$$V_\epsilon(t + T, k) = V_\epsilon(t, k), \quad V_\epsilon(0, k) = I = V_\epsilon(T, k). \tag{II.69}$$

In [36], the authors considered a topological invariant $W_\epsilon$ of the 2d gapped Floquet systems defined by

$$W_\epsilon = \text{deg}(V_\epsilon) = \frac{1}{2\pi} \int_{[0, T] \times BZ} V_\epsilon^* H, \tag{II.70}$$

see (II.17), i.e. as the homotopy invariant of the map $V_\epsilon : \mathbb{R}/(TZ) \times BZ \to U(N)$. For two gaps with $-\frac{2\pi}{T} < \epsilon_1 < \epsilon_2 < 0$,

$$V_{\epsilon_2}(t, k) = V_{\epsilon_1}(t, k) e^{\frac{2\pi i}{T} P_{\epsilon_1, \epsilon_2}(k)}, \tag{II.71}$$
due to \((\text{II.67})\). As \(\deg(V)\) is additive under the multiplication of maps, it follows from relation \((\text{II.17})\) that

\[ W_{\epsilon_2} - W_{\epsilon_1} = c_{\epsilon_1, \epsilon_2}, \tag{\text{II.72}} \]

where \(c_{\epsilon_1, \epsilon_2}\) is the 1st Chern number of the vector bundle \(E_{\epsilon_1, \epsilon_2}\) with fibers \(P_{\epsilon_1, \epsilon_2}(k) \mathbb{C}^N\), i.e. spanned by the eigenstates of \(\hat{U}(t, k)\) with the quasi-energies between the two gaps. In particular, we may have the bundles of states between two gaps topologically trivial with \(c_{\epsilon_1, \epsilon_2} = 0\) but the Floquet systems still topologically nontrivial with \(W_{\epsilon_1} = W_{\epsilon_2} \neq 0\).

In \([3, 4]\), we considered the time-reversal invariant gapped Floquet systems with

\[ H_{\epsilon}(-t) = \theta H_{\epsilon}(t) \theta^{-1} \quad \text{or, equivalently,} \quad \hat{H}(-t, -k) = \theta \hat{H}(t, k) \theta^{-1}. \tag{\text{II.73}} \]

In this case,

\[ \hat{U}(-t, -k) = \theta \hat{U}(t, k) \theta^{-1}, \quad H_{\epsilon}^{\text{eff}}(-k) = \theta H_{\epsilon}^{\text{eff}}(k) \theta^{-1} \tag{\text{II.74}} \]

and

\[ V_{\epsilon}(T - t, -k) = V_{\epsilon}(-t, -k) = \theta V_{\epsilon}(t, k) \theta^{-1}. \tag{\text{II.75}} \]

The latter symmetry property implies that in 2d the index \(W_{\epsilon}\) of \([36]\) vanishes. Instead, we introduced an index \(K_{\epsilon} \in \mathbb{Z}_2\) defined by the relation

\[ (-1)^{K_{\epsilon}} = \mathcal{K}(V_{\epsilon}), \tag{\text{II.76}} \]

where \(\mathcal{K}(V_{\epsilon})\) is the 3d index with values in \(\pm 1\) defined in Sec.\(\text{II.G}\) for equivariant maps. Index \(K_{\epsilon}\) is a topological invariant of time reversal symmetric gapped Floquet systems in 2d. In the case of two gaps with \(-\frac{2\pi}{25} < \epsilon_1 < \epsilon_2 < 0\),

\[ K_{\epsilon_2} - K_{\epsilon_1} = KM_{\epsilon_1, \epsilon_2}, \tag{\text{II.77}} \]

where \(KM_{\epsilon_1, \epsilon_2} \in \mathbb{Z}_2\) is the Kane-Mele index of the vector bundle \(E_{\epsilon_1, \epsilon_2}\) with fibers \(P_{\epsilon_1, \epsilon_2}(k) \mathbb{C}^N\). \(KM_{\epsilon_1, \epsilon_2}\) is well defined since \(P_{\epsilon_1, \epsilon_2}(-k) = \theta P_{\epsilon_1, \epsilon_2}(k) \theta^{-1}\). The proof of relation \((\text{II.77})\) uses the fact that

\[ \mathcal{K}(V_{\epsilon_2}) = \mathcal{K}(V_{\epsilon_1} \Phi) = \mathcal{K}(V_{\epsilon_1}) \mathcal{K}(\Phi), \tag{\text{II.78}} \]

for \(\Phi(t, k) = e^{\frac{2\pi i}{25} \rho(k)}\) (the 3d index is not multiplicative in general, but in this case it is) and the relation \((\text{II.49})\).

Finally, for gapped 3d Floquet systems, we may define 6 week indices \(K_{\epsilon}(i,a) \in \mathbb{Z}_2\) for \(i = 1, 2, 3\) and \(a = 0, \pi\) from 6 2d sub-tori \(T^2(i,a)\) in the 3d Brillouin torus \(BZ \cong T^3\), see Fig.\([4]\) and one strong index \(K_{\epsilon}^s \in \mathbb{Z}_2\) expressed by the 3d index for the equivariant map \(BZ \ni k \mapsto V_{\epsilon}(\frac{k}{2}, k)\),

\[ (-1)^{K_{\epsilon}^s} = \mathcal{K}(V_{\epsilon}|_{l = 2}). \tag{\text{II.79}} \]

Again for two gaps with \(-\frac{2\pi}{25} < \epsilon_1 < \epsilon_2 < 0\),

\[ (-1)^{K_{\epsilon_2}^s} = \mathcal{K}(V_{\epsilon_2}|_{l = 2}) = \mathcal{K}(V_{\epsilon_1}|_{l = 2})(1 - 2P_{\epsilon_1, \epsilon_2}) \]

\[ = \mathcal{K}(V_{\epsilon_1}|_{l = 2})\mathcal{K}(1 - 2P_{\epsilon_1, \epsilon_2}) = (-1)^{K_{\epsilon_1}^s} (-1)^{KM_{\epsilon_1, \epsilon_2}}, \tag{\text{II.80}} \]

where we used the multiplicativity of the 3d index holding for maps with no winding of determinants and the relation \((\text{II.58})\) of Sec.\(\text{II.E}\). Thus

\[ K_{\epsilon_2}^s - K_{\epsilon_1}^s = KM_{\epsilon_1, \epsilon_2}^s, \tag{\text{II.81}} \]

similarly as in 2d, see \((\text{II.77})\). One also has

\[ K_{\epsilon}^s = K_{\epsilon}(i, \pi) - K_{\epsilon}(i, 0) \tag{\text{II.82}} \]

for each \(i = 1, 2, 3\), similarly as for the 3d Kane-Mele indices, see \((\text{II.50})\). For \(i = 1\) this is proven by using the fundamental domain \(F_R = BZ_+\) for the involution \(\rho : k \mapsto -k\) of \(BZ\) and observing that the relation

\[ \int_{\partial BZ_+} V_{\epsilon}^* H = 0 \tag{\text{II.83}} \]
for $\mathcal{B}Z_+ = [0, \frac{1}{2}] \times BZ_+$ implies that

$$
\int_{\mathcal{B}Z_+} (V_\epsilon|_{t=\frac{T}{2}})^* H = \int_{[0, \frac{1}{2}] \times T^1, \pi} V_\epsilon^* H - \int_{[0, \frac{1}{2}] \times T^1, 0} V_\epsilon^* H
$$

so that

$$
\mathcal{K}(V_\epsilon|_{t=\frac{T}{2}}) = \frac{\mathcal{K}(V_\epsilon|_{k_1=\pi})}{\mathcal{K}(V_\epsilon|_{k_1=0})}.
$$

The latter equality, together with the 2d relation (II.76), implies (II.82) for $i = 1$. The proof for $i = 2, 3$ goes the same way by choosing the fundamental domains for $\rho$ corresponding to the restrictions $k_i \in [0, \pi]$.

### H. Bulk-edge correspondence

Physically, the most interesting aspect of topological phases of insulators, the mean of their detection, and the essential feature for present and future application, is that, in finite geometry, they may carry currents localized on the boundary of the samples that are protected against sufficiently weak disorder or interactions. In particular, in the half-space geometry, such edge currents are localized near the boundary hyperplane, see the left part of Fig. 11. The massless modes carrying the edge currents can be detected in the spectrum of the half-crystal Hamiltonian Fourier transformed in the directions parallel to the boundary hyperplane. They correspond to the intersections with the Fermi energy level of the energy bands that appear in such boundary Hamiltonians within the gap of the original crystalline Hamiltonian, see the right part of Fig. 11.

![FIG. 11: The edge current (left) and the spectrum of Bloch Hamiltonians for the half-space geometry (right)](image)

In particular, in a 2d Chern insulator, the 1st Chern number $c_1$ of the infinite-crystal valence states bundle counts with chirality (i.e. direction) the massless modes of the half-crystal Bloch Hamiltonians with energies close to the Fermi energy $\epsilon_F$ ($= 0$ in Fig. 11 corresponding to $c_1 = 1$), see e.g. [37]. For 2d time reversal invariant insulators, the Kane-Mele invariant $KM$ counts the parity of the number of Kramers pairs of massless edge modes of opposite chirality, see Fig. 12 taken from [38] that corresponds to $KM = 1$.

![FIG. 12: Pairs of chiral edge currents (left) and the typical spectrum of time reversal symmetric half-space Bloch Hamiltonians (right)](image)

The bulk-edge correspondence in this case was proven rigorously in [39]. Similarly, the strong Kane-Mele 3d invariant should count the parity of the number of Dirac cones intersecting the Fermi energy inside the bulk gap.
It was shown in [36] that for the gapped Floquet systems the invariant $W$ enumerates with chirality the edge massless modes appearing in the quasi-energy gap around $\epsilon$ even in situations when the 1st Chern numbers of quasi-energy bands vanish, as in Fig. 13 extracted from [40].

Similarly, for time reversal invariant $2d$ gapped Floquet systems, invariant $K_\epsilon$ should count modulo two the number of Kramers pairs of massless edge modes in the bulk quasi-energy gap around $\epsilon$, as confirmed by simulations reported in [5] of a simple periodically driven model in a strip geometry, see Fig. 14.

We discussed how $\Theta$-equivariant structures on a bundle gerbe $\mathcal{G}$ over manifold $M$ equipped with involution $\Theta$ may be used to fix the square root of the WZ amplitudes of maps from $2d$ surfaces with orientation preserving involutions to $M$. Using such square roots, we defined an index $K(\Phi) = \pm 1$ of equivariant maps $\Phi$ from a $3d$ manifolds equipped with an orientation reversing involutions to $M$. Such index was applied to the situation when $M = U(N)$, $\mathcal{G}$ is the basic gerbe on $U(N)$ with the bi-invariant curvature, and $\Theta$ is given by the adjoint action of an anti-unitary transformation of $\mathbb{C}^N$ that squares to $-I$. The problem with the absence of a $\Theta$-equivariant structure on $\mathcal{G}$ was solved by passing to the double cover of $U(N)$. We discussed how index $K(\Phi)$ may be used to express the Kane-Mele $\mathbb{Z}_2$-valued invariant of $2d$ and $3d$ time-reversal invariant insulators and to obtain its generalization to periodically driven crystalline systems.

The approach discussed here, based on the geometry of bundle gerbes, may be also extended to topological insulators in other symmetry classes that lead to torsion invariants, and, potentially, to insulators with more crystalline symmetries. It should be also useful to describe the bulk-edge correspondence, but that remains to be done constituting the main challenge for this line of thought. A possible extension of the present approach to non-commutative geometry should be investigated.

I. Conclusions
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