A theorem regarding families of topologically non-trivial fermionic systems

B. Mera

Instituto Superior Técnico
CeFEMA and Physics of Information Group

11th July 2016

outline

Topological Insulators and Superconductors

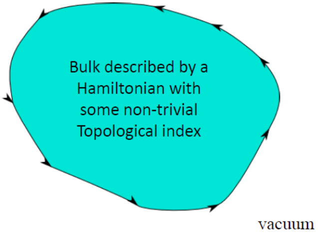
Topological Band Theory

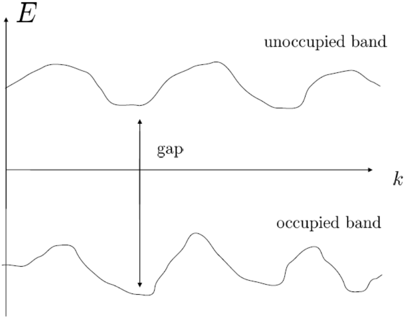
A class of non-trivial examples

Topological Insulators and Superconductors

Topological Insulators and Superconductors

Topological insulators (superconductors) are *gapped states* of matter (thus "insulators") in d spatial dimensions with the following property (bulk-to-boundary correspondence): If we terminate the topological insulator (superconductor) against a "topologically trivial" state (e.g. vacuum), *gapless degrees of freedom* will necessarily appear at the *boundary* between the topologically trivial and the topologically non-trivial states.





As long as we keep the gap fixed, by adding a perturbation to the Hamiltonian, the phase will be the same. Only “generic” symmetries, like time reversal and particle-hole symmetry, have to be preserved. An example of a symmetry which is not generic is translation invariance: we can add a term to the Hamiltonian which explicitly breaks it without violating the gap condition.

In this talk, we will focus on phases of matter that can be understood in terms of non-interacting fermions and topological band theory. We point out that some topological phases of matter, such as the fractional quantum hall effect, cannot be understood using these methods.

Topological insulators

The Hamiltonian describing an insulator, discretized on a lattice, is given by,

$$\mathcal{H} = \frac{1}{2}\sum_{i,j}\psi_i^* h_{ij}\psi_j,$$

where the sum is taken over the degrees of freedom of the system (lattice sites, spin, etc) and the ψ_i, ψ_i^*'s are fermion annihilation and creation operators. The matrix $H = [h_{ij}] = H^*$. We can choose a representative with translation invariance, giving, in the continuum limit,

$$\int_{\mathcal{B}\cong\mathbb{T}^d} d^d k \sum_{i,j}\psi_i^*(k)h_{ij}(k)\psi_j(k).$$

Observe that the transformations $\psi_i \mapsto e^{i\theta_i}\psi_i$ preserve $\mathcal{H}$. These symmetries are generated by the charges $Q_i = \psi_i^* \psi_i$ and form a $U(1) \times ... \times U(1)$ Lie group.

If we impose that the theory is symmetric not under this Lie group but under the subgroup $\mathbb{Z}_2 \times ... \times \mathbb{Z}_2$ given explicitly by the transformations $\psi_i \mapsto \pm\psi_i$ (and realized by the unitary operators $(-1)^{Q_i}$), we obtain a Hamiltonian which can support superconductivity.

Topological Superconductors

By writing the Hermitian operators

$$\gamma_{2i} = \psi_i + \psi_i^* \text{ and } \gamma_{2i+1} = -i(\psi_i - \psi_i^*),$$

we see that they satisfy Clifford algebra relations

$$\{\gamma_i, \gamma_j\} = \gamma_i\gamma_j + \gamma_j\gamma_i = 2\delta_{ij},$$

and the most general Hamiltonian on a lattice has then the form

$$\mathcal{H} = \frac{i}{8}\sum_{i,j} \gamma_i a_{ij} \gamma_j,$$

where $A = [a_{ij}] \in \mathfrak{so}(2n)$ ($n \equiv$ number of dof).

Notice that topological insulators and superconductors are significantly different.

Solve for the spectrum of an insulator $\Leftrightarrow$ diagonalize an Hermitian matrix through a unitary matrix.

$$H = U.\mathrm{diag}(d_1, ..., d_n).U^*, \ \ U \in \mathrm{U}(n)$$

Solve for the (quasi-particle) spectrum of a superconductor $\Leftrightarrow$ $\mathfrak{so}(2)$-block diagonalize a real skew-symmetric matrix through a special orthogonal matrix.

$$A = S.\left(\oplus_{i=1}^{n} \begin{bmatrix} 0 & \xi_i \\ -\xi_i & 0 \end{bmatrix}\right).S^t, \ \ S \in \mathrm{SO}(2n)$$

Where does topology come into play? One way to see this is to take a translation invariant representative and study the map $H : k \mapsto H(k) = [h_{ij}(k)]$ modulo the right equivalence relation, i.e., deformations preserving the finite gap condition. In what follows, we will focus on the topological insulator case with no symmetries (namely no time-reversal nor particle hole symmetry), but it is enough to understand the general picture.

Topological Band Theory

Smooth Families of Hamiltonians and associated Eigenbundles: Berry phases

We consider smooth families of Hamiltonians parameterized by a smooth manifold,

$$\{H(x) : x \in M\}, \text{ with } H : M \to \mathrm{Herm}(\mathbb{C}^n)$$

We assume constant maximal rank ($\sim$ gap condition).
Eigenvalue problem assumes the local form,

$$H(x)v = \lambda v,$$

Roots of the Characteristic Polynomial give the band spectrum,

$$p_x(\lambda) := \det(H(x) - \lambda I) = 0 \Rightarrow \{\lambda_j(x)\}_{j\in J},\ x \in M.$$

Eigenvector bundles

Locally solve for the Eigenspaces,

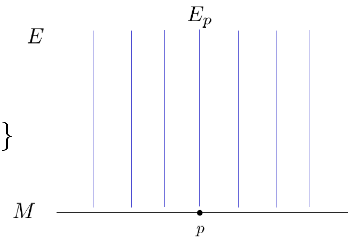
$$E_x^j := \{v \in \mathbb{C}^n : (H(x) - \lambda_j(x)I)v = 0\},\ x \in M$$

And take,

$$E_x^+ := \{v : v \in E_x^j \text{ for some } j \in J \text{ s.t. } \lambda_j(x) > 0\},$$
$$E_x^- := \{v : v \in E_x^j \text{ for some } j \in J \text{ s.t. } \lambda_j(x) < 0\}$$

Form the Unoccupied/Occupied (or Positive/Negative energy) "Eigenbundles"

$$E^\pm := \{(x, v) \in M \times \mathbb{C}^n : v \in E_x^\pm\}$$
$$\downarrow \pi^\pm$$
$$M$$



Where $\pi^\pm$ is just the projection onto the first factor.

Local Triviality

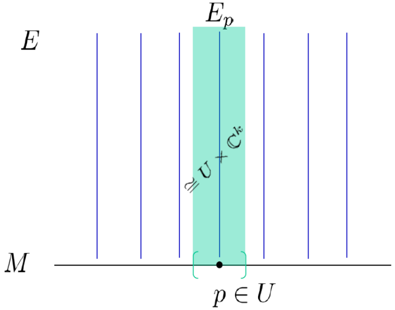
Locally, in some coordinate neighbourhood $U \subset M$, it is possible to find solutions of the eigenvalue problems, and these solutions provide a local trivialization of the eigenbundles.

$$E_p^+ = \mathrm{span}_{\mathbb{C}}\{v_i(p) : i = 1, \ldots, k\}, \ \forall p \in U \subset M$$

Any vector in E_p^+, $\forall p \in U$, can be written as a linear combination,

$$v = \sum_{i=1}^{k} a^i v_i(p).$$

Thus, $E^+|_U \cong U \times \mathbb{C}^k$.



Remark

If M is connected, the dimension of E^+ is locally constant (gap condition), therefore constant. We will assume that this is the case.

Local choice of basis: Gauge transformations

Any local section, i.e., a map $s : U \subset M \to E^+$, such that,

$$\pi^+ \circ s = \mathrm{id}_U$$

can be written as a linear combination, with smooth functions as coefficients:

$$s(p) = \sum_{i=1}^{k} a^i(p) v_i(p), \;\; p \in U \subset M,$$

$$\begin{array}{c} E^+ = \bigcup_{p \in M} E_p^+ \\ {\scriptstyle \pi^+} \big\downarrow \big\uparrow {\scriptstyle s} \\ U \subset M \end{array}$$

Local choice of basis: Gauge transformations

There is no preferred choice of local basis of the eigenbundles, hence if

$$\{s_1, ..., s_k\} \text{ and } \{e_1, ..., e_k\}$$

are two local frames for E^+ in an open neighbourhood U of $p \in M$, there exists a map $g : U \subset M \to \mathrm{GL}(k; \mathbb{C})$ such that

$$[s_1, ..., s_k] = [e_1, ..., e_k].g.$$

Remark

If there were a global choice of basis, the eigenbundle would be a trivial vector bundle, i.e., $E^+ \cong M \times \mathbb{C}^k$.

Unitary/Hermitian Structure

The eigenbundles $E^{\pm}$ come equipped with an Hermitian structure: the canonical Hermitian inner product in $\mathbb{C}^n$ yields an Hermitian structure, $\langle .,. \rangle$, in the trivial bundle $M \times \mathbb{C}^n$ which, by restriction, yields an Hermitian structure in $E^{\pm} \subset M \times \mathbb{C}^n$.

Berry Connection

A connection is an $\mathbb{R}$-linear map $\nabla : \Gamma(E) \to \Omega^1(E)$, satisfying the Leibniz rule. Since $E^{\pm}$ are sub-bundles of the trivial bundle, there exists a natural connection on them given as follows. If $P_{\pm}$ denotes the orthogonal projection (fiberwise) onto $E^{\pm} \subset M \times \mathbb{C}^n$, then we can define,

$$\nabla s = P_{\pm} ds, \ \forall s \in \Gamma(E^{\pm}),$$

where in the RHS d is understood as the flat connection on the trivial bundle $M \times \mathbb{C}^n$. If $\{s_1, ..., s_k\}$ is a local orthonormal frame for E^+, then the connection coefficients are local 1-forms given by,

$$\omega^i_j = \langle s_i, ds_j \rangle, \ 1 \leq i, j \leq k.$$

Berry Connection

If the eigenbundle's fibers are one-dimensional, then the Berry connection assumes the familiar form

$$\omega = \langle s, ds \rangle \equiv -iA \text{ (gauge field)}.$$

The local sections are interpreted as local wave-functions and parallel transport along a closed curve γ on the base space, given by solving $\nabla_{\dot{\gamma}} s = 0$ for some initial condition $s(\gamma(0))$, yields the so-called Berry phase (Holonomy)

$$s(\gamma(1)) = \exp(i \int_{\gamma} A).s(\gamma(0)).$$

Berry Curvature

If $\gamma = \partial\Sigma$, then, by Stokes' thereom,

$$\exp(i \int_{\gamma=\partial\Sigma} A) = \exp(i \int_{\Sigma} dA).$$

The quantity $F \equiv dA$ is the so-called Berry curvature. If it were trivial, then the Berry phase would, in this case, be irrelevant. The Berry curvature measures the non-triviality of parallel transport along an infinitesimal closed curve.

Berry Curvature and Characteristic classes

In general, the Berry curvature is locally given by the 2-forms

$$F^i_j = -i\Omega^i_j, \text{ (Physics literature)}$$

$$\Omega^i_j = d\omega^i_j + \sum_{l=1}^{k} \omega^i_l \wedge \omega^l_j, \ 1 \leq i \leq k.$$

One can write Gauge-invariant polynomials on the Berry curvature, and it turns out that these define de Rham cohomology classes which do not depend on the choice of the connection. These classes are called characteristic classes, since they depend only on the “twisting” of the vector bundle and not on additional structures.

Berry Curvature and Characteristic Classes

The Chern class is the de Rham cocycle associated to

$$\det(I_k + \frac{i\Omega}{2\pi}) = 1 + \mathrm{tr}(\frac{i\Omega}{2\pi}) + ...$$

The first non-trivial term is the 1st Chern class which appears in most practical examples in Condensed Matter. Notice that if a vector bundle admits a flat connection the above implies that the Chern class is trivial.

Remark

For our purposes, we may assume that there are only two constant eigenvalues, ± 1.

The maximal rank condition gives,

$$E^+ \oplus E^- = M \times \mathbb{C}^n,$$

and, in fact, due to the fact that we are dealing with families of Hermitian matrices, E^+ and E^- are orthogonal to each other. The previous condition imposes,

$$\begin{aligned} c(E^+)c(E^-) &= 1, \\ c_1(E^+) + c_1(E^-) &= 0. \end{aligned}$$

Topological Classification

Due to the previous discussion, we can find an orthonormal local basis of sections of E^+ and E^-, respectively, $[s_1, ..., s_k]$ and $[s_{k+1}, ..., s_n]$, such that $S = [s_1, ..., s_n]$, satisfies,

$$H(x).S(x) = S(x).\begin{bmatrix} I_k & 0 \\ 0 & -I_{n-k} \end{bmatrix}, \ \forall x \in U \subset M$$

Thus, the problem is locally diagonalized. Notice that multiplication on the right of $S(x)$ by a matrix function $g : U \to \mathrm{U}(k) \times \mathrm{U}(n-k)$, leaves the Hamiltonian invariant and, thus, $H(x)$ defines an element of $\mathrm{U}(n)/(\mathrm{U}(k) \times \mathrm{U}(n-k))$, i.e., the complex Grassmannian of k-planes in the standard n-dimensional complex vector space, denoted by $\mathrm{Gr}_k(\mathbb{C}^n)$.

Topological Classification

We can then think of a smooth family of Hamiltonians (with maximal rank) as a smooth assignment

$$H : M \to \mathrm{Gr}_k(\mathbb{C}^n)$$

If one wants to see an explicit realization of this map, one uses the identification of $\mathrm{Gr}_k(\mathbb{C}^n)$ as the space of orthogonal projectors of rank k and then the map assigns to each point $p \in M$ the projection onto E_p^+.
There is a canonical vector bundle over $\mathrm{Gr}_k(\mathbb{C}^n)$. Namely, the tautological bundle,

$$E = \{(W, v) \in \mathrm{Gr}_k(\mathbb{C}^n) : v \in W\}.$$

We then realize that

$$\begin{aligned} E^+ &= \{(p, v) \in M \times \mathbb{C}^n : v \in E_p^+ = H(p)\} \\ &\cong \{(p, (W, v)) \in M \times E : W = H(p)\} =: H^*(E) \end{aligned}$$

Topological Classification

The Chern class is natural with respect to pullbacks,

$$c(H^*(E)) = H^*(c(E)).$$

Thus, since coholomogy is an homotopy invariant, the Chern class does not change if we make a smooth perturbation of the Hamiltonian. Is the same true with the vector bundle? Yes!

Proposition

Let $\{H_t : M \to \mathrm{Herm}(\mathbb{C}^n)\}_{t\in[0,1]}$ be a smooth family of Hamiltonians. Then the associated Eigenbundles are all isomorphic.

Remark

This justifies our, not so innocent, choice for constant eigenvalues. The associated continuous transformation is called spectrum flattening.

Topological Classification

If n is sufficiently large, the homotopy classes of maps $H : M \to \mathrm{Gr}_k(\mathbb{C}^n)$ are in bijection with the isomorphism classes of vector bundles of rank k over M: $\mathrm{Vect}_k^{\mathbb{C}}(M) \cong [M, \mathrm{BU}(k)]$ with $\mathrm{BU}(k) = \mathrm{Gr}_k(\mathbb{C}^\infty)$.

Physically, allowing n to be sufficiently large is equivalent to allow one to augment the system by a trivial one (add extra flat bands): it may be possible that the two systems cannot be smoothly deformed into each other, but after augmenting they can be (stable equivalence).

A class of non-trivial examples

(joint work with M. A. N. Araújo and V. R. Vieira)

Model Hamiltonian and SO(4)

Consider the following Hamiltonian describing fermions on a 2D-lattice:

$$H(k) = \begin{pmatrix} h(k)\cdot\tau & i\bar{D}(k)\tau_2 \\ -iD(k)\tau_2 & -(h(k)\cdot\tau)^t \end{pmatrix},\ k \in \mathcal{B} \cong \mathbb{T}^2$$

with $h = (h^0, \vec{h})$, $\tau = (\tau_0, \vec{\tau})$ and $D = D^1 + iD^2$. The above Hamiltonian can be written as,

$$H(k) = \vec{h}(k)\cdot\vec{S} + \vec{h'}(k)\cdot\vec{T},$$

where $\vec{h'}(k) = (h^0(k), D^1(k), D^2(k))$, and

$$[S_i, S_j] = 2i\varepsilon_{ijk}S_k,\ [T_i, T_j] = 2i\varepsilon_{ijk}T_k,\ [S_i, T_j] = 0,$$

generate a Lie algebra $\mathfrak{so}(4) \cong \mathfrak{so}(3) \oplus \mathfrak{so}(3)$. In fact, there exists a matrix S such that,

$$S.H(k).S^* = iA(k),\ \text{with } A(k) \in \mathfrak{so}(4)$$

Hodge Duality

The Lie algebra $\mathfrak{so}(4)$, identified as the vector space of real skew-symmetric 4×4 matrices, has a notion of duality provided by the Levi-Civita symbol:

$$(*A)_{ij} = \frac{1}{2} \sum_{k,l=1}^{4} \varepsilon_{ijkl} A_{kl}, \ 1 \leq i, j \leq 4.$$

Now $** = 1$, meaning that we can decompose the matrices into self-dual (S's) and anti-self-dual matrices (T's).

Facts of life: A skew-symmetric matrix can be put in canonical form by a rotation matrix in SO(4). There is a natural SO(4)$-$ invariant (thus, Gauge-invariant): The Pfaffian polynomial (a squareroot of the determinant).

The Pfaffian and ground state parity

A simple example gives us a natural interpretation for the sign of Pf(A). Consider a single fermionic harmonic oscillator

$$\mathcal{H} = \omega(\psi^* \psi - \frac{1}{2}) = \frac{i}{4}\omega\gamma_1\gamma_2 = \frac{i}{8}\left[\gamma_1 \ \gamma_2\right] \cdot \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix} \cdot \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}.$$

Now, Pf(A) $= \omega$. If $\omega > 0$ the ground state is $|0\rangle$, with energy $-\omega/2$. If $\omega < 0$, the ground state is $|1\rangle = \psi^*|0\rangle$ with energy $\omega/2$. In other words, the sign of the Pfaffian measures the parity of the many-body ground state.

By a spectrum flattening transformation, depending on the sign of $\mathrm{Pf}(A(k))$, one sees that $A(k)$ can be put into the canonical form,

$$A(k) = S(k). \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \pm 1 \\ 0 & 0 & \mp 1 & 0 \end{bmatrix} .S^t(k).$$

Mathematically, under the equivalence of perturbing the Hamiltonian while keeping the gap open, the SO(4)- adjoint orbits, $\mathcal{O}(A) = \{S.A.S^t : S \in \mathrm{SO}(4)\}$, (which, because the Hodge operator commutes with special rotations, can only be, modulo diffeos, $\{\mathrm{pt}\}$, S^2, $S^2 \times S^2$) can all be represented by spheres S^2 (self-dual or anti-self-dual). The following theorem holds.

Theorem [J. Phys.: Condens. Matter 27 465501 (2015)]

If a physical system is modelled by the previous Hamiltonian, such that a gap condition is satisfied, then,

(i) The pfaffian polynomial of $A(k)$ is either positive or negative everywhere. In the first case, $H(k)$ can be smoothly deformed into $\vec{h}(k) \cdot \vec{S}$. On the second case $H(k)$ can be smoothly deformed into $\vec{h'}(k) \cdot \vec{T}$;

(ii) The first Chern number of E^- (occupied Eigenbundle) is given by twice the degree of $\Phi_+ : k \mapsto \vec{h}(k)/|\vec{h}(k)|$ (for positive Pfaffian) or $\Phi_- : k \mapsto \vec{h'}(k)/|\vec{h'}(k)|$ (for negative Pfaffian);

(iii) If H is a BdG Hamiltonian, then one has to account for the doubling of the degrees of freedom and we have to divide the Chern number by a factor of 2.

Applications

Now consider the associated second quantized Hamiltonian of fermions on a lattice, i.e.,

$$\mathcal{H} = \int_{\mathcal{B}\cong\mathbb{T}^2} d^2k \; \psi^\dagger(k) H(k) \psi(k),$$

Then, depending on what the physical meaning of ψ we will have different applications. We found the following non-trivial applications,

1) *Chern insulator*, considering spinless fermions on a lattice with four orbitals per site, in the basis $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)$;
2) *Single orbital superconductor* $\psi = (\psi_\uparrow, \psi_\downarrow, \psi_\uparrow^\dagger, \psi_\downarrow^\dagger)$ or $\psi = (\psi_\uparrow, \psi_\downarrow, \psi_\downarrow^\dagger, -\psi_\uparrow^\dagger)$;
3) *Multiorbital superconductor*. This requires the decoupling of a higher dimensional BdG matrix.

A few remarks

This is an improvement with respect to the usual single band models which are an over simplification because topological materials are, in a realisitic physical setup, multiorbital.

It can be regarded as an extension of previous suggestions for practical realization of Majorana modes in TI/Sc heterojunctions [Alicea, RPP 2012] which did not identify the physical significance of the topological criterion found as a $\mathbb{Z}_2$ topological invariant.

If this behaviour is realized experimentally, then this would allow for potential applications in topological quantum computation as this could be a way to control Majorana fermions.

Acknowledgements

I thank the support from the DP-PMI and Fundação para a Ciência e a Tecnologia (Portugal), namely through scholarship SFRH/BD/52244/2013.
A very special acknowledgement goes to M. Abreu for very fruitful discussions regarding the mathematical concepts behind the paper [J. Phys.: Condens. Matter 27 465501 (2015)].