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Executive Summary of the Thesis

A C*-Algebraic Approach to Topological Phases for Insulators

Laurea Magistrale in Mathematical Engineering - Ingegneria Matematica

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1. Introduction

The goal of this work is to give the basis for the understanding of what topological insulators are and what it means to classify them. In particular we will consider a particular classification for topological insulators proposed in [2] by the co-advisor of this Master thesis. The prerequisites are of two types: physical and mathematical ones. At first, we will recall concepts from quantum physics to describe qualitatively insulators and conductors: we will recall the "tight binding" approximation to describe a solid and the "band theory" for a crystal. Then, we will be able to talk about topological insulators, which are a kind of exotic materials which display characteristics both of conductors and insulators. A first experimental example is the *Quantum Hall* insulators, which is briefly described. Their key property is their stability to "continuous" deformations: we can measure with great precision some quantities even if a perturbation is present! To study rigorously their behaviour, we need some mathematical tools, in particular from operator algebra. We will introduce the concept of C^*-algebra, which is the topological space where our topological insulators live. Then, we will introduce K-theory, a branch of operator algebra useful to study the structure of C^*-algebras. With these tools we are ready for the description of the classification of topological insulators which is proposed. Here, "Classification" means to describe, given a particular physical situation, the classes of insulators and their relations. Two insulators are in the same class if we can deform continuously one insulator into the other (preserving some properties). In particular, the key aspect of the approach is to consider some classical physical symmetries. Then, we will see some examples/exercises of real topological insulators (in particular the well-known Haldane's model) on which I prove some properties and finally, some exercises (fundamental for real applications) on C^*-algebras with symmetries.

2. Physical and mathematical recalls

In quantum physics, a physical system is described by its hamiltonian, a self-adjoint operator over an Hilbert space. We can consider a particular sub-space of this space, namely a C^*-algebra. We can define the spectrum of an element of the C^*-algebra and identify it with the set of possible values for the energy of the electrons of the system. Using the "tight binding" approximation, we see the appearance of energy bands in the spectrum of the operator which are functions of the quasi-momentum k: we see that we could have regions of forbidden energy ("gaps" in the spectrum).

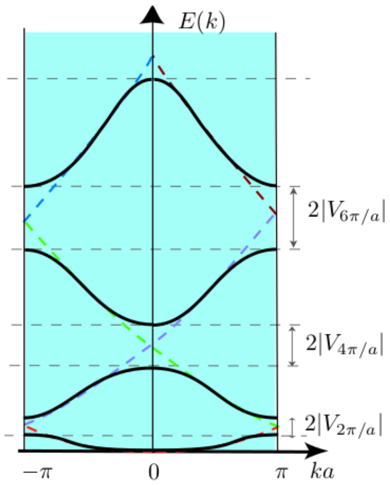

Figure 1: Energy bands.

To define insulators and conductors, we give the definition of Fermi energy: it is the energy of the last electron added at $0K$ temperature. A material is a conductor if the Fermi energy belongs to one of the bands, an insulator if the Fermi energy is in a gap. Without loss of generality (in most cases), we can assume the Fermi energy to 0: therefore, an insulator is a invertible self-adjoint element of the C^*-algebra. Concerning the mathematical part, C^*-algebras are particular Banach spaces with a convolution satisfying the condition $\|a^*a\| = \|a\|^2$ for every a in the C^*-algebra. They have a quite rigid structure and one of the fundamental result about them is the "Gelfand-Naimark" theorem: it states that every C^*-algebra is isomorphic to a sub-C^*-algebra of $\mathcal{B}(H)$, the bounded linear operators over some Hilbert space H. To define symmetries over a C^*-algebra, we define the concept of *grading* γ (an order two $\mathbb{C}$-linear $*$-isomorphism) and of *real structure* $\mathfrak{r}$ (an order two anti-linear $*$-isomorphism). We have five cases of symmetries: no symmetry, chiral symmetry (we consider the elements such that $\gamma(a) = -a$), time reversal symmetry (TRS, $\mathfrak{r}(a) = a$), particle hole symmetry (PHS, $\mathfrak{r}(a) = -a$) and chiral symmetry with time reversal symmetry ($\gamma(a) = -a$ and $\mathfrak{r}(a) = a$).

The goal of K-theory is to associate to homotopy classes of particular elements in the C^*-algebra A (either projections or unitaries) an abelian group: it will be called $K_0(A)$ in the case of projections and $K_1(A)$ in the case of unitaries. We are interested in Van Daele's approach to K-theory: he menages to associate an abelian group to the homotopy classes of a subset of the elements of the C^*-algebra which satisfy a symmetry condition. Clifford algebras will help us to adapt each type of symmetry of topological insulators in order to use Van Daele's construction.

3. Description of the approach

Paper [2] has two main goals. The first one is to give a classification of possible cases of symmetries. PHS and TRS correspond to a real structure on a C^*-algebra and we could have potentially infinitely many of them. Considering further assumptions to simplify the mathematical problem, the author presents a compact classification of possible symmetries. The key idea is to consider a reference real structure: in this way, it is possible to define a relation between all the other real structures and classify them. We define the concept of **inner related** and **inner conjugate** real structures. Given the C^*-algebra A, $\mathfrak{r}$ and $\mathfrak{s}$ are inner related if it exists $u \in A$ (the generator) s.t. the following diagram commutes.

$$\begin{array}{ccc} A & \xrightarrow{\mathfrak{r}} & A \\ & \searrow^{\mathrm{Ad}_u} & \downarrow \mathfrak{s} \\ & & A \end{array}$$

$\mathfrak{r}$ and $\mathfrak{s}$ are inner conjugate if it exists $w \in A$ s.t. the following diagram commutes.

$$\begin{array}{ccc} A & \xrightarrow{\mathfrak{r}} & A \\ \mathrm{Ad}_w \downarrow & & \downarrow \mathrm{Ad}_w \\ A & \xrightarrow{\mathfrak{s}} & A \end{array}$$

We can show that inner conjugation implies inner relation. An important result obtained in the paper is that, under further technical hypothesis, given a reference real structure, up to stabilisation and inner conjugation, there is a **finite number of real structures** inner related to the first one. Given a reference real structure, we can distinguish between an even and odd TRS and PHS.

The second goal is: given one of the previous cases of symmetry, we want to give a description of the algebraic structure of the topological phases. Also in this case, the idea is to choose a reference element and to define an equivalence relation. Then, it is possible to apply Van Daele's construction to obtain an abelian group. Van Daele's construction applies straightforwardly just in the case of chiral symmetry. In the other cases (i.e. the grading is trivial) we do not have any odd elements: the key idea is to use Clifford algebras to produce odd elements. For example, in the case of no symmetry, we replace the C^*-algebra A with $A \otimes \mathbb{C}l_1$. In the paper, the author associates to each symmetry case a K-group (we note with DK Van Daele's group and with K_n Van Daele's groups of higher oder, as defined in [3]). Two classifications are presented. The first one is a "rough" one, under minimal assumptions. To give an example of the type of groups we are dealing with, in the case of no symmetry, the classes of topological insulators in the C^*-algebra A are isomorphic to

$$DK\left(A \otimes \mathbb{C}l_1, \mathrm{id} \otimes \phi\right) = K_0(A, \mathrm{id}) \cong KU_0(A)$$

where $KU_0(A)$ is the standard K_0-group of A seen as ungraded complex C^*-algebra. When we just have chiral symmetry, we have

$$DK(A, \gamma) = K_1(A, \gamma)$$

The second classification is finer and it is a classification with respect to a reference real structure. The case with no symmetry and with just chiral symmetry do not change. Instead, now we can distinguish an even and odd TRS and PHS and four cases corresponding to TRS with chiral symmetry: we have a total of ten possible symmetries (two complex cases and eight real cases). For each of them, the author proposes a K-group.
In the case of chiral symmetry and time reversal symmetry we get the following table

$\eta_{\mathfrak{t},\mathfrak{f}}$	K-group
$(+1, +1)$	$K_1\left(A^{\mathfrak{f}}, \gamma\right)$
$(+1, -1)$	$K_{-1}\left(A^{\mathfrak{f}\circ\gamma}, \gamma\right)$
$(-1, +1)$	$K_5\left(A^{\mathfrak{f}}, \gamma\right)$
$(-1, -1)$	$K_3\left(A^{\mathfrak{f}\circ\gamma}, \gamma\right)$

If the grading is trivial (no chiral symmetry) we get

Symmetry	$\eta^{(1)}_{\mathfrak{r},\mathfrak{f}}$	K-group
TRS even	$+1$	$KO_0\left(A^{\mathfrak{f}}\right)$
TRS odd	-1	$KO_4\left(A^{\mathfrak{f}}\right)$
PHS even	$+1$	$KO_2\left(A^{\mathfrak{f}}\right)$
PHS odd	-1	$KO_6\left(A^{\mathfrak{f}}\right)$

In both cases, the classification can be improved if we assume the grading to be inner (i.e. $\gamma = \mathrm{Ad}_\Gamma$ for $\Gamma \in A$).

4. Examples

The first example is an easy application of the Bloch-Floquet transform to compute the energy band of a crystal. We consider the Hilbert space $\ell^2(\mathbb{Z})$ and the hamiltonian

$$H = T + T^* + V$$

where T is the right-shift operator and V is a periodic potential given by

$$(V\psi)(n) = \psi(n)V(n) \quad V(n) = (-1)^n a,\ a \in \mathbb{R}_+$$

It is interesting to see that, even if we are neglecting the spin of electrons, the fact that atoms are not identical (the potential is 2-periodic) introduces two internal degrees of freedom. Indeed, using Bloch-Floquet transform we find

$$H \mapsto \hat{H} = \begin{pmatrix} a & 1 + \mathrm{e}^{\mathrm{i}k} \\ 1 + \mathrm{e}^{-\mathrm{i}k} & -a \end{pmatrix}$$

The eigenvalues $E(k)$ of $\hat{H}$ are (figure 2)

$$E(k) = \pm\sqrt{2\cos k + 2 + a^2}$$

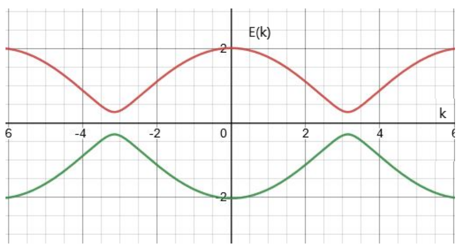

Figure 2: Bands in the spectrum of H ($a = 0.25$).

The second example is the demonstration that the insulator of Haldane's model is a non trivial insulator. We consider a tight-binding model of spinless electrons on a two-dimensional hexagonal (honeycomb) lattice. The unit cell contains two types of atoms A and B (see figure 3).

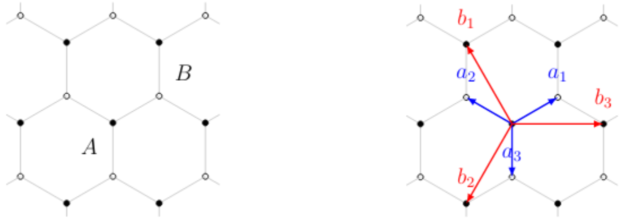

Figure 3: Honeycomb lattice used in Haldane's model.

We consider as Hilbert space the space of square integrable functions over the sites of type A and B. The form of the hamiltonian for Haldane's model is:

$$\begin{aligned}\hat{H} =& t\sum_{\langle i,j\rangle}|i\rangle\langle j| + t_2\sum_{\langle\langle i,j\rangle\rangle}|i\rangle\langle j| \\ &+ M\left[\sum_{i\in A}|i\rangle\langle i| - \sum_{j\in B}|j\rangle\langle j|\right]\end{aligned}$$

Using Bloch-Floquet transform, we obtain the hamiltonian in the quasi-momentum domain

$$H(k) = \sum_{j\in\{0,x,y,z\}} h^j(k)\sigma_j$$

where σ_j are the Pauli matrices ($\sigma_0 = I_2$) and h_j are real functions. We can compute the energy bands, i.e. the eigenvalues of $H(k)$

$$\epsilon_{\pm}(k) = h_0(k) \pm h(k)$$

where $h_0(k)$ and $h(k)$ are real functions. There are two bands and this hamiltoninan describes an insulator. We can compute the **Chern number** of the insulator: if it is different from 0, then the insulator is not trivial. Chern number c_1 is a topological invariant and it is obtained by integrating a function of the Fermi projector P (the projector over the subspace of the normalised eigenstate u corresponding to the lower band energy) over the Brioullin zone S of the crystal. It is given by

$$c_1 = \frac{1}{2\pi\mathrm{i}}\int_S \mathrm{Tr}(P)\mathrm{d}P\mathrm{d}P$$

Using Stokes theorem, we show that

$$c_1 = \lim_{\varepsilon\to 0}\frac{1}{2\pi\mathrm{i}}\int_{C_\varepsilon}\langle u|\mathrm{d}u\rangle$$

where C_ε is the boundary of the surface $S_\varepsilon \subset S$ where we removed a small surface of measure of order ε containing the singularities of u. We reduce the computation of the previous integral to the computation of the index of some curves in the complex plane depending on u. We find that, under certain choices for the parameters, the Chern number of the Haldane model is 1 and therefore, the insulator is not trivial.

Finally, we consider some easy examples of C^*-algebra and we compute gradings and real structures on it: we consider the cases $\mathbb{C}$, $\mathbb{C}\oplus\mathbb{C}$, $M_2(\mathbb{C})$ and $M_n(\mathbb{C})$. On one side, these examples allowed me to practise on *concrete* examples and on the other, to prove some properties about gradings and real structures which are assumed in [2]. In the case $\mathbb{C}$, we have that the only grading is the identity and the only real structure is complex conjugation. In $\mathbb{C}\oplus\mathbb{C}$, the only balanced grading is the flip isomorphism ($\phi(a,b) = (b,a)$) and the possible real structures are $\mathfrak{r}(s,t) = (\bar{s},\bar{t})$ and $\mathfrak{r}(s,t) = (\bar{t},\bar{s})$. In the case $M_2(\mathbb{C})$, up to a changing of the basis, the only balanced grading is $\gamma = \mathrm{Ad}_{\sigma_z}$. Analogously, in the case $M_n(\mathbb{C})$ we find that the gradings have the form Ad_Γ, where Γ is one of the $\Gamma_k \in M_n(\mathbb{C})$

$$\Gamma_k = \begin{pmatrix} I_k & 0_{k,n-k} \\ 0_{n-k,k} & -I_{n-k}\end{pmatrix}, \quad k\in\{0,1\dots n\}$$

Moreover, to have a balanced grading, we must have $n = 2k$ (therefore, n must be even). A corollary shown in the paper tells us that there are just four real structures up to stabilisation and inner conjugation: we find three of them for $n = 2$ and the last one just in the cases $n = 4l$, $l\in\mathbb{N}$. The real strucutures are given in the following table.

Real structures on $M_n(\mathbb{C})$

	n	**real structure**
r_1	2	$\mathfrak{c}$
r_2	2	$\mathrm{Ad}_{\sigma_x}\circ\mathfrak{c}$
r_3	2	$\mathrm{Ad}_{\sigma_y}\circ\mathfrak{c}$
r_4	4	$\mathrm{Ad}_{\sigma_y}\circ\mathfrak{c}\otimes\mathfrak{c}$

where $\mathfrak{c}$ is complex conjugation. Moreover, we link the study of these fundamental C^*-algebras to the typical cases that we can find in applications. Indeed, the typical C^*-algebra (after tensoring with $\mathbb{C}l_1$ to apply Van Daele's construction) is

$$\mathcal{C}(\mathbb{S}^1)\otimes M_N(\mathbb{C})\otimes \mathbb{C}l_1 \cong \mathcal{C}(\mathbb{S}^1)\otimes M_N(\mathbb{C})\oplus M_N(\mathbb{C})$$

We can see how the study of the real structures over C^*-algebras of the type $M_N(\mathbb{C})$ is important, as they appear recurrently.

5. Conclusions

To conclude, we mention a few applications of topological insulators. Topological insulators are extremely interesting for the development of topological quantum computers thanks to their property to be stable to exterior perturbations: stable edge currents could encode information with a low risk of error. Aside from quantum computers, other promising applications are in the field of photodetectors, magnetic devices, field-effect transistors and lasers.
Concerning the continuation of this project, the idea is to compare the mathematical approach to classify topological phases of [2] to another one, namely the one presented in [1]. Also in the second approach Van Daele's picture is used to classify topological phases but taking a different starting point: it would be interesting to find the link between the results of the two approaches and determine if they are equivalent.

References

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