Topological Classification of Insulators and Superconductors

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Abstract

In this thesis a topological classification is made of condensed matter systems. The presence or absence of discrete symmetries divide the systems into ten different classes. Mathematically the symmetries restrict the space of Hamiltonian matrices, so first the matrix form of time-reversal, particle-hole and chiral symmetry are discussed. This will result in the ten symmetry classes with their properties.

The Hamiltonians of the classes will be related to the bandstructure using projection operators and the properties of each symmetry class will restrict the allowed bandstructures. After a short introduction of homotopy theory, the homotopy groups will be used to find the classes where topologically different bandstructures are possible. The result is that for any dimension there are five classes with non-trivial topology. Finally for the physical relevant dimensions a few examples are given of topological states and the experimental discoveries are discussed.
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Chapter 1

Introduction

1.1 Personal Motivation

Over the past three years I have completed bachelor degrees in Mathematics and in Physics. These two studies are combined into one program because of the connection between the subjects. That connection was however not apparent in the normal classes and therefore I started looking for a bachelor project that would connect the two.

Originally I wanted to do a project in high energy physics, were it not for a presentation I had to give in the Condensed Matter Physics class. After a few talks with my supervisor in which the subject of my project changed a bit, I landed on my current choice: “The Topological Classification of Insulators and Superconductors”.

Judging from the title I expected this subject to require at least some knowledge from both the mathematical area of Topology as the field of Condensed Matter Physics. As you will notice upon reading the rest of this thesis, this was correct. So after three years I finally am able to use my knowledge from both fields together. I think therefore that this thesis really completes the two bachelors.

1.2 Scientific Motivation

The use of topology in condensed matter physics is fairly new. The first example was about 30 years ago in the quantum Hall effect (QHE). It turned out that the quantized Hall conductance was irrespective of the shape and size of the sample, thereby giving an example of a topological invariant in condensed matter systems.

The subject of topological insulators and superconductors has only started developing in the last 5 years [4], when it was realized that the QHE was not the only topological state possible. Examples where found of a new spin quantum
Hall effect (SQHE) and now the experimental search is on for more topologically special states.

This thesis will focus on the theoretical part of the field, which finds its roots in random matrix theory, first studied around 1930 [7]. In the study of random matrices the question was how the eigenvalues where distributed for a matrix with random values. Around 1950 physicists became interested when this turned out to be a model for slow neutron resonances in nuclear physics. The systems where so chaotic that it was impossible to find the relevant Hamiltonians so they were modeled using random values.

About ten years later Wigner and Dyson where the first to use time-reversal symmetry to classify these systems [7]. This resulted in the first three classes of the now ten symmetry classes that will be the main topic of this thesis. The search for (likely all) the classes was only completed in 1997 with the discovery of the last four classes [2].

When it turned out that the QHE was an example of one of the classes that Wigner and Dyson found [3], it was clear that the symmetry classes could also be realized in condensed matter systems. Here the precise interaction of all particles is to complex to give a Hamiltonian, so by representing it by random matrices it is possible to study general properties. This means that Hamiltonians will usually not be given explicitly, which has the effect that the theory is very generally applicable but also a bit abstract.

By studying these classes using topology it is possible to see where states like the quantum Hall state are possible. These states are protected by their topology from being destroyed, which for the QHE results in a fixed conductance because the electrons cannot fall back to a lower energy state and have to keep moving. The hope is that in one of the classes a material can be found that could be used for a quantum computer. The protected states could then be used as quantum bits that have the property that the bits are protected from being destroyed by accidental measuring of the state.

1.3 Dutch Summary

Dit bachelor project gaat over de classificatie van topologische isolatoren en supergeleiders. De classificatie gebeurt aan de hand van een aantal symmetrieën van veel-deeltjes systemen. Dat zijn tijd-symmetrie, die de richting van de tijd omdraait, deeltje-antideeltje-symmetrie, dat de naam deeltjes en antideeltjes omdraait, en hun combinatie chirale symmetrie, die tegelijk beide doet. Eerst kijk ik hoe deze symmetrieën worden weergegeven in de natuurkundige taal van veel deeltjes systemen. Daarna kan ik aan de hand van deze symmetrieën tien verschillende symmetrie klassen identificeren.
1.4. General Outline

The basic goal for this thesis is to understand the classification of topological insulators and superconductors. This means that I will largely follow the paper of Schnyder et al [3], where this classification was first given in its complete form. The classification is based on symmetries that are possible in condensed matter systems so I will begin by discussing these. After that I can construct the distinct classes and give their defining equations. The interesting question then is in which classes topologically distinct states are possible, so I will need to introduce the concept of homotopy groups and then compute these for the classes. As a conclusion I will try to find example materials for each of the nontrivial classes.
Chapter 2
Symmetries

All physical systems discussed in this thesis will be non-interacting fermionic systems\(^1\). They can be described by a Hamiltonian, a matrix, acting on the Hilbert space of the system. The symmetries that will be discussed are time-reversal, particle-hole and chiral symmetry. The objective of this chapter is to find how they can be expressed in the language of matrices.

2.1 General Form of a Symmetry

Any symmetry will need to act on the Hilbert space of the system. The question is: what are the possible actions of the symmetry operator? This question can be answered by Wigner’s Theorem \([8]\).

**Theorem 1. Wigner’s Theorem**

Let \( \mathcal{H} \) be a complex Hilbert space and \( S : \mathcal{H} \to \mathcal{H} \) a surjective map with the property 
\[ |\langle Sx, Sy \rangle| = |\langle x, y \rangle|, \forall x, y \in \mathcal{H}. \]

Then \( S \) is of the form \( Sx = \phi(x)Ux \), where \( U \) is an unitary or antiunitary operator and \( \phi(x) \) is a phase-function, so \( |\phi(x)|^2 = 1 \).

Symmetries like time-reversal or particle hole symmetry must do nothing observable to a physical system when the symmetry operation is applied twice. Therefore these symmetries need to be represented by surjective maps on the Hilbert space. It is also natural to demand that a symmetry operator has the property \( |\langle Sx, Sy \rangle| = |\langle x, y \rangle| \), which just means that comparing states before or after a symmetry operation should yield the same answer. Thus Wigner’s Theorem applies here and time-reversal and particle hole symmetry need to be represented by either unitary or antiunitary operators.

\(^1\)The Hamiltonian of the system should not have an interaction term as described in section 2.3.
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2.2 Time-Reversal Symmetry

Since time-reversal symmetry (TRS) is unitary or antiunitary it can be represented by $T = C$ or by $T = CK$ where $C$ is a unitary matrix and $K$ stands for complex conjugation. This means that if $T$ is unitary it has the property $\langle Tx, Ty \rangle = \langle x, y \rangle$, $\forall x, y \in \mathcal{H}$, however if it is antiunitary then $\langle Tx, Ty \rangle = \langle x, y \rangle$, $\forall x, y \in \mathcal{H}$ holds.

Now there are (at least) two distinct ways to tell which one it is. Take for example the commutator of time and energy, $[t, E] = i\hbar$. If time is reversed, it means that $t \rightarrow -t$, but energy remains the same. Thus in order to conserve the commutator it is necessary that $T(i) = -i$, so the TRS operator must be antiunitary.

A more mathematical way [13] with the same result is by noting that if $T$ is unitary the generator of time translations must pick up a minus sign when the symmetry acts.

$$ e^{iHt} = C^d e^{-iHt} C \Rightarrow -H = C^d HC $$
$$ \Rightarrow -H|n\rangle = C^d HC|n\rangle $$
$$ \Rightarrow -E|n\rangle = C^d HC|n\rangle $$
$$ \Rightarrow -EC|n\rangle = HC|n\rangle. $$

On an infinite lattice, where there are an infinite amount of energy states, this would mean that under time-reversal there is no state with a lowest energy, so a system could never reach its groundstate. Therefore the time-reversal operator should be antiunitary. On a finite lattice it is then natural to also choose the operator to be antiunitary. In that way there is no problem in the limit of bigger and bigger systems.

To see how TRS does work on the hamiltonian, take two states $\phi$ and $\psi$. They transform as

$$ T\phi = C\phi^* $$

and therefore (by the antiunitarity of $T$)

$$ \langle \psi | H | \phi \rangle = \langle T\phi | T(H) | T\psi \rangle $$
$$ \overline{\langle \phi | H^T | \psi \rangle} = \langle C\phi^* | T(H) | C\psi^* \rangle $$
$$ \langle \phi^* | H^T | \psi^* \rangle = \langle \phi^* | C^{-1}T(H)C | \psi^* \rangle $$
$$ H^T = C^{-1}T(H)C $$
$$ T(H) = CH^T C^{-1}. $$

There are still two ways that time-reversal symmetry can be implemented [7]. The difference is that there is still a choice $C^T = \pm C$. To see this remember that
acting twice with the symmetry has to do nothing to the physical system. A state can only pick up a non-measurable phase.

\[ T^2 = \alpha \cdot 1, \quad |\alpha| = 1. \]

This means that by combining

\[ T^2 = CKCK = CC^* KK = CC^* = \alpha \cdot 1 \]

and the unitarity \( C^T C^* = 1 \), this becomes

\[ C = \alpha C^T = \alpha (\alpha C^T)^T = \alpha^2 C. \]

Therefore \( \alpha = \pm 1 \) and \( C^T = \pm C \).

Both options are valid TR symmetries and they will be denoted by TRS+1 and TRS-1. TRS+1 is the time-reversal symmetry that has the properties \( H = CH^T C^{-1} \), \( CC^\dagger = 1 \) and \( C = C^T \), while TRS-1 has the same properties except for the last one which is replaced by \( C = -C^T \).

## 2.3 Particle-Hole Symmetry

Particle-Hole Symmetry (PHS) is a symmetry that relates the description of a system using particles to the same system being described by holes. On a lattice it is possible to construct the Fermi sphere of a system, that is the sphere of all occupied Fourier-modes of the lattice. In a normal material the Fermi-sphere would be comprised of all electrons with their respective \( k \)-value, their momenta. All modes that are not filled are called holes.

On a (finite) lattice there is a maximum number of states, so there is a maximum number of holes. This means that it is possible to describe a system by its holes. Instead of filling the Fourier-modes from below with particle, the description fills the Fourier-modes from the top with holes. This allows for two descriptions of the same system. If the description are the same, i.e. an excitation of a particle is the same as an excitation of a hole, then the system is particle-hole symmetric.

This is best described in the language of second quantization. This is just a fancy word for describing particles and anti-particles in terms of creation and annihilation operators on the vacuum state. For example when solving the quadratic potential in quantum mechanics the Hamiltonian can described by two operators, \( a \) and \( a^\dagger \). The \( a^\dagger \) is the raising operator and applying it to the groundstate raises the energy with \( \hbar \omega \) making it the first excited state, with the lowering operator \( a \) it is possible to go down again.

In the same way it is possible to define creation \( c^\dagger \) and annihilation \( c \) operators. Instead of raising the energy, these creation operators raise the number of particles
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by one. The annihilation operator then of course lowers the number of particles by one, but this can also be seen as creating a hole. This means that in the language of second quantization a system has PHS if it is symmetric under the interchange of the \( c^\dagger \) and \( c \) operators.

To see what happens use the Hubbard model as an example. The Hubbard model has as Hamiltonian [1]:

\[
H = -t \sum_{\langle i,j \rangle} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2}) - \mu \sum_i \sum_{\sigma} n_{i,\sigma}
\]

Here \( n \) is the number operator, that also appeared in the quadratic potential. There it gave the number of energy quanta added, so the total energy had the form \( \hbar \omega (n + \frac{1}{2}) \), here it gives the number of particles but has the same form. The sum over \( \langle i,j \rangle \) means that the sum is over all neighboring states \( i \) and \( j \) and the \( \sigma \) stands for spin up or spin down.

The Hubbard Hamiltonian has three terms. The first one, with a strength parameter \( t \), is the hopping term. It annihilates a particle in state \( j \) and creates a particle in the state next to it, so the particle hops to the next state. In the model the Coulomb interaction between particles is simplified to only work on the same lattice site as this is the largest contribution. This results in the second term, the interaction term, with strength parameter \( U \). The last term is a chemical potential, it just measures the amount of particles present. When a system has a fixed number of particles this term remains constant.

Now changing particles to holes and holes to particles (\( c^\dagger \leftrightarrow c \)) this becomes

\[
H_{PHS} = -t \sum_{\langle i,j \rangle} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i (c^\dagger_{i,\uparrow} c_{i,\uparrow} - \frac{1}{2})(c^\dagger_{i,\downarrow} c_{i,\downarrow} - \frac{1}{2}) - \mu \sum_i \sum_{\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}.
\]

To rewrite this the commutation relations are needed. Since the particles are all fermions the anticommutators are given by

\[
\{c^\dagger_i, c_j\} = c^\dagger_i c_j + c_j c^\dagger_i = \delta_{i,j}.
\]

This gives the result

\[
H_{PHS} = t \sum_{\langle i,j \rangle} c^\dagger_{j,\sigma} c_{i,\sigma} + U \sum_i (1 - c^\dagger_{i,\uparrow} c_{i,\uparrow} - \frac{1}{2})(1 - c^\dagger_{i,\downarrow} c_{i,\downarrow} - \frac{1}{2}) - \mu \sum_i \sum_{\sigma} (1 - c^\dagger_{i,\sigma} c_{i,\sigma})
\]

\[
= t \sum_{\langle i,j \rangle} c^\dagger_{j,\sigma} c_{i,\sigma} + U \sum_i (c^\dagger_{i,\uparrow} c_{i,\uparrow} - \frac{1}{2})(c^\dagger_{i,\downarrow} c_{i,\downarrow} - \frac{1}{2}) - \mu \sum_i \sum_{\sigma} (1 - c^\dagger_{i,\sigma} c_{i,\sigma})
\]

\[
= t \sum_{\langle i,j \rangle} c^\dagger_{j,\sigma} c_{i,\sigma} + U \sum_i (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2}) - \mu \sum_i \sum_{\sigma} (1 - c^\dagger_{i,\sigma} c_{i,\sigma}).
\]
2.4. CHIRAL SYMMETRY

Now, by comparing between the Hamiltonians before and after the PHS, it becomes clear what the particle-hole operator does. The chemical potential term fixes an energy scale of the system and the interaction and hopping term then raise or lower the energy. Since a fixed particle number leaves this term constant, it is possible to measure energy with respect to this point and this means that it possible to set \( \mu = 0 \). This leaves

\[
H_{\text{PHS}} = t \sum_{\langle i,j \rangle} c_{j,\sigma}^\dagger c_{i,\sigma} + U \sum_i (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2}).
\]

Now, it is necessary to restrict to free fermion systems only, because then \( U \) is zero and there is a symmetry

\[
H_{\text{PHS}} = t \sum_{\langle i,j \rangle} c_{j,\sigma}^\dagger c_{i,\sigma} = -H.
\]

Because chemical potential is set to zero, the energy levels are now exactly symmetrical around zero because the excitation from the hopping term get a minus sign under PHS.

Again, by the commutator of \([t, H] = i\hbar\), PHS needs to be antiunitary. By the same argument as with TRS, there are two types of PHS. The properties of PHS+1 are: \( H = -DHTD^{-1}, DD^\dagger = 1 \) and \( D = DT \). For PHS-1 the last one is again \( D = -DT \). Notice the minus sign in \( H = -DHTD^{-1} \), it comes from the fact that the excitation energies all get a minus sign under the symmetry.

2.4 Chiral Symmetry

If both of the above two symmetries are present, so \( H = CH^T C^{-1} \) and \( H = -DHTD^{-1} \) there is also a relation

\[
H = -DHTD^{-1} = -DC^{-1}HCD^{-1} = -(DC^{-1})H(DC^{-1})^{-1} = -UHU^{-1}.
\]

This new type of relation is a property of chiral symmetry. Notice that it is different from the other symmetries because this relation does not contain a transposed Hamiltonian. By the above construction chiral symmetry (CS) automatically arises if both TRS and PHS are, in any form, present. The converse also holds: if CS and either TRS or PHS are present, then all three are present. By defining \( D = UC \) or \( C = U^{-1}D \) it is easy to prove both cases. On its own CS does not imply the presence of TRS or PHS.

Besides \( H = -UHU^{-1} \) chiral symmetry has the properties,

\[
UU^\dagger = DC^{-1}(DC^{-1})^\dagger = DC^{-1}CD^\dagger = 1
\]
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and

$$UU = 1.$$  

Physically this last one is easy to understand: it should not matter in the definition of CS if the PHS or the TRS is applied first. This means that both $U = DC^{-1}$ and $U = CD^{-1}$ should be good definitions, so $U = U^{-1} = U^\dagger$.

2.5 Consequences for the Bandstructure

Each of the above symmetries has an effect on the bandstructure of a material. The matrix properties of each of the symmetries that were derived in the preceding sections do not give a clear hint to what these effects might be. Therefore in this section the effects on the bandstructure will be derived in order to make it easier to tell from experimental results which symmetries are present.

The first one under consideration is TRS-1. This symmetry has the property that $T^2 = -1$, which for example is a symmetry for an odd number of half-integer-spin particles. In that case Kramers’ Theorem gives a constraint on the bandstructure.

**Theorem 2. Kramers’ Theorem**

*If there are an antiunitary operator $T$ with the property that $T^2 = -1$, a Hamiltonian $H$ which is invariant under $T$, i.e. $TH = HT$ and a eigenstate of $H |\phi\rangle$. Then $|\phi\rangle$ and $T|\phi\rangle$ are two orthogonal degenerate eigenstates.*

**Proof.** The degeneracy is fairly easy to see:

$$H|\phi\rangle = E|\phi\rangle \Rightarrow HT|\phi\rangle = TH|\phi\rangle = ET|\phi\rangle.$$  

Then the orthogonality:

$$\langle \phi|T\phi\rangle = -\langle T^2\phi|T\phi\rangle^{\text{antiunitary}} = -\langle \phi|T\phi\rangle \Rightarrow \langle \phi|T\phi\rangle = 0.$$

This means that at time-reversal momenta, i.e. at $k = 0$, $k = \pi/a$ and so on, there are two states with the same energy. Figure 2.1 shows the general form of such a bandstructure. Between the time-reversal momenta the bandstructure can have any form, but there must always be doublets, called Kramers’ Doublets, at the time-reversal points.

For PHS it was already noted in section 2.3 that there is a symmetry $E \rightarrow -E$. This of course means that the bandstructure should be symmetric around zero energy. The general form of the bandstructure is again shown in figure 2.1.
2.5. CONSEQUENCES FOR THE BANDSTRUCTURE

For chiral symmetry the property $H = -UHU^{-1}$ also implies a symmetry in the energy spectrum

$$H|\psi\rangle = E|\psi\rangle \Rightarrow HU|\psi\rangle = -UH|\psi\rangle = -EU|\psi\rangle.$$  

In section 3.2.1 an example is given, including the bandstructure, of a system with only CS. Here it is perhaps best understood by the PHS figure of 2.1 but instead of a mirror symmetry in the line $E = 0$, this time the states that are related are the ones that end up on one another by rotating the picture 180 degrees around the origin.
Chapter 3

Symmetry Classes

Now that all the symmetries are introduced and all the defining properties are known it is relatively easy to find all symmetry classes. Since there are two types of TRS and two types of PHS this means that there must be four classes with only one symmetry. Then there are another four classes coming from all possible combinations of TRS±1 and PHS±1, where each one also has chiral symmetry. This would mean that there are 9 classes if the class without any symmetry is also taken into account. There are however 10 classes, the one that is still missing is the class with only CS. That last class is perhaps a bit of a surprise and in section 3.2.1 it is discussed how it is possible to have only chiral symmetry.

3.1 Wigner-Dyson Classes

The first classes that were found are called the Wigner-Dyson classes after Wigner and Dyson, who were the first to classify random matrices by the property of time reversal symmetry [7]. They found three classes: the no symmetry class (A), the TRS+1 class (AI) and the TRS-1 class (AII).

The letters that are used to name each class are from the mathematical classification of symmetric spaces by Cartan. Originally the class AI was the one that was first developed in physics because it is relevant for the study of atomic nuclei [2]. Later it turned out that also class A and AII had physical realizations in the quantum Hall-effect for class A and in the quantum spin Hall-effect for the class AII, see also section 6.1.

3.1.1 A

Class A is called the unitary symmetry class. Because all matrices under consideration should be the Hamiltonian of a physical system, the matrices should be
hermitian for all classes. Other than being hermitian the matrices from this class have no constraints. Thus class A can be summarized as
\[ H = H^\dagger. \]

### 3.1.2 AI

Class AI is called the orthogonal symmetry class. This class is obtained from class A by requiring the matrices to have TRS+1. By section 2.2 this means that there is a constraint \( H = CH^T C^{-1} \). It is possible to choose \( C \) to be the third Pauli-matrix
\[ C = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_z = \sigma_z^T, \quad \sigma_z \sigma_z^\dagger = 1. \]
Then TRS+1 becomes
\[ H = H^T. \]

### 3.1.3 AII

Class AII is called the symplectic symmetry class. It has TRS-1, which means that it has the constraint \( H = CH^T C^{-1} \) but now \( C \) needs to have different properties. A good choice for \( C \) this time is \( i \sigma_y \), the second Pauli-matrix
\[ C = i \sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_y = -\sigma_y^T, \quad \sigma_y \sigma_y^\dagger = 1. \]
In that case TRS-1 becomes
\[ H = \sigma_y H^T \sigma_y. \]

### 3.2 Chiral Classes

The chiral classes are found by demanding CS on the above classes [3]. This means by section 2.4 that all these classes have to have the property \( H = -U H U^{-1} \). This matrix \( U \) can be chosen to be the third Pauli-matrix
\[ U = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_z^2 = 1, \quad \sigma_z \sigma_z^\dagger = 1. \]

### 3.2.1 AIII

Class AIII is called the chiral unitary class. As stated this class if found by demanding CS on class A. This means that besides being hermitian the only constraint is the one above
\[ H = -\sigma_z H \sigma_z. \]
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Figure 3.1: Left: Drawing of the example used in section 3.2.1. An applied magnetic field (blue arrows) forces the electrons to rotate (yellow arrows) in circles. This results in an current around the side of the slab. Right: Sketch of the bandstructure from the example. It has chiral symmetry but no TRS or PHS.

This class is interesting in that it only has the combination of both TRS and PHS symmetry simultaneously and none of the symmetries on their own. To get an idea of how this is possible imagine a slab of material with an applied magnetic field perpendicular to the slab. Because of the magnetic field the electrons in the material circle around to create a current along the edge of the slab. If the time is reversed the motion of the electrons is reversed which results in a opposite direction of the current. Also if the electrons are changed into holes, so with positive charge, the direction of the current is also reversed. This means that on their own neither TRS or PHS is present. However by changing the direction of time and the electrons to holes at the same time, the current is reversed twice, which means that it remains the same, so there is chiral symmetry. An example of the bandstructure is shown in figure 3.1.

3.2.2 BDI

Class BDI is called the chiral orthogonal group. Starting from class AI and adding CS this class has the following properties

\[ H = H^T, \quad H = -\sigma_z H \sigma_z. \]

Immediately it is clear that \( H = -\sigma_z H^T \sigma_z \) is also a symmetry. Which means that class BDI has PHS+1, since \( \sigma_z = \sigma_z^T \).
3.2.3 CII

Class CII is called the chiral symplectic class. This class is obtained by adding CS to class AII, so it must have

\[ H = \sigma_y H^T \sigma_y, \quad H = -\sigma_z H \sigma_z. \]

This implies that there is a symmetry

\[ H = - (\sigma_z \otimes \sigma_y) H^T (\sigma_z \otimes \sigma_y), \]

since \((\sigma_z \otimes \sigma_y) = - (\sigma_z \otimes \sigma_y)^T\) this means that class CII has PHS-1.

3.3 BdG Classes

The last classes are the Bogoliubov-de Gennes classes and all of them have a form of PHS [3]. These classes were the last ones to be discovered and don’t have any name yet besides their letter from the Cartan symmetric spaces classification.

3.3.1 D

This is the class with only PHS+1. The way to represent this symmetry is to take \(D = \sigma_x\). This means that Hamiltonians in this class have the property

\[ H = -\sigma_x H^T \sigma_x. \]

3.3.2 DIII

To get class DIII from class D there needs to be the extra constraint of TRS-1. This means that this class is defined by

\[ H = -\sigma_x H^T \sigma_x, \quad H = \sigma_y H^T \sigma_y. \]

These can be combined to show the explicit chiral symmetry

\[ H = - (\sigma_x \otimes \sigma_y) H (\sigma_x \otimes \sigma_y). \]

3.3.3 C

This class has PHS-1, which is chosen to be represented as \(D = \sigma_y\). This then implies that all Hamiltonians in class C have the property

\[ H = -\sigma_y H^T \sigma_y. \]
### 3.3.4 CI

The last class is CI, found by adding TRS+1 to class C. This means that the constraints are

\[ H = -\sigma_y H^T \sigma_y, \quad H = H^T. \]

Then there is also a chiral symmetry present in the form

\[ H = -\sigma_y H \sigma_y. \]

All the results are summarized in table 3.1.

Table 3.1: Summary all the classes with their constraints. For TRS and PHS the 0 means that it is not present while the +1 means that TRS+1 or PHS+1 is present and −1 means that TRS-1 or PHS-1 is present. For CS the 1 just means that the class has chiral symmetry and the zero that it doesn’t.

<table>
<thead>
<tr>
<th>Class name</th>
<th>TRS</th>
<th>PHS</th>
<th>CS</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>(H = H^\dagger)</td>
</tr>
<tr>
<td>AI</td>
<td>+1</td>
<td>0</td>
<td>0</td>
<td>(H = H^T)</td>
</tr>
<tr>
<td>AII</td>
<td>−1</td>
<td>0</td>
<td>0</td>
<td>(H = \sigma_y H^T \sigma_y)</td>
</tr>
<tr>
<td>AIII</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>(H = -\sigma_z H \sigma_z)</td>
</tr>
<tr>
<td>BDI</td>
<td>+1</td>
<td>+1</td>
<td>1</td>
<td>(H = H^T, \quad H = -\sigma_z H \sigma_z)</td>
</tr>
<tr>
<td>CII</td>
<td>−1</td>
<td>−1</td>
<td>1</td>
<td>(H = \sigma_y H^T \sigma_y, \quad H = -\sigma_z H \sigma_z)</td>
</tr>
<tr>
<td>D</td>
<td>0</td>
<td>+1</td>
<td>0</td>
<td>(H = -\sigma_x H^T \sigma_z)</td>
</tr>
<tr>
<td>DIII</td>
<td>0</td>
<td>−1</td>
<td>0</td>
<td>(H = -\sigma_x H^T \sigma_y, \quad H = \sigma_y H^T \sigma_y, \quad H = H^T)</td>
</tr>
<tr>
<td>C</td>
<td>−1</td>
<td>+1</td>
<td>1</td>
<td>(H = -\sigma_y H^T \sigma_y)</td>
</tr>
<tr>
<td>CI</td>
<td>+1</td>
<td>−1</td>
<td>1</td>
<td>(H = -\sigma_y H^T \sigma_y, \quad H = H^T)</td>
</tr>
</tbody>
</table>
Chapter 4

Q-matrices

All the symmetry classes were introduced in chapter 3 and now it is possible to start with the interesting question of where the topologically different states are possible. In this chapter the first step to this goal is made by looking at projector operators from the Brillouin zone to the energy spectrum. With these projection operators it will be possible to define Q-matrices and the allowed Q-matrices will be different for each class. First the idea is made clear in a few examples and then the rest of the classes will just be given.

4.1 Projectors

To construct the bandstructure in any material the Hamiltonian at every point of the Brillouin zone (BZ) has to be solved, yielding a set of energy states for that specific point of the BZ. Then by connecting the different points of the BZ for one n-th energy state one finds the n-th energy band of the material. This means that the bandstructure is completely determined by assigning a Hamiltonian to every point of the BZ.

Mathematically this means that there is a map which sends $k \in \mathbb{T}^d \rightarrow H(k)$. Note that the BZ of a $d$-dimensional material is isomorphic to $\mathbb{T}^d$, the d-dimensional torus. Then at every $k$ there is the eigenvalue equation

$$H(k)|\psi_i(k)\rangle = E_i(k)|\psi_i(k)\rangle,$$

where the $i$ runs over all possible states. By plotting a figure of $E_i(k)$ against $k$ for all $i$ the familiar bandstructure is obtained, but that is not necessary here. Instead define an operator [3]

$$P(k) = \sum_{i}^{\text{filled}} |\psi_i(k)\rangle \langle \psi_i(k)|.$$
This is clearly a projection operator on the filled states since $P(k)^2 = P(k)$ and $P(k)$ is the identity on the filled states.

With $P(k)$ it is possible to define a Q-matrix

$$Q(k) = 2P(k) - I,$$

where $I$ is the identity matrix. By choosing a basis of $m$ filled and $n$ empty states it is clear that $\text{tr} Q = 2m - (m + n) = m - n$. Also $Q^2 = I$,

$$Q(k)^2 = (2P(k) - I)^2 = 4P(k)^2 - 4P(k) + I^2 = I,$$

since $P(k)$ is a projection operator.

### 4.2 Class A and AI

Any Q-matrix can be viewed as a set of $m + n$ complex eigenvectors and these can be represented as an element from the $(m + n)$-dimensional complex unitary matrices: $U(m + n)$. However if the filled states are chosen in a different order the Q-matrix would not change so there is a abundant $U(m + n)$ freedom. The same thing holds for the choice of the empty states, this gives a $U(n)$ freedom. This means that any Q-matrix is an element of $U(m + n)/(U(m) \times U(n)) \cong G_{m,m+n}(\C)$.

$G_{m,m+n}(\C)$ is a complex Grassmannian manifold. It is the space of all complex $m$-dimensional subvectorspaces in complex $(m + n)$-dimensional vectorspace. So for example $G_{1,3}(\C)$ are all the complex lines in complex three-dimensional space. There is a natural isomorphism $G_{m,m+n}(\C) \cong G_{n,m+n}(\C)$ because every subspace can also be determined by its orthogonal complement.

For class A there are no addition constraint, so $Q(k) \in G_{m,m+n}(\C)$. But in class AI there was an addition constraint of $H = H^T$, which has its effect on the bandstructure and thereby the Q-matrices. It is possible to use a simple example to see what happens to the Q-matrices.

If the (quasi)particles in a material can be described by free waves, i.e. $|\psi(k)\rangle = e^{ikx}$, then the TRS+1 has the effect that $e^{ikx} \to e^{-ikx}$, which is the same as taking the complex conjugate. So $|\psi(k)\rangle = |\psi(-k)\rangle^*$. Also the constraint of class AI can be expressed as $H = H^*$ (because $H = H^\dagger$) and together this means that if

$$H|\psi(k)\rangle = E|\psi(k)\rangle,$$

then by taking the complex conjugate

$$H^*|\psi(k)\rangle^* = E^*|\psi(k)\rangle^* \Rightarrow H|\psi(-k)\rangle = E|\psi(-k)\rangle.$$

Since the waves with opposite momenta have the same energy either both are filled or both are empty states. This means that $P(k) = P(-k)^*$ which in turn implies that $Q(k)^* = Q(-k)$ for all Q-matrices in class AI.
4.3 Class AIII and BDI

For class AIII and all classes with a chiral symmetry something changes. The Q-matrices are completely specified by a smaller matrix called $q$ which is an element of $U(m)$. Again there is a simple example to show the mechanism. In class AIII there was the constraint $H = -\sigma_z H \sigma_z$ and to see what this implies lets try this out on a spin-up and spin-down vector.

$$H := \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad H \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix} = \begin{pmatrix} a |\uparrow\rangle + b |\downarrow\rangle \\ c |\uparrow\rangle + d |\downarrow\rangle \end{pmatrix},$$

and also

$$H \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix} = -\sigma_z H \sigma_z \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix} = \begin{pmatrix} -a |\uparrow\rangle + b |\downarrow\rangle \\ c |\uparrow\rangle - d |\downarrow\rangle \end{pmatrix}.$$  

This means that $a = d = 0$ and because $H = H^\dagger$ also $b = c^\dagger$ therefore

$$H = \begin{pmatrix} 0 & b \\ b^\dagger & 0 \end{pmatrix}.$$ 

The same thing can be done with $Q$, by a change of basis [3] it can be represented as

$$Q = \begin{pmatrix} 0 & q \\ q^\dagger & 0 \end{pmatrix}.$$ 

Because $Q^2 = I$ this means that $qq^\dagger = 1 = q^\dagger q$ and therefore $q \in U(m)$ for class AIII.

Finding the constraint on the $q$-matrices for class BDI is really simple. In section class A and AI the constraint was $Q(k)^* = Q(-k)$, but this simply means that the same thing holds for $q$

$$\begin{pmatrix} 0 & q(k)^* \\ q(k)^\dagger & 0 \end{pmatrix} = Q(k)^* = Q(-k) = \begin{pmatrix} 0 & q(-k) \\ q(-k)^\dagger & 0 \end{pmatrix}.$$  

So for class BDI the $q$-matrices must have $q(k)^* = q(-k)$.

4.4 All Classes

In a similar way it is possible to find the constraints on all the classes, with the results [3] summarized in table 4.1. For the classes without CS the symmetries provide constraints on the Q-matrices which are elements form $G_{m,m+n}(\mathbb{C})$, while for the classes with CS the symmetries give constraints on the $q$-matrices, elements from $U(m)$. 
Table 4.1: Summary of the Q and q-matrix spaces allowed for each different symmetry class.

<table>
<thead>
<tr>
<th>Symmetry Class</th>
<th>Space of Q-matrices</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>{Q(k) \in G_{m,m+n}(\mathbb{C})}</td>
</tr>
<tr>
<td>AI</td>
<td>{Q(k) \in G_{m,m+n}(\mathbb{C}) \mid Q(k)^* = Q(-k)}</td>
</tr>
<tr>
<td>AII</td>
<td>{Q(k) \in G_{m,m+n}(\mathbb{C}) \mid \sigma_y Q(k)^* \sigma_y = Q(-k)}</td>
</tr>
<tr>
<td>AIII</td>
<td>{q(k) \in U(m)}</td>
</tr>
<tr>
<td>BDI</td>
<td>{q(k) \in U(m) \mid q(k)^* = q(-k)}</td>
</tr>
<tr>
<td>CII</td>
<td>{q(k) \in U(m) \mid \sigma_y q(k)^* \sigma_y = q(-k)}</td>
</tr>
<tr>
<td>D</td>
<td>{Q(k) \in G_{m,m+n}(\mathbb{C}) \mid \sigma_x Q(k)^* \sigma_x = -Q(-k)}</td>
</tr>
<tr>
<td>DIII</td>
<td>{q(k) \in U(m) \mid q(k)^T = -q(-k)}</td>
</tr>
<tr>
<td>C</td>
<td>{Q(k) \in G_{m,m+n}(\mathbb{C}) \mid \sigma_y Q(k)^* \sigma_y = -Q(-k)}</td>
</tr>
<tr>
<td>CI</td>
<td>{q(k) \in U(m) \mid q(k)^T = q(-k)}</td>
</tr>
</tbody>
</table>
Chapter 5

Homotopy Groups

The goal is still to find the classes where special materials are possible. In this chapter the spaces found in table 4.1 are studied using homotopy groups. The first section explains how the homotopy groups give information about the spaces and therefore the classes. After that the mathematical tools are defined and explained. Then it is possible to calculate the homotopy groups, but since this is a long and difficult calculation it will be done for one class only. The rest is then summarized in the last section.

5.1 The Idea behind Homotopy Groups

The first homotopy group is the easiest to start with. It is also known as the fundamental group and it is the algebraic group of loops on a topological space. The basic question is how many loops there are that cannot be changed into one another by only moving, stretching and shrinking (part of) the loop. With the example of figure 5.1 it is easy to see how this tells us something about the space.

In $\mathbb{R}^2$ it is possible to shrink the loop (or any loop) to a point, but with a hole in it, it becomes possible to wrap the loop around the hole, so it can no longer be shrunk to a point. Of course figure 5.1 only depicts one possibility, one immediately sees that there are more loops possible. Wrapping the loop twice or three or four times around the circle are all different. In fact there are an infinity amount of possibilities. All the possible loops together form a group and it is clear that the addition of a hole made the group a lot bigger. Therefore the group tells us something about the structure, or topology, of the space.

For the higher homotopy groups the idea is basically the same. The second homotopy group uses spheres instead of loops. So in $\mathbb{R}^3$ this can detect a missing ball in the space, in the same way as the fundamental group could detect a missing disk. The third homotopy group then uses 3-spheres (this is the unit sphere in $\mathbb{R}^4$).
Figure 5.1: The upper two pictures are two spaces. The left one is $\mathbb{R}^2$ and the right one is $\mathbb{R}^2$ with a hole in it. In the lower two pictures a loop is laid in the spaces. It is easy to see that on the left it is possible to shrink the loop to a point, but on the right not without leaving the space.

four dimensional space) and the n-th homotopy group uses n-spheres.

It is not necessary to use the n-th homotopy group in n+1 dimensional space, as one might think from the preceding discussion. The first homotopy group can just as well be used in $\mathbb{R}^3$ to detect missing infinite cylinders. If the cylinder would be finite, then it would be possible to move the loop up over the cylinder, so then it would only be detectible by the second homotopy group. This shows that all homotopy groups give information about a space.

Of course it is now possible to use this technique on the spaces of Q-matrices found in table 4.1, but how could that be relevant to our search for different materials? As discussed in section 4.1 the bandstructure of a material is mathematically just a mapping from the Brillouin zone torus to the space of Hamiltonians. From each Hamiltonian a unique Q-matrix follows and this means that the bandstructure is a map from spheres to the Q-matrix space. The final piece of the puzzle is that a torus can be viewed as a product of two spheres, meaning that the bandstructure is a map from spheres to the Q-matrix space. Thus if there exist non-zero homotopy groups for the Q-matrix spaces, then this means that there exist bandstructures that can not be deformed into one another. Physicists then say that the bandstructures are topologically
5.2 Homotopy Groups and Covering Spaces

The next two sections will contain a lot of mathematics, so for readers who are afraid of that it is possible to skip them and go directly to the answers in section 5.4. However all concepts are explained and the text is intended to be understandable for physics bachelors.

5.2.1 Homotopies and Homotopy Groups

In the last section it was made clear that homotopy groups measure how many different loops there are in a space. To see if two loops are topologically “equal” it must be possible to deform them. This is done with homotopies, which will now be defined.

Definition. Let $X, Y$ be topological spaces and $I = [0, 1]$ the unit interval. If there are two continuous maps $f : X \to Y$ and $g : X \to Y$ then they are said to be homotopic, denoted by $f \sim g$, if there exists a continuous map $F : X \times I \to Y$ with the property that $F(x, 0) = f(x)$ and $F(x, 1) = g(x)$. The map $F$ is called a homotopy from $f$ to $g$.

Let $C(X,Y)$ denote the space of all continuous maps from $X$ to $Y$ and let $C((X,x_0), (Y,y_0))$ be the space of all continuous maps from $X$ to $Y$ where $x_0 \in X$ is mapped to $y_0 \in Y$.

Proposition. $f \sim g$ is an equivalence relation on $C(X,Y)$.

Proof. Reflectivity: $f \sim f$ because there exists the homotopy $F(x,t) = f(x)$. Symmetry: $f \sim g \Rightarrow g \sim f$ because $F(x,t)$ is a homotopy from $f$ to $g$ then $G(x,t) = F(x,1-t)$ is a homotopy from $g$ to $f$. Transitivity: If $f \sim g$ with a homotopy $F$ and $g \sim h$ with a homotopy $G$ then $f \sim h$ because there exists a homotopy $H$

$$H(x, t) = \begin{cases} F(x, 2t) & \text{if } 0 \leq t \leq \frac{1}{2} \\ G(x, 2t - 1) & \text{if } \frac{1}{2} \leq t \leq 1. \end{cases}$$

The fact that being homotopic is an equivalence relation just means that it works like a =-sign. The properties that were checked in the proof are all properties of the normal =-sign. So now it is allowed to say that two loops are the same if they can be deformed into one another.
CHAPTER 5. HOMOTOPY GROUPS

Since the same equivalence relation holds on \( C((X,x_0), (Y,y_0)) \) it is now possible to define for \( k \geq 1 \) the pointed loop space: \( \Omega^k(X,x_0) := C((S^k, *), (X,x_0)) \), where \( S^k = \{ x \in \mathbb{R}^{k+1} | \|x\| = 1 \} \) is the unit k-sphere, the \( x_0 \) is any point in \( X \) and \( * \in S^k \) can be any point, but fix it on the north pole of the k-sphere. Then the pointed homotopy groups are found by dividing out the homotopy equivalence relation
\[
\pi_k(X,x_0) := \Omega^k(X,x_0)/\sim.
\]

**Theorem 3.** The pointed homotopy groups are groups.

For a proof see for example [9]. The elements from the groups are denoted by \([f]\) and they stand for the equivalence class of maps that are homotopic to \( f \). The group operation is composition of maps. It is possible to leave out all the “pointed” adjectives if the space \( X \) is path-connected, which just means that there is a path from any point in \( X \) to any other point in \( X \). This is because of the following theorem.

**Theorem 4.** Let \( X \) be path-connected and \( x_0, x_1 \in X \) two points. Then \( \pi_k(X, x_0) \simeq \pi_k(X, x_1) \).

Again the proof can be found in [9]. Since for path-connected spaces these isomorphisms exist the special point can be dropped and then the loop space is \( \Omega^k(X) := C(S^k, X) \) and the homotopy groups are \( \pi_k(X) := \Omega^k(X)/\sim \).

The definition above did not include the case \( k = 0 \), because then the homotopy group is not a group anymore. Instead it counts the number of path-connected components of \( X \), this is relatively easy to see. For \( k = 0 \) the maps are maps from points to \( X \) and they are homotopic if there is a line in \( X \) connecting them, because the homotopy can then run over this line. This means that for every path-connected component of \( X \) there is a single map in \( \pi_0(X) \).

Let’s do a simple example and calculate \( \pi_1(\mathbb{R}^n, x_0) \). \( \mathbb{R}^n \) is clearly path-connected, so \( \pi_0(\mathbb{R}^n) = 0 \) and the choice of base point is irrelevant, so set \( x_0 = 0 \). Then any map \( f: S^1 \to \mathbb{R}^n \) can be expressed as
\[
f(x) = \{s_1(x), s_2(x), ..., s_n(x)\},
\]
where \( s_i(t) \) are the coordinate functions. By rewriting this in polar coordinates it becomes
\[
f(x) = \{r(x), \phi_1(x), \phi_2(x), ..., \phi_{n-1}(x)\}.
\]
Now it is easy to give a continuous homotopy to the constant map
\[
F(x, t) = \{t \cdot r(x), \phi_1(x), \phi_2(x), ..., \phi_{n-1}(x)\}.
\]
Thereby it is clear that any map is homotopic to the constant map, so \( \pi_1(\mathbb{R}^n) = 0 \).

If it would be necessary to compute all groups for all spaces individually it would be a very long exercise. However there are theorems to speed up the process.
5.2. HOMOTOPY GROUPS AND COVERING SPACES

**Definition.** Let $X,Y$ be topological spaces. $X$ and $Y$ are of the same homotopy type, written as $X \simeq Y$, if there exists continuous maps $f : X \to Y$ and $g : Y \to X$ such that $f \circ g \sim \text{Id}_Y$ and $g \circ f \sim \text{Id}_X$. $f$ is the homotopy equivalence between $X$ and $Y$.

Please note that between spaces $\simeq$ means that the spaces are of the same homotopy type, while $\simeq$ between groups means an isomorphism exists.

**Theorem 5.** Let $f : X \to Y$ be a homotopy equivalence between $X$ and $Y$. Then there is an isomorphism: $\pi_k(X, x_0) \simeq \pi_k(Y, f(x_0))$.

For a proof see [14]. By using this theorem it is possible to calculate all higher homotopy groups of $\mathbb{R}^n$ at the same time. The map $f : \mathbb{R}^n \to \ast$ by $f(x) = \ast$ is a homotopy equivalence ($g$ sends $\ast$ to zero) since the homotopy is given by $F(\bar{x}, t) = (1 - t)\bar{x}$.

This means that $\pi_k(\mathbb{R}^n) \simeq \pi_k(\ast), \forall k$ and since every map to a single point is the same i.e. $\pi_k(\ast) = 0, \forall k$, it is clear that $\pi_k(\mathbb{R}^n) = 0, \forall k$.

This holds in general for any space that is contractible, that is homotopy equivalent to a point.

5.2.2 Covering Spaces and the Exact Sequence

A covering space of a base space is a bigger space that, just as the word says, covers the base space. It can cover the space multiple times which means that every point of the base space has multiple points in the covering space that are mapped to it. The collection of all these points in the covering space, that are mapped to one point, is called a fiber.

**Definition.** A covering space is a space $E$, such that there is a projection $p : E \to B$ on the base space $B$ and for every $x \in B$ there should be an open set $U$ around $x$ such that $p^{-1}(U) = U \times F$, where the fiber $F = p^{-1}(x)$.

The reason for looking at the covering spaces is that the homotopy groups of the covering space are related to the homotopy groups of the base space via a so called exact sequence. So the first thing to do is to introduce this notion and its basic properties.

**Definition.** A (long) exact sequence is a sequence of groups $(A_n)$ with maps $(f_n)$ between them

$$\ldots \xrightarrow{f_{n+2}} A_{n+1} \xrightarrow{f_{n+1}} A_n \xrightarrow{f_n} A_{n-1} \xrightarrow{f_{n-1}} \ldots$$

such that $\forall n, \text{im}(f_{n+1}) = \text{ker}(f_n)$. 

Chapter 5. Homotopy Groups

It is not always necessary to write the maps, so they can be left out. Exact sequences can be very useful and have a lot of applications but the only thing that will be required is the following proposition.

**Proposition.** If (part of an) exact sequence has the form

\[ \cdots \rightarrow 0 \xrightarrow{f_{n+1}} A_n \xrightarrow{f_n} A_{n-1} \xrightarrow{f_{n-1}} 0 \rightarrow \cdots \]

then \( A_n \cong A_{n-1} \).

**Proof.** Because \( f_{n+1} : 0 \rightarrow A_n \) must map zero to zero it must be that \( \text{im}(f_{n+1}) = 0 = \ker(f_n) \), this means that \( f_n \) is injective. On the other hand \( f_{n-1} : A_{n-1} \rightarrow 0 \) must map the entire group \( A_{n-1} \) to zero, so \( \ker(f_{n-1}) = A_{n-1} = \text{im}(f_n) \), this means that \( f_n \) is surjective. Together this means that \( f_n \) is an isomorphism, i.e \( A_n \cong A_{n-1} \).

**Theorem 6.** Let \( E \) be the covering space of \( B \), \( F = p^{-1}(b) \) the fiber at the point \( b \in B \) and \( x \in F \subset E \), then there exists an exact sequence

\[ \cdots \rightarrow \pi_k(F, x) \rightarrow \pi_k(E, x) \rightarrow \pi_k(B, b) \rightarrow \pi_{k-1}(F, x) \rightarrow \cdots . \]

This sequence ends with

\[ \cdots \rightarrow \pi_0(F, x) \rightarrow \pi_0(E, x) \rightarrow \pi_0(B, b) \rightarrow 0. \]

The prove for this can be found in [14], but it is more useful to look at an example to see how this can be used.

Take as a base space the circle \( S^1 \) and as a covering space take \( \mathbb{R} \) with the projection \( p : \mathbb{R} \rightarrow S^1 \) by \( p(x) = e^{2\pi x} \). The circle is now viewed as the unit circle in the complex plane. The fiber \( F \) at any point is (isomorphic to) \( \mathbb{Z} \) because adding \( 2\pi i k, k \in \mathbb{Z} \) in the exponential gives the same point in the base space.

Since it is already known that \( \pi_k(\mathbb{R}) = 0, \forall k \) by the proposition there are isomorphism \( \pi_k(S^1, 1) \cong \pi_{k-1}(\mathbb{Z}, 0), \forall k \geq 1 \). Now it is easy to calculate \( \pi_k(\mathbb{Z}, 0) \), because it consists of disconnected points, therefore every continuous map is a constant map and all homotopy groups are zero except for the zeroth. The number of disconnected components is exactly the numbers in \( \mathbb{Z} \) so it must that \( \pi_0(\mathbb{Z}, 0) = \mathbb{Z} \). This results in the homotopy groups for \( S^1 \)

\[ \pi_k(S^1) = \begin{cases} \mathbb{Z} & \text{if } k = 1 \\ 0 & \text{otherwise.} \end{cases} \]
5.3 Calculation of $\pi_k(U(m))$

Now that all the technical tools are introduced it is time to start with the actual relevant groups. The simplest case is the class AIII with q-matrices in the group $U(m)$. To see if there are topologically different states possible it is necessary to calculate the homotopy groups for this space $U(m)$.

$U(m)$ is the space of all unitary matrices in $GL(m, \mathbb{C})$, that is all unitary $m \times m$-matrices with complex entries. From linear algebra it is known that these matrices have eigenvalues on the complex unit circle and since the determinant of a matrix is equal to the product of its eigenvalues this means that there is a projection map: $\det : U(m) \to S^1$. Taking 1 to be the base point in $S^1$ the fiber is the subspace of matrices in $U(m)$ with determinant 1, this space is called $SU(m)$.

Now I would like to show that the choice of base point is irrelevant, because all spaces in question are path-connected. For the circle this was already known, but the other two are more difficult to see.

**Proposition.** $U(m)$ and $SU(m)$ are path-connected.

**Proof.** Again from linear algebra it is possible to decompose any matrix $U \in U(m)$ as $U = \Lambda D \Lambda^{-1}$ where $D$ is a diagonal matrix, with the eigenvalues of $U$ on the diagonal. For $D$ the homotopy to the identity is given by

$$D(t) = \begin{pmatrix} e^{ix_1 t} & 0 & \cdots & 0 \\ 0 & e^{ix_2 t} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{ix_m t} \end{pmatrix}.$$

At every $t$ this $D(t)$ gives a matrix $U(t) = \Lambda D(t) \Lambda^{-1}$ and this is a homotopy from $U(0) = \Lambda D(0) \Lambda^{-1} = \Lambda \text{Id} \Lambda^{-1} = \text{Id}$ to $U(1) = \Lambda D(1) \Lambda^{-1} = U$. This implies that $U(m)$ is connected for all $m$.

The same trick can be done in $SU(m)$ but the determinant should always remain one. The new homotopy is most easily constructed with induction in $m$. For $m = 2$ it is easy

$$D(t) = \begin{pmatrix} e^{ix_1 t} & 0 \\ 0 & e^{-ix_1 t} \end{pmatrix}.$$

To reduce the case $m$ to the case $m - 1$ the homotopy is

$$D(t) = \begin{pmatrix} e^{ix_1 (1-t)} & 0 & \cdots & 0 \\ 0 & e^{i(x_2 + tx_1)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{ix_m t} \end{pmatrix}.$$
At every \( t \) the determinant remains
\[
\det(U(t)) = \det(\Lambda)\det(D(t))\det(\Lambda)^{-1} = \det(D(t)) = \prod_j e^{ix_j} = \exp[i \sum_j x_j] = 1.
\]
So also \( SU(m) \) is path-connected for all \( m \).

This means that all base points are irrelevant and the exact sequence is given by
\[
\cdots \to \pi_k(SU(m)) \to \pi_k(U(m)) \to \pi_k(S^1) \to \pi_{k-1}(SU(m)) \to \cdots,
\]
since all spaces are pathconnected and \( \pi_2(S^1) = 0 \) this sequence ends with
\[
0 \to \pi_1(SU(m)) \to \pi_1(U(m)) \to \pi_1(S^1) \to 0.
\]
The homotopy groups of \( S^1 \) where all zero, except for the first one which means that there are isomorphism \( \pi_k(SU(m)) \simeq \pi_k(U(m)), \forall k \geq 2 \).

The calculation of the homotopy groups of \( U(m) \) is now reduced to the calculation of the homotopy groups of \( SU(m) \) and this can be done for the first two homotopy groups with another covering space construction and induction.

The map \( p : SU(n) \to S^{2n-1} \) is a projection with fibers \( SU(n-1) \). To see this, recall that to specify a rotation in three dimensional (real) space one has to choose an axis, which is a point on the 2-sphere and then the rotation around that axis. This last rotation is just a two dimensional rotation. This means that by projecting a three dimensional rotation on the axis of rotation a two dimensional rotation group is projected to the same point. This means that \( SO(3) \to S^2 \) has fibers \( SO(2) \), but the same construction can be done in any dimension and also for complex spaces. \( SU(n) \) is the rotation group of the complex n-space, this has real dimension \( 2n \), so the group is projected on a \( (2n-1) \)-dimensional sphere while the \( SU(n-1) \) rotations are send to the same point.

The starting point is \( SU(1) \), which are all the one by one matrices which determinant one. Since there is only one possible matrix, this is the trivial group and its homotopy groups were already computed
\[
\pi_k(SU(1)) \simeq \pi(*) = 0, \forall k.
\]
By the exact sequence then \( \pi_k(SU(2)) \simeq \pi_k(S^3), \forall k \). The first two homotopy groups of \( S^3 \) are easy (the higher ones are an absolute disaster, but they are not needed). Any map from \( S^1 \) or \( S^2 \) to \( S^3 \) is homotopic to a map that is not surjective \([5]\). This means that there is at least one point on \( S^3 \) not in the image, so use that point as a basis for a stereographic projection onto \( \mathbb{R}^3 \). There it is easy to contract the image to a point. This is also possible in higher dimensions, meaning that any map \( S^i \to S^j \) is homotopic to the constant map if \( i < j \). To get a physical
intuition of why this is true, wrap a shoestring around a ball and tie the ends together. Whatever you do, it is always possible to remove the shoestring without untying the ends. This means that now

\[ \pi_1(SU(2)) = 0, \quad \pi_2(SU(2)) = 0. \]

The next step is the induction step. The end of the exact sequence is given by

\[
\cdots \to \pi_3(SU(n-1)) \to \pi_3(SU(n)) \to \pi_3(S^{2n-1}) \\
\to \pi_2(SU(n-1)) \to \pi_2(SU(n)) \to \pi_2(S^{2n-1}) \\
\to \pi_1(SU(n-1)) \to \pi_1(SU(n)) \to \pi_1(S^{2n-1}) \to 0.
\]

Since the lowest case is \( n = 3 \) by the above argument about maps of spheres this becomes

\[
0 \to \pi_2(SU(n-1)) \to \pi_2(SU(n)) \to 0 \\
\to \pi_1(SU(n-1)) \to \pi_1(SU(n)) \to 0.
\]

Meaning that by induction

\[ \pi_1(SU(m)) = 0, \quad \pi_2(SU(m)) = 0. \]

These results imply an isomorphism \( \pi_1(U(m)) \simeq \pi_1(S^1) = \mathbb{Z} \) and also give the second homotopy group, \( \pi_2(U(m)) \simeq \pi_2(SU(m)) = 0 \). To finish of the calculation the Bott-periodicity Theorem is needed. This theorem gives the following isomorphism [5]

\[ \pi_k(U(m)) = \pi_{k+2}(U(m)), \text{ if } m > (k+1)/2. \]

Since the \( m \) stands for the number of occupied states and the dimension of the Brillouin zone is usually 2 or 3, this theorem can be applied, yielding as a final result

\[ \pi_k(U(m)) = \begin{cases} 
\mathbb{Z} & \text{if } k \text{ is odd} \\
0 & \text{if } k \text{ is even}.
\end{cases} \]

### 5.4 Homotopy Groups for all Classes

As is probably clear from the calculation of the homotopy groups of \( U(m) \), it can get very complicated to calculate homotopy groups of spaces [6]. Therefore the rest of the groups will just be given in table 5.1, taken from [4].
Table 5.1: The homotopy groups for all the different classes. The dimension in the table stands for the dimensions of space and at the same time the number of the homotopy group. The interesting pattern that emerges comes from the Bott-periodicity Theorem mentioned in section 5.3. Besides the 2-periodicity used there for complex matrix spaces, it also gives a 8-periodicity for the other (real) matrix spaces. The group $\mathbb{Z}_2$ is the group of two elements $\{0, 1\}$.

<table>
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<th>2-dim</th>
<th>3-dim</th>
<th>4-dim</th>
<th>5-dim</th>
<th>6-dim</th>
<th>7-dim</th>
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Chapter 6
Discussion

In the last chapter the homotopy groups of the Q-matrix spaces were computed. This gave an answer to the question in which symmetry classes topologically distinct states of matter are possible. The question is now if it is possible to find experimental examples for each of these interesting classes.

6.1 2-dimensional examples

As stated in section 1.2 the first example of a topological state was the quantum Hall effect (QHE). The QHE happens when an electric field is added to the example of section 3.2.1. If the electric field makes the electrons move to the left of the sample then the applied magnetic field bends them upward, resulting in a potential difference between the two sides of the sample. Because the magnetic field breaks TRS and the electric field breaks PHS there are no symmetries. This means that the QHE belongs to class A and that there should be a $\mathbb{Z}$ quantization. Indeed there is a quantized Hall conductivity $\sigma = Ne^2/h$, $N \in \mathbb{Z}$ [4].

Only a few years ago a new topological state was found and this was named the quantum spin Hall effect (QSHE) [10]. In the QHE the places were particles that move forward and move backward are separated by the magnetic field, since the magnetic field deflects particles that move to the left upwards, while particles moving rightward get deflected downwards. In the QSHE there is no applied magnetic field, but instead strong spin-orbit coupling creates two different channels. Now spin-up forward movers together with spin-down backward movers are in one channel while on the other side of the sample spin-down particle move forward and spin-up particle move backwards. Instead of a net charge transport in the QHE, in the QSHE there is a net spin transport from one side of the sample to the other, hence the name quantum spin Hall effect.

In the QSHE there is no magnetic field so the time-reversal symmetry remains
unbroken and these systems have TRS-1, meaning that the QSHE is an example of the class AII. In this class there is a $\mathbb{Z}_2$ homotopy group in 2-dimensions, so there should only be two topologically different states. These two are given by the two bandstructures figure 6.1 [4].

![Figure 6.1: The two topologically different bandstructures of the QSHE. Only the positive k-value side is drawn because TRS implies the right side to be the mirror image. In red the valence band, blue the conduction band and the states in the gap are in yellow and green. Left: The two state have Kramer doublets at both $k = 0$ and $k = \pi/a$ and therefore can be moved adiabatically (continuously) into the valence band. Right: The gap states have only one doublet in common, resulting in a link between the valence and conduction band that cannot be removed adiabatically.]

An actual experimental example was found in mercury telluride quantum wells [10]. By adjusting the thickness of the layer HgTe between the layers of CdTe it is possible create both the left and the right picture of figure 6.1. For the other classes there are no experimental examples yet, however there has been a suggestion [12] that the material Sr$_2$RuO$_4$ might be a topological superconductor in the class DIII. Also a method for the construction of a material in the class D was given [11]. By combining layers of s-wave superconductors and quantum hall insulator it might be possible to construct a new topological state in the region where the two materials meet.

### 6.2 3-dimensional examples

In three dimensions it is not possible to have a QHE, because the third homotopy group of that class is trivial. However the QSHE is possible because it again has a $\mathbb{Z}_2$ group. In three dimensions, materials from this class are called topological insulators and most experimental research is focussed on them. Examples in this
class are BiSb, Bi$_2$Se$_3$, Bi$_2$Te$_3$ and Sb$_2$Te$_3$ [4]. In figure 6.2 the experimental bandstructure of Bi$_2$Se$_3$ and Bi$_2$Te$_3$ are shown, taken from [4].

![Figure 6.2: ARPES measurements of the bandstructure of Bi$_2$Se$_3$ (a and c) and of Bi$_2$Te$_3$ (d). Figure a: The valence and conduction band are visible with between them two bands that cross the gap. On the left the Kramer doublet is visible, but adding magnetic disorder (the right) destroys the doublet, by breaking TRS. Figure c and d: Adding non-magnetic disorder does not break TRS, so the Kramer doublet remains intact. The bands are shifted a bit, but the topology of the bandstructure remains the same.](image)

The figure shows what this thesis was about. By adding magnetic impurities the symmetries of the system change en thereby the topology of the bandstructure. The magnetic impurities here have broken TRS and thus destroyed the Kramer doublet, separating the valence and conduction band. However by adding normal impurities the symmetries remain intact and the bandstructure still has the same topology. The bandstructure looks a bit different but it can be changed back continuously.

From the other classes that have a non-trivial homotopy group (AIII, DIII, CII, CI) only for the class DIII an example is known in the form of helium-3 in the B phase [3]. None of the other classes have been experimentally observed. This means there is still a lot of possible research to be done. The classification might be complete, but theorists could try to predict the materials where the new states are realized. It should not be to hard to calculate most of the bandstructures, since all material should approximately be free fermion systems. Right now almost all the experimental searches are focussed on the class AII, but there are still a lot
of classes without experimental examples, so guided by the theoretical prediction, there should be a lot of new discoveries possible.
Bibliography


