

Research Project - M1 General Physics

A First Encounter With Topological Matter

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Abstract

This report gives a brief overview of the formalism of second quantization and the worked solutions to some simple exercises. Next, hopping in 1-dimensional homogeneous and dimerized chains is described using second quantization. For chains with periodic boundary conditions the Hamiltonians are solved analytically and compared to the numerical solution of chains with open boundary conditions. The topological phase transition that occurs in the Su-Schrieffer-Heeger model at $t = t'$ is shown and the corresponding topological invariants are discussed.

1 Introduction

The purpose of this research project is to lay the theoretical foundations for a subsequent in-depth internship. The topic of this internship will be *New topological states from inhomogeneous spin-orbit coupling*, which neatly states the subject that needs to be tackled in this research project: Topological states of matter. In order to do this, a firm footing in the formalism of second quantization is needed, which is why an extensive review on second quantization is given in this report based on various lecture notes and books [1–4].

Once a certain familiarity has been developed with second quantization, it will be applied to 1-dimensional homogeneous and dimerized chains of atoms. The dimerized chain will show us how a topological phase transition occurs in a 1-dimensional chain and how this leads to localised edge states. Furthermore, it will bring us the notion of topological invariants, which are the winding number and number of edge states in the case of the 1-dimensional dimerized chain.

This report will end with an outlook on what needs to be learned still, before the true search for new topological states from inhomogeneous spin-orbit coupling can begin. With topological materials playing a pivotal role in today's research in superconductivity, spintronics and quantum computing [5, 6], it is hardly necessary to stress the excitement and satisfaction one can gain from studying this topic.

2 Second Quantization Formalism

2.1 Many-particle Hilbert space

Before explaining what second quantization is and why it is useful, let us first consider many-particle states in regular 'first' quantization. An n -particle wavefunction lives in the Hilbert space H_n generated by the tensor product of its n single-particle Hilbert spaces H_1 . A system of indistinguishable particles has the added condition that a state must be untouched by the exchange of two particles. Defining the permutation operator of any two arbitrary particles $S_{ab} |\psi(a, b)\rangle = \alpha |\psi(a, b)\rangle$, it can easily be shown that $\alpha = \pm 1$ are the only possible eigenvalues for a system of indistinguishable particles [3, p. 262]. This restricts the total direct product space of dimension $n!$ to exactly state two vectors: The bosonic totally symmetric and the fermionic totally anti-symmetric wavevectors. The Hilbert space spanned by these two vectors is denoted F_n . Note that for $n = 2$, these two vectors form a complete basis $H_2 = F_2$, but for $n \geq 3$, $F_n \subset H_n$. The case where $n = 1$ is trivial ofcourse, since no permutation is possible. From now on, we will restrict ourselves to the discussion of fermionic (anti-symmetric) wavevectors to describe many-electron states in condensed matter. The totally anti-symmetric wavevector is often denoted as the Slater determinant

$$\Psi(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\lambda_1}(x_1) & \phi_{\lambda_2}(x_1) & \cdots & \phi_{\lambda_N}(x_1) \\ \phi_{\lambda_1}(x_2) & \phi_{\lambda_2}(x_2) & \cdots & \phi_{\lambda_N}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\lambda_1}(x_N) & \phi_{\lambda_2}(x_N) & \cdots & \phi_{\lambda_N}(x_N) \end{vmatrix} \quad (1)$$

$$= \frac{1}{\sqrt{N!}} \sum_{\mathbf{x} \in S_N} (-1)^P \phi_{\lambda_1}(x_1) \dots \phi_{\lambda_N}(x_N), \quad (2)$$

where $\phi_{\lambda_1}(x_1)$ denotes one spin-orbital wavefunction at position x_1 with eigenvalue λ_1 and the summation runs over all possible permutations of \mathbf{x} . P counts the number of permutations of the *ordered product*. It is straightforward to verify that the determinant is zero if any two electrons share the same eigenvalue or position, in good correspondence with the Pauli principle. Bear in mind that, for ease of imagination, we have chosen the position basis to project the wavefunctions onto $\langle x_1 | \phi_{\lambda_1} \rangle = \phi_{\lambda_1}$, but this could of course have been any arbitrary basis. It is easily noted that for large N , writing down the determinant becomes rather cumbersome. However, we will see that in second quantization, we can let go completely of the determinant, once we have understood exactly how they relate to one another.

2.2 The Occupation Basis & Fock Space

Now, instead of clinging on to the idea that we have to keep track of the position of every electron, we can make smart use of the indistinguishability of the

particles again to write the wavefunction in a more succinct way. Think of an enormous set \mathcal{S} of single-particle states, which many more states than needed to describe the wavefunction in eq.(1). The electrons of our wavefunction in eq.(1) then only occupy certain states in \mathcal{S} . To write down our wavefunction, we merely list all states in \mathcal{S} in order of increasing λ and just write an $n_\lambda = 0, 1$ when the state is occupied ($n_\lambda = 0$) or not ($n_\lambda = 1$):

$$|n_\lambda\rangle = |0 \dots \overset{\lambda_1}{1} \dots 0 \dots \overset{\lambda_2}{1} \dots 0 \dots \overset{\lambda_N}{1}\rangle. \quad (3)$$

Since the wavefunction only lives on the subset of \mathcal{S} which contains its own N single-particle states, we could drop all the zeros in eq.(3). However, accounting for the possibility of creation and annihilation of electrons, it is more general to write the wavefunction as

$$\Psi_{\lambda_1, \dots, \lambda_\infty}(x_1, \dots, x_\infty) = |n_{\lambda_1}, \dots, n_{\lambda_\infty}\rangle, \quad (4)$$

where n_{λ_1} denotes the number of electrons occupying the orbital corresponding to λ_1 . As mentioned before, n_λ can only take the values 0 or 1, since any other value would mean that two or more electrons share the same eigenvalue which is forbidden by the Pauli principle. The representation of wavefunctions in occupation basis is referred to as *second quantization*.

If we now release the constraint of a fixed number of electrons, we can define the space in which a system with a variable number of electrons lives as the direct sum of all F_n as defined above, called the *Fock space*

$$F(H) = \bigoplus_{n=0}^{\infty} F_n = \bigoplus_{n=0}^{\infty} \bigoplus_{\nu=\pm} S_\nu H^{\otimes n} = \mathbb{C} \oplus H \oplus (S_+(H \otimes H)) \oplus \dots, \quad (5)$$

where S_ν denotes the operator which (anti-)symmetrizes the tensor it acts upon. Thus, we have the fermionic (bosonic) Fock space by keeping only S_- (S_+) in eq.(5). The Fock space is the natural space of quantized fields (usually referred to as 'the second quantization'), much like the Hilbert spaces are the natural spaces of quantized particles (first quantization).

At this point it is important to realise that the number of electrons at a certain-point in time actually fixes the Hilbert space that you are working in, explaining why writing states in occupation basis is so convenient. Adding an electron adds $N + 1$ new terms to the fully anti-symmetric basis in Hilbert space, whereas in Fock space it just turns a zero into a one.

We thus define the creation and annihilation operators in second quantization as follows

$$c_{\lambda_1}^\dagger |\dots \overset{\lambda_1}{0} \dots\rangle = |\dots \overset{\lambda_1}{1} \dots\rangle \quad c_{\lambda_1} |\dots \overset{\lambda_1}{1} \dots\rangle = |\dots \overset{\lambda_1}{0} \dots\rangle. \quad (6)$$

In order to satisfy the anti-symmetric properties of fermionic particles as described in first quantization, these operators have to satisfy the following anti-commutation relations

$$\{c_\alpha^\dagger, c_\beta^\dagger\} = \{c_\alpha, c_\beta\} = 0 \quad (7)$$

$$\{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha, \beta}. \quad (8)$$

From the same argument, it follows that $c_{\lambda_\alpha}^\dagger |\dots \overset{\lambda_\alpha}{1} \dots\rangle = 0$. Like we defined the ordered product in eq.(2), we will take the convention of writing our state as the result of successively applying the creation operator on the vacuum in the same order of eigenvalues as that we write the occupation number in the ket

$$|n_{\lambda_1} \dots n_{\lambda_N}\rangle = c_{\lambda_1}^\dagger \dots c_{\lambda_N}^\dagger |0\rangle. \quad (9)$$

When having a combination of both annihilation and creation operators, it often proves useful to write them using the commutation relation in normal order with respect to the vacuum $|0\rangle$, meaning all the annihilation operators closest to the ket and the creation operators after

$$c_{\lambda_1}^\dagger \dots c_{\lambda_N}^\dagger c_{\lambda_{N'}} \dots c_{\lambda_1'} |0\rangle.$$

Since the expectation value of normal ordered products is zero, all the terms you obtained from commuting the creation and annihilation operators can be striped away when calculating the expectation value.

As you have probably observed, the creation and annihilation operators are the second quantization analogues of the ladder operators for the quantum harmonic oscillator (QHO) and just like the QHO, we can define the counting operator as

$$\hat{N}_{\lambda_\alpha} |\dots n_{\lambda_\alpha} \dots\rangle = c_{\lambda_\alpha}^\dagger c_{\lambda_\alpha} |\dots n_{\lambda_\alpha} \dots\rangle = n_{\lambda_\alpha} |\dots n_{\lambda_\alpha} \dots\rangle. \quad (10)$$

To get a better feel of how first and second quantization formalism relate to each other and to convince ourselves of the utility of writing many-electron systems and operators in occupation basis, we will, at the risk of being pedantic, work out explicitly some basic exercises in both first and second quantization formalism before tackling many-particle systems.

Exercise 1

Let $H = \{\uparrow, \downarrow\}$ be the Hilbert space of a single electron.

- Write the basis of the (first quantization) Hilbert and (second quantization) Fock space of two electrons.
- Write the total spin operator $\hat{\mathbf{S}}$ in the first quantization basis.
- Write $\hat{\mathbf{S}}$ in the second quantization basis and test its action on a state.
- The complete basis of a 2-particle Hilbert space is given by the direct product

$$H_2 = H_1 \otimes H_1 = \{\{\uparrow_1, \downarrow_1\} \otimes \{\uparrow_2, \downarrow_2\}\} = \{\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow\}. \quad (11)$$

We know however, that the only acceptable (normalized) basis for two indistinguishable fermions is in fact as in eq.(1)

$$H_2^A = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \longrightarrow F_2 = |\overset{\uparrow\downarrow}{11}\rangle, \quad (12)$$

which we know is equivalent to F_2 as written above in occupation basis. Remember however, that the *complete* Fock basis is defined as in eq. (5) to also account for the for a variable number of particles.

- b) The single-particle spin operator is defined as the vector of Pauli matrices

$$\hat{\mathbf{S}} = \frac{\hbar}{2} \hat{\boldsymbol{\sigma}} = \frac{\hbar}{2} (\sigma_x, \sigma_y, \sigma_z) = \frac{\hbar}{2} \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right). \quad (13)$$

For two particles we have to extend the operator to operate in H_2 by taking the sum of two single-particle spin operators, each acting on one of the two single-particle Hilbert spaces and leaving the other invariant

$$\hat{\mathbf{S}} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 = \hat{\mathbf{S}}_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \hat{\mathbf{S}}_2. \quad (14)$$

$$= \frac{\hbar}{2} \left(\begin{bmatrix} \hat{\sigma}_x & \mathbb{1} \\ \mathbb{1} & \hat{\sigma}_x \end{bmatrix}, \begin{bmatrix} \hat{\sigma}_y & -i\mathbb{1} \\ i\mathbb{1} & \hat{\sigma}_y \end{bmatrix}, \begin{bmatrix} \mathbb{1} + \hat{\sigma}_z & 0 \\ 0 & -\mathbb{1} + \hat{\sigma}_z \end{bmatrix} \right). \quad (15)$$

When writing out the operator explicitly using the basis of H_2 as defined in eq. (11) and acting it on state (12), we see that the total spin is zero, no matter along which axis we measure

$$\hat{\mathbf{S}} \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{\hbar}{2\sqrt{2}} (\vec{0}, \vec{0}, \vec{0}).$$

- c) It is a straightforward exercise to show that single- and two-particle operators can be written in occupation basis [4] as

$$\hat{O}_1 = \sum_{i,j} \langle i|\hat{o}|j\rangle c_i^\dagger c_j \quad \hat{O}_2 = \sum_{ijkl} \langle ij|\hat{o}|kl\rangle c_i^\dagger c_j^\dagger c_l c_k. \quad (16)$$

Applying this to the one-particle Pauli spin matrices, we obtain

$$\sigma_x = c_\downarrow^\dagger c_\uparrow + c_\uparrow^\dagger c_\downarrow \quad \sigma_y = c_\downarrow^\dagger c_\uparrow - c_\uparrow^\dagger c_\downarrow \quad \sigma_z = c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow. \quad (17)$$

Using the matrices as defined in eq. (14) and the Fermi exclusion principle ($c_\uparrow^\dagger c_\uparrow^\dagger, c_\uparrow c_\uparrow \rightarrow 0$), we can very rapidly determine the action of, for example, the two-particle S_x on the two-particle state

$$\hat{S}_x |11\rangle = (c_\uparrow^\dagger c_\uparrow^\dagger + c_\downarrow^\dagger c_\downarrow^\dagger) (c_\downarrow c_\uparrow + c_\uparrow c_\downarrow) |11\rangle = 0. \quad (18)$$

Exercise 2

Consider the Hilbert space $H_1 = \{a, b\} \otimes \{\uparrow, \downarrow\}$ of a single electron.

- a) Write the basis of the (first quantization) Hilbert and (second quantization) Fock space of two electrons.
- b) Write the operators S_z , $\hat{\mathbf{S}}$ and S^2 in the first quantization basis.

- c) Use the states written in second quantization to infer the spectrum of the system.
- a) We could write down the 16 basisvectors of the 2-particle Hilbert space and then look for the anti-symmetric combinations, but instead, let us rewrite the two-particle Hilbert space as

$$H_2 = \left\{ \sum_{\alpha\sigma\beta\rho} |\alpha\sigma\rangle^{(1)} \otimes |\beta\rho\rangle^{(2)} \right\} = \left\{ \sum_{\alpha\sigma\beta\rho} (|\alpha^{(1)}\beta^{(2)}\rangle \otimes |\sigma^{(1)}\rho^{(2)}\rangle) \right\}.$$

We recognise now that we have the tensor product of the Hilbert space of two two-level systems. To make life easier we can anti-symmetrize both levels separately as shown in table 1. Taking the direct products of the symmetric kets of one two-level system with the anti-symmetric ket of the other two-level system and vice versa, gives us the 6 antisymmetric basis states of a 2-particle two-level system.

Table 1: Splitting of 2-level 2-particle state into symmetric parts

| | $ \alpha\rangle \otimes \beta\rangle$ | $ \sigma\rangle \otimes \rho\rangle$ |
|----------------|---|---|
| Symmetric | $ aa\rangle$ | $ \uparrow\uparrow\rangle$ |
| | $ bb\rangle$ | $ \downarrow\downarrow\rangle$ |
| | $\frac{1}{\sqrt{2}} ab\rangle + ba\rangle$ | $\frac{1}{\sqrt{2}} \uparrow\downarrow\rangle + \downarrow\uparrow\rangle$ |
| Anti-symmetric | $\frac{1}{\sqrt{2}} ab\rangle - ba\rangle$ | $\frac{1}{\sqrt{2}} \uparrow\downarrow\rangle - \downarrow\uparrow\rangle$ |

The naive way of going to occupation basis would be to immediately write down the six simple states that we can think of

$$F_2 = \left\{ \begin{bmatrix} a\uparrow & a\downarrow & b\uparrow & b\downarrow \\ 1 & 1 & 0 & 0 \end{bmatrix}, |1010\rangle, |0101\rangle, |0011\rangle, |0110\rangle^\times, |1001\rangle^\times \right\}. \quad (19)$$

However, in this system, we have to realise that the spins and the a, b eigenvalues can be *independently permuted*

$$S_{a \leftrightarrow b} |0110\rangle = -|1001\rangle.$$

Therefore, a superposition of two "simple" states in occupation basis is needed to guarantee that the states are at least eigenstates under the permutation of a single eigenvalue and that they are anti-symmetric under permutation the two particles. This exact condition is explicitly displayed in the table above when writing the symmetric and anti-symmetric parts of Hilbert space. Taking the direct product in Hilbert space of the anti-symmetric states with the symmetric states that consist of a superposition of two states will guarantee us with the right states in occupation basis

$$\begin{aligned} (|ab\rangle - |ba\rangle) \otimes (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) &= |1001\rangle + |0110\rangle \\ (|ab\rangle + |ba\rangle) \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) &= |1001\rangle - |0110\rangle. \end{aligned}$$

- b) Notice that we only have to extend the space of the operators to leave the $\{a, b\}$ space invariant

$$\begin{aligned}
\hat{\mathbf{S}} &= \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 = (\mathbb{1}_\alpha \otimes \hat{\mathbf{S}}_1) \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes (\mathbb{1}_\beta \otimes \hat{\mathbf{S}}_2) \\
&= \mathbb{1}_\alpha \otimes (\hat{\mathbf{S}}_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \hat{\mathbf{S}}_2) \\
&= \mathbb{1}_\alpha \otimes (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2) \\
\hat{S}_z &= \mathbb{1}_\alpha \otimes (\hat{S}_{z_1} + \hat{S}_{z_2}) \\
\hat{S}^2 &= \mathbb{1}_\alpha \otimes (\hat{\mathbf{S}} \cdot \hat{\mathbf{S}}).
\end{aligned}$$

As known from elementary quantum mechanics, S^2 is diagonalized by the product spin-states as defined in table 1, with eigenvalues of \hbar (hence total spin 1) for the symmetric and 0 for the anti-symmetric states.

- c) Knowing that the operators above are diagonalized by the spin-states with which we have formed our space, we can easily group them to retrieve the well-known triplet and singlet states. For example, the state $|1100\rangle = |aa\rangle \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ will have total spin value 0, because it was formed with the anti-symmetric spin state. The values of S^2 and S_z have been tabulated below. Note that contrary to the classical example of helium, we have three $S^2 = 0$ states here, which is a result of taking into account the $\{a, b\}$ level.

Table 2: Splitting of the states into 'singlets' and triplets

| $S^2 = 0$ | | | $S^2 = 1$ | S_z |
|----------------|----------------|---|---|-------|
| | | | $ 1010\rangle$ | +1 |
| $ 1100\rangle$ | $ 0011\rangle$ | $\frac{1}{\sqrt{2}}(1001\rangle - 0110\rangle)$ | $\frac{1}{\sqrt{2}}(1001\rangle + 0110\rangle)$ | 0 |
| | | | $ 0101\rangle$ | -1 |

Exercise 3

Let a state be an element of Fock space $|\psi\rangle \in F$ such that

$$\langle\psi|c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger|\psi\rangle \neq 0. \quad (20)$$

What is a possible state $|\psi\rangle$?

Having now absorbed the idea of Fock space as an extended Hilbert space where states with unequal number of particles can exist at the same time, it only takes a moment's thought to come up with the following state that satisfies the requirement

$$|\psi\rangle = |0\rangle \pm |1001\rangle. \quad (21)$$

Now that the formalism of second quantization is part of the routine, we can start tackling some more exciting problems.

3 1D Chain

As explained in the motivation, the study of 1-dimensional chains of atoms using the tight-binding model will introduce us to many concepts relevant to topology. From first quantization we know that in a homogeneous chain, tight-binding can explain the formation of bands in a material and that it predicts the formation of band-gapped structures for dimerized chains. After retrieving these results using the formalism of second quantization, we can show even more (topological) structure formation for open chains. Since we will often have to change to k-space, the change of basis (a discrete Fourier transform) from coordinate to k-space in second quantization is given without proof below

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-i\mathbf{k} \cdot \mathbf{r}_j} c_k^\dagger \quad c_j = \frac{1}{\sqrt{N}} \sum_k e^{i\mathbf{k} \cdot \mathbf{r}_j} c_k. \quad (22)$$

3.1 Periodic Homogeneous Chain

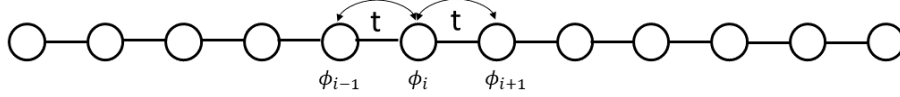


Figure 1: Homogeneous chain with hopping parameter t from one orbital ϕ to a nearest neighbour.

Let the wavefunction of the system be a linear combination of orthonormal atomic orbitals

$$|\psi\rangle = \sum_{j=0}^{N-1} \alpha_j |\phi_j\rangle, \quad \langle \phi_i | \phi_j \rangle = \delta_{ij}.$$

Discarding the self energy, which would only raise the energy arbitrarily, we can define the hopping with the off-diagonal Hamiltonian

$$\langle \phi_i | \hat{H} | \phi_j \rangle = -t(\delta_{i,j+1} + \delta_{i,j-1}), \quad (23)$$

which we know by now how to transform to occupation basis

$$\hat{H} = \sum_{i,j} c_i^\dagger H_{ij} c_j = \sum_j -t(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j). \quad (24)$$

Using eq.(22) we can diagonalize the Hamiltonian in k-space as

$$H = -\frac{t}{N} \sum_j \sum_{kk'} e^{-ikr_j} c_k^\dagger e^{ik'r_{j+1}} c_{k'} + e^{-ikr_{j+1}} c_k^\dagger e^{-ik'r_j} c_{k'} \quad (25)$$

$$= \sum_k -2t \cos(ka) c_k^\dagger c_k. \quad (26)$$

To reach eq.(26), we have invoked the periodic boundary condition $c_0^\dagger = c_{N-1}^\dagger$, which gives that $k = \frac{2\pi}{Na}n, n \in \mathbb{Z}$. We can then use this, together with the periodicity of the lattice $r_{j+1} = r_j + a$, to prove that

$$\sum_{j=0}^{N-1} e^{i(k'-k)r_j} = \delta_{kk'}.$$

Then summing over k' gives us the fully diagonalised Hamiltonian as shown in eq.(26), from which we recover the familiar dispersion relation $\epsilon_k = -2t \cos ka$.

3.2 Open Homogeneous Chain

Since we do not have periodic boundary conditions anymore and transforming to k-space would therefore make less sense, we will opt for a numerical approach to solve the Hamiltonian. Let us rewrite the Hamiltonian from eq.(24) as a matrix to put into

$$H = \begin{pmatrix} 0 & -t & 0 & \cdots & 0 \\ -t & 0 & -t & & 0 \\ 0 & -t & 0 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & -t \\ 0 & 0 & \cdots & -t & 0 \end{pmatrix}, \quad (27)$$

Note that to make this system periodic, you would only have to insert a $-t$ at the top-right and bottom-left entry of the matrix. This can be useful as a check when solving the system numerically to verify that indeed you have the right matrix, in which case you should retrieve the same energy spectrum as for the exact solution (see figure 2). Opening up the chain again and computing

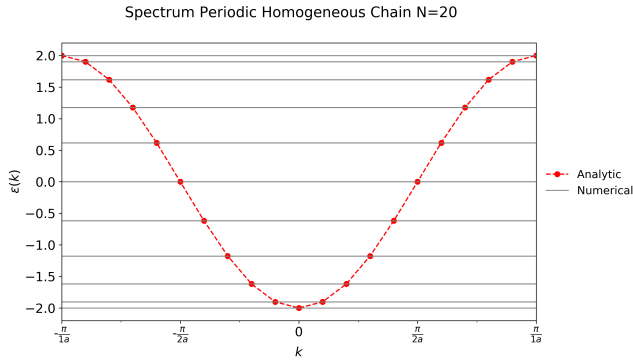


Figure 2: Correspondence of analytical (red) and numerical (grey) solutions found for periodic boundary conditions.

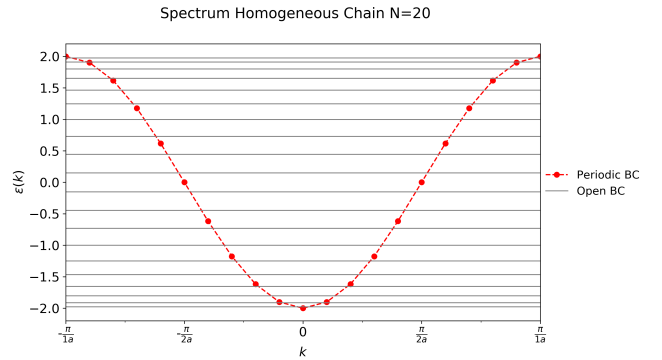


Figure 3: Spectrum of homogeneous chain with $N = 20$ atoms. In red is the analytical solution to the periodic boundary condition. In grey is the numerical solution to the open boundary condition.

the eigenvalues numerically, we see in figure 3 that there is a clear difference between the spectrum of chains with periodic and open boundary conditions. Although more can be said about the difference between periodic (semi-infinite) and open chains, let us move on to the next examples which are more relevant for the topic of topological insulators.

3.3 Periodic Dimerized Chain

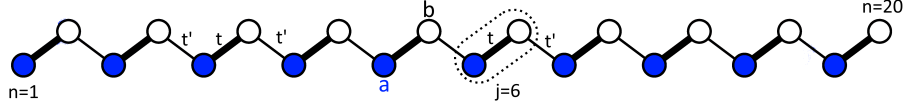


Figure 4: Dimerized chain with $N = 20$ atoms, $j = 10$ cells and t and t' being the intracellular and intercellular hopping parameters respectively. Adapted from [7].

In figure 4, we have already hinted at possible dimers of orbitals a and b . In first quantization we would write the wavefunction as a linear combination of the two distinct orbitals

$$|\psi\rangle = \sum_{j=0}^{N-1} \alpha_j |\phi_{ja}\rangle + \beta_j |\phi_{jb}\rangle \quad \langle\phi_{i\alpha}|\phi_{j\beta}\rangle = \delta_{ij}\delta_{\alpha\beta}$$

with the hopping terms in the Hamiltonian as

$$\langle\phi_{ia}|\hat{H}|\phi_{jb}\rangle = -t\delta_{ij} - t'\delta_{i,j+1}, \quad (28)$$

This would be rewritten in second quantization as

$$\hat{H} = \sum_j -t(c_{ja}^\dagger c_{jb} + c_{jb}^\dagger c_{ja}) - t'(c_{j+1,a}^\dagger c_{jb} + c_{jb}^\dagger c_{j+1,a}). \quad (29)$$

Transforming the creation and annihilation operators to k-space using eq.(22) and invoking the same arguments of periodic boundary condition and periodicity of the lattice (although here $r_{j+1} = r_j + 2a$) as was done in section 3.1, we arrive at the Hamiltonian

$$H = \sum_k c_{ka}^\dagger c_{kb} e^{ik\delta} (-t - t' e^{-ik2a}) + c_{kb}^\dagger c_{ka} e^{-ik\delta} (-t - t' e^{ik2a}) \quad (30)$$

$$= \sum_k (c_{ka}^\dagger c_{kb}^\dagger) \begin{bmatrix} 0 & -t - t' e^{ik2a} \\ -t - t' e^{-ik2a} & 0 \end{bmatrix} \begin{pmatrix} c_{ka} \\ c_{kb} \end{pmatrix}, \quad (31)$$

where $\delta = |r_a - r_b|$ the distance between orbital a and b in the same cell/dimer. The second equality is obtained by realising that we can write the Hamiltonian more beautifully as a 2x2 matrix by taking the vector $e^{ik\delta} \begin{pmatrix} c_{ka} \\ c_{kb} \end{pmatrix}$. The eigenvalues of this matrix are $\epsilon = \pm \sqrt{t^2 + t'^2 + 2tt' \cos(2ka)}$, which are plotted for the first Brillouin zone for the values $t = 1$ and $t' = 0.5$ in figure 5.

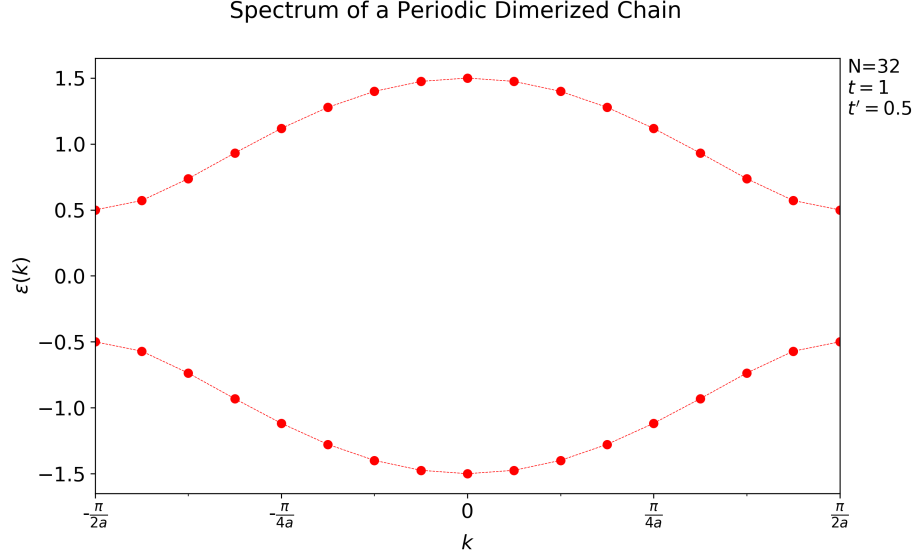


Figure 5: Spectrum of a dimerized chain made up of $N = 32$ atoms, plotted for $t = 1$ and $t' = 0.5$.

3.4 Open Dimerized Chain - SSH Model

If we now cut the dimerized chain open, we obtain what is called the Su-Schrieffer-Heeger model, discovered for a chain of polyacetylene in 1979 [8]. It is the simplest model that portrays a topological phase transition, which will be discussed in further detail in section 3.5. First, let us again rewrite the Hamiltonian (29) to get a more practical formulation using the vector $\mathbf{c}_j^\dagger = (c_{aj}^\dagger \ c_{bj}^\dagger)$

$$H = \sum_{i,j}^N \mathbf{c}_i^\dagger H_{ij} \mathbf{c}_j \quad (32)$$

$$= \begin{pmatrix} U & T & 0 & \cdots & 0 \\ T^\dagger & U & T & & 0 \\ 0 & T^\dagger & U & & \vdots \\ \vdots & & & \ddots & T \\ 0 & 0 & \cdots & T^\dagger & U \end{pmatrix}, \quad (33)$$

where

$$U = \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix} \quad T = \begin{pmatrix} 0 & 0 \\ -t' & 0 \end{pmatrix}.$$

Note that, like in the homogeneous chain, to make this system periodic, you only have to insert a T^\dagger and a T at the top-right and bottom-left entry of the corner,

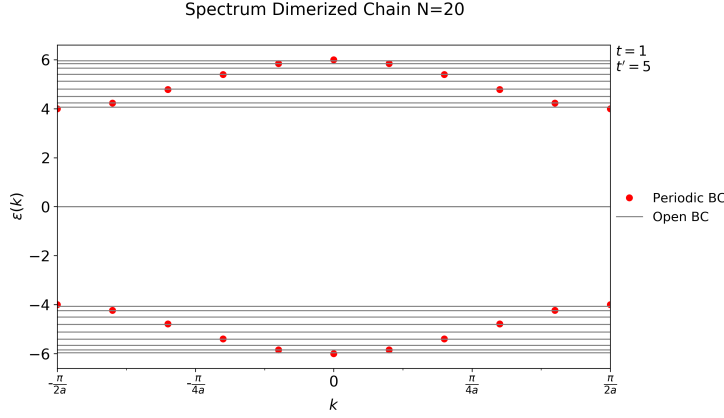


Figure 6: Energy spectrum of the dimerized chain: The dots are the energies found for the periodic chain, whereas the lines are the energies found for the open chain.

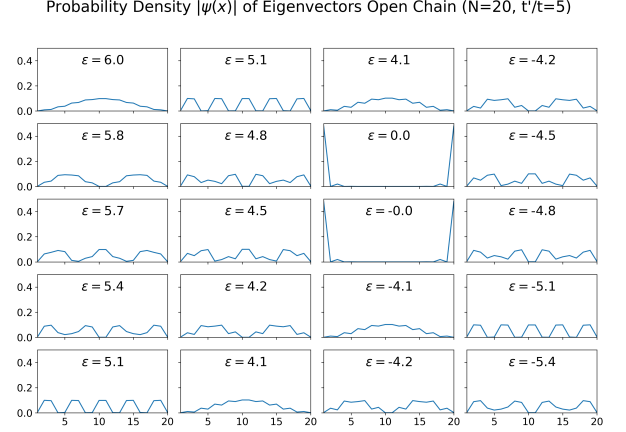


Figure 7: Probability density of the eigenvectors versus the position of the atoms.

respectively. By solving the above Hamiltonian numerically, we can obtain the eigenenergies and *spatial* eigenvectors, which will prove to be useful in a moment. The energies in the first Brillouin zone for a system of $N = 20$ particles and for $t' = 5t$ as well as the probability distribution of all 20 eigenvectors versus the position of the atoms are plotted in figures 6 and 7.

The most important thing to notice in this figure is the appearance of states at $\epsilon = 0$ that are not existent in chains with periodic boundary conditions for this particular choice of t'/t . Even more striking is the probability distribution of the two eigenvectors corresponding to $\epsilon = 0$ in figure 7. It seems as though these states are fully localised on the *edges* of the chain. The SSH model has just given us the first example of a topological state. Let us try to answer the next question that arises: When does it happen?

3.5 Topological Phase Transition

To discover what happens in the SSH model, the energy spectrum for various values of t and t' has been plotted in figure 8. The bulk spectrum, which can be seen as periodic in the thermodynamic limit $N \rightarrow \infty$, is plotted in red and the eigenenergies found for the open chain are plotted in grey. We see that the gap of width $\Delta = |t - t'|$ slowly closes as the ratio t'/t increases until the state becomes conducting in the bulk at $t = t'$. Then, as the ratio t'/t increases further, the band gap is opened again for the bulk state, but there appears a zero-energy state (actually two states) for the open chain which remains for as long as $t' > t$.

Since apparently the system undergoes some kind of change around $t' = t$, it makes sense to take a second look at the Hamiltonian for a clue as to what might happen. First, let us review the Hamiltonian of the bulk as was written

in eq.(31). Notice that, since it is a 2x2 matrix, it can be written in terms of the Pauli matrices

$$\begin{bmatrix} 0 & -t - t'e^{ik2a} \\ -t - t'e^{-ik2a} & 0 \end{bmatrix} = (-t - t' \cos(2ka))\hat{\sigma}_x + t' \sin(2ka)\hat{\sigma}_y. \quad (34)$$

Letting this matrix evolve from one end of the Brillouin zone to the other, we recognise that it traces out a closed circle of radius t' , centred at $(t, 0)$ in the σ_y, σ_x plane, as plotted in figure 8 [7]. The transition in the bulk happens when the circle intersects the point $(0, 0)$. Hence, we might be inclined to say that whether or not the Hamiltonian encloses the origin, as for a system where $t' > t$, defines whether or not we have these topological $\epsilon = 0$ edge states. The number of times that the Hamiltonian encloses the origin when traversing the Brillouin zone is known as the *winding number* and is indeed intricately connected to the edge states through something called the *bulk-boundary correspondance*.

Now, let us have a look at the open chain again. We can make sense of the appearance of zero-energy states for $t' > t$ (or a lack thereof for $t' < t$) by looking at the extreme cases of fully dimerized chains as sketched in figure 9.

Full dimerization happens when either t or t' is zero and they look similar enough, but they correspond to completely different *topological* configurations. Looking at the top case in figure 9, we see that for $t' = 0$, all states, including the edge states, are comprised of two sites. These both contribute an orbital, so we can make an even or odd superposition of the two orbitals a definite energy of $\pm\epsilon(k)$. However, in the case that $t = 0$, the two edge states are all on their own. Although the bulk is dimerized between cells and thus have energies of $\pm\epsilon(k)$, there is no self-energy term in the SSH model, thus the eigenenergy of the

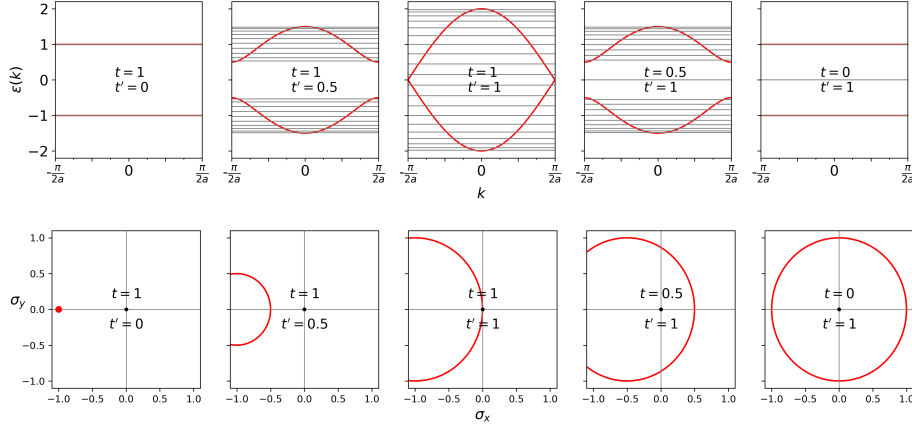


Figure 8: Top row: The energy spectrum for the bulk (red) and edge states (grey) are plotted in the first Brillouin zone for different values of t and t' . Bottom row: The trajectory that the bulk k-space Hamiltonian describes going from one side of the Brillouin to the other for different values of t and t' .

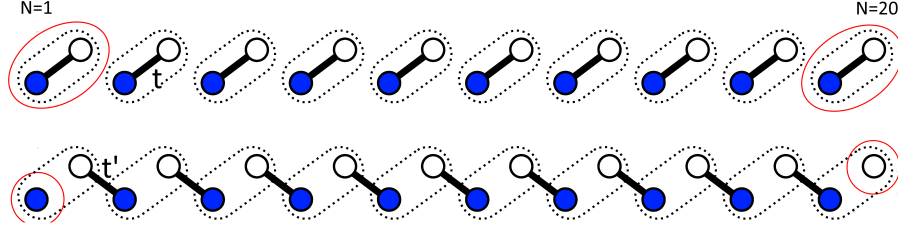


Figure 9: Fully dimerized states of the chain. Adapted from [7].

single states must be 0. What we saw in figure 7 was that the two eigenstates corresponding to $\epsilon = 0$ are localized at *both* edges, suggesting that those states are even and odd superpositions of the individual edges.

One can define an integer number characterising a Hamiltonian as *topological invariant* if it does not change under adiabatic deformation of the Hamiltonian. Adiabatic deformation here means that

1. the parameters in the Hamiltonian (t and t') are changed continuously
2. the symmetries in the system are maintained (not swapping t and t')
3. the bulk gap at $E = 0$ remains open (not crossing $t = t'$ when changing parameters).

We recognise from our previous discussion that the winding number falls neatly under the definition of a topological invariant. Hence, we can make official what we suspected already: the insulating system for $t' < t$ with $w = 0$ is topologically different from the system where $t' > t$ with $w = 1$! Furthermore, one can show using the winding number, that the number of edge states on either edge of this system is a topological invariant integer as well, namely 0 if $t' < t$ and 1 if $t' > t$ [7]. This is called the *bulk–boundary correspondence*, which states that a bulk topological invariant goes hand in hand with an edge topological invariant.

4 Conclusion & Outlook

In this report a brief overview of the formalism of second quantization has been given and tested on some simple exercises. Next, the second quantization formalism was used to write the Hamiltonian that describes hopping in 1-dimensional homogeneous and dimerized chains. For chains with periodic boundary conditions these Hamiltonians were solved analytically and compared to the numerical solution of the Hamiltonians of chains with open boundary conditions. It was shown that a topological phase transition occurs in the Su-Schrieffer-Heeger model at $t = t'$ after which the corresponding topological invariants, the winding number and number of edge states, were discussed.

The notions learned from the SSH model will be very applicable to the study of new topological states in the subsequent internship. One of the first things to understand after the SSH model will be the quantum Hall state (QHS), which occurs when electrons are confined to two dimensions and placed in a strong magnetic field. The theoretical prediction of the quantized Hall effect in a two-dimensional electron gas in 1975 by Ando et al. [9] soon led to the experimental realisation by Klitzing et al. [10] in 1980. As a corollary, they showed the geometric invariance of the Hall resistance ρ_{xy} , which marked the start of a new paradigm of classifying materials based on their *topological order* [11]. A step forward to grasping the importance of spin-orbit coupling in topology will be to understand the proof, due to Haldane in 1988, of the existence of a QHS in graphene by application of a periodic magnetic field [12]. The last step will be to recover the quantum *spin* Hall insulator, predicted in 2005 [13] for graphene and later produced in HgCdTe wells in 2007 [14, 15]. The quantum spin Hall insulator has, amongst other eccentric properties, two opposite spin-polarized currents that run in opposite directions along the edges of the material [16] and can be obtained by taking into account the spin-orbit coupling of the electrons with the material.

After finally understanding the role of spin-orbit coupling in topological materials, the time will be ripe to start investigating the possibility of the existence of topological states of matter under the application of *inhomogeneous* spin-orbit coupling.

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