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Edge states of a 1D topological insulator

Bachelor thesis

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Abstract

One of the most famous quasi particles is the exciton, a bound state of an electron and an electron hole. It is still being intensively researched, because it is very interesting. The exciton is an excitation of a topological insulator. We want to know all the properties of the edge states of topological insulators in one dimension. More specifically, we want to know the wave function and its energy. We found that edge states always have the same energy as the energy halfway the band gap. And that the wave functions peak at the topological side of the edge. We also found that we can rewrite the Hamiltonian to that of the Zeeman interaction, from which we can deduce the topological class of the Hamiltonian. The difference in topological classes explains why the edge states always have the same energy as halfway the band gap. Because the boundary between the topological classes has that energy. By researching the properties of edge states of a topological insulators in one dimension, we can obtain more knowledge about excitons and their edge states in the future.

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1 Introduction

Insulators are a great part of condensed-matter research. One-dimensional chains are also useful to research. The starting point of this thesis is a one-dimensional insulator. But we are not necessarily interested in a normal insulator, but in a topological insulator. The band structure of a topological insulator is similar to the band structure of a normal insulator. Since they both have a band gap. The difference is that the topological insulator has in some sense a knot in the band structure. That is why it is called a topological insulator. We will elaborate on the topological properties in later chapters. We are interested in what happens at the edge between a topological insulator and a normal insulator. This is called an edge state. Specifically, we are interested in the wave function of the edge state between the topological insulator and the normal insulator.

Our research question is: "What are the properties of an edge state of a one-dimensional topological insulator?" More specifically, we want to compute the wave function. We also want to know the energy of this bound state and why it has that energy. Previous work by Kathibi et al[1] is the starting point, since we use the same Hamiltonian. We continue in a different direction, as mentioned. Namely, researching the edge states of topological insulators.

We found that the edge states have the same energy as the energy halfway the band gap. And we also computed the according wave functions of these edge states. Furthermore, we explained the energy of the edge states by rewriting the Hamiltonian to include a fictional magnetic field. From that fictional magnetic field we deduced whether the Hamiltonian described a normal insulator or a topological insulator. The other parts of this thesis are organized as follows. Chapter 2 is about explaining the 1D chain. Chapters 3 and 4 are about the Hamiltonian and the fictional magnetic field we introduce. After that we introduce a mathematical explanation of how we distinguish the topological case from the trivial case, namely, the Berry phase. In Chapter 6 we describe the edge states and its properties. In Chapter 7 we show the results and, finally, in Chapter 8 we conclude this Bachelor thesis.

2 1D Chain

We construct a model of an infinite 1D chain of atoms with s and p orbitals and a distance between the atoms of a. The electrons on the atoms are spinless and do not interact with each other. The energy in the s orbital is ϵ_s. The energy in the p orbital is ϵ_p. There are also tunneling parameters from one orbital to another. The tunneling parameter going from one p orbital to the neighboring p orbital is t_p. Parameter t_s is the tunneling parameter between two s orbitals of nearest neighbors. The tunnel parameter for going from an s orbital to a p orbital or vice versa is V_{sp},V_{ps} respectively. The tunnel parameters are also shown in Figure 1.

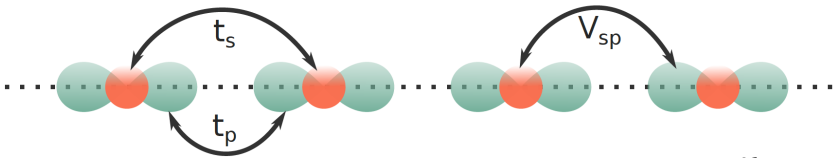


Figure 1: Representation of the 1D Chain[1].

3 Hamiltonian

We obtain the Hamiltonian in position space[1]:

$$
\begin{aligned}
H = \epsilon_s \sum_j \Psi^*_{s,j}\Psi_{s,j} + \epsilon_p \sum_j \Psi^*_{p,j}\Psi_{p,j} \\
- t_s \sum_j (\Psi^*_{s,j}\Psi_{s,j+1} + \Psi^*_{s,j+1}\Psi_{s,j}) + t_p \sum_j (\Psi^*_{p,j}\Psi_{p,j+1} + \Psi^*_{p,j+1}\Psi_{p,j}) \\
+ V_{sp} \sum_j (\Psi^*_{s,j}\Psi_{p,j+1} - \Psi^*_{s,j+1}\Psi_{p,j}) - V_{ps} \sum_j (\Psi^*_{p,j}\Psi_{s,j+1} - \Psi^*_{p,j+1}\Psi_{s,j}), \quad (1)
\end{aligned}
$$

where $\Psi_{s,j}$ is the wave function of the s orbital of the jth atom and $\Psi_{p,j}$ the wave function of the p orbital of the jth atom. To understand this Hamiltonian we look at the representation of this chain in Figure 1. We want to understand the signs in front of the tunneling parameters. First of all, we have to define which side of the p orbitals is the positive phase of the wave function and which side is the negative phase. We define the left lobe of the p orbital to be the positive phase of wave function, as seen in Figure 2.

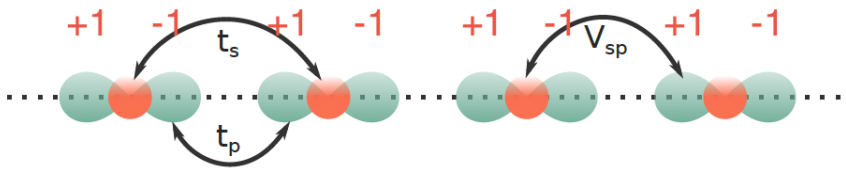


Figure 2: The sign of the phase of the wave functions of the p orbitals of the 1D Chain.

Tunneling parameter t_s describes the tunneling from one s orbital to another between nearest neighbors. If you hop from one s orbital to another you widen the wave function, thus decreasing k. That means that the kinetic energy decreases as well and thus we obtain a minus sign in front of t_s. Hopping between two nearest neighbor p orbitals means that the wave function has to go from either the positive phase of the wave function to the negative phase of the wave function, or vice versa. That takes energy, that is why the sign in front of t_p is negative. Now we look at the final four terms concerning the hybridization energies, V_{sp} and V_{ps}. Namely, the hopping from an s orbital to a p orbital or vice versa. In this case the sign depends on whether the p orbital is the positive phase of the wave function or the negative phase. The first term describes the hopping from an s orbital to the p orbital of the neighbor to the right. This means that this p orbital has a positive phase. That means the sign in front of this term and the corresponding parameter is plus. Then the sign in front

of the second term has to be minus, because the hopping takes place between an s orbital and the negative phase of the wave function of the p orbital. We continue the same reasoning for the third and fourth term.

Now we apply a Fourier transform from position space to momentum space by

$$\Psi_j(k,t) = Ce^{\mathrm{i}kaj}e^{\frac{-\mathrm{i}E_k t}{\hbar}}. \tag{2}$$

Here, C is a constant coefficient and E_k is the energy of the wave function. We can enter this into the Schrödinger Equation as

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi_j = \sum_{j'} H^{jj'}\Psi_{j'}. \tag{3}$$

We can do this for each combination of s and p orbitals. For example for $j = s$ and $j' = s$ we obtain

$$E\Psi_j = [\epsilon_s - 2t_s\cos ka]\Psi_j. \tag{4}$$

Then we do the same calculation for all 4 components, leading to

$$H = \begin{pmatrix} \epsilon_s - 2t_s\cos ka & 2\mathrm{i}V_{sp}\sin ka \\ \text{-}2\mathrm{i}V_{ps}\sin ka & \epsilon_p + 2t_p\cos ka \end{pmatrix}. \tag{5}$$

We have obtained a 2x2 Hamiltonian in momentum space. This Hamiltonian is much easier to manipulate than the Hamiltonian in position space.

3.1 Simplification

Since the Hamiltonian has a lot of variables, we want to simplify it. First of all, we assume $t = t_p = t_s$ and $t = V_{sp} = V_{ps}$. And finally we set $a = 1$. We then write the Hamiltonian as

$$H = \begin{pmatrix} \epsilon_s - 2t\cos k & 2\mathrm{i}t\sin k \\ \text{-}2\mathrm{i}t\sin k & \epsilon_p + 2t\cos k \end{pmatrix}. \tag{6}$$

From now on we redefine the energy in units of t. That means we have to divide by t in the Hamiltonian

$$H = \begin{pmatrix} \epsilon_s/t - 2\cos k & 2\mathrm{i}\sin k \\ \text{-}2\mathrm{i}\sin k & \epsilon_p/t + 2\cos k \end{pmatrix}. \tag{7}$$

The Hamiltonian is Hermitian, since it is equal to its own conjugate transpose.

3.2 Eigenvalues

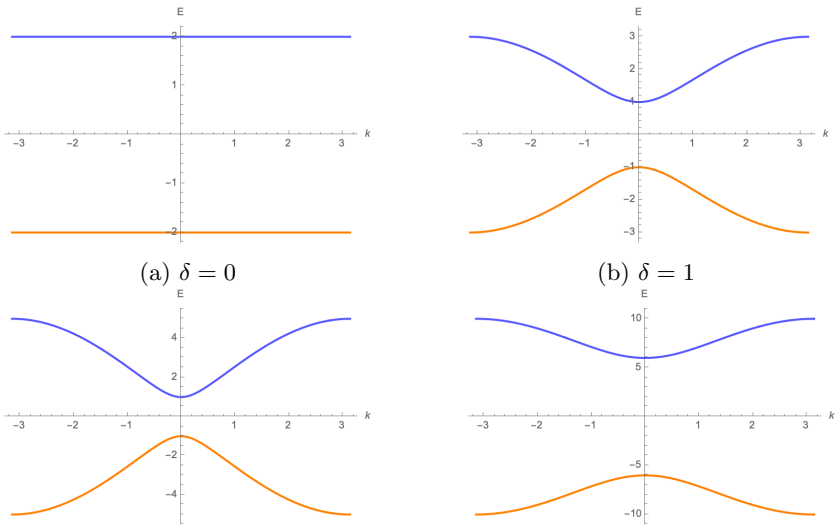
Since we have obtained the Hamiltonian, we can construct the band structure by calculating the eigenvalues. The eigenvalues of H are

$$E_{\pm} = \frac{\epsilon_s + \epsilon_p}{2t} \pm \sqrt{(\frac{\epsilon_s - \epsilon_p}{2t})^2 - 2(\frac{\epsilon_s - \epsilon_p}{t})\cos k + 4}. \tag{8}$$

We can compact this expression by renaming certain expressions. We call $E_0 = \frac{\epsilon_s + \epsilon_p}{2t}$ the zero point energy. And we define $\delta = \frac{\epsilon_s - \epsilon_p}{2t}$. We take $\delta \geq 0$ for simplicity sake. Substituting these expressions into the eigenvalues, we obtain

$$E_{\pm} = E_0 \pm \sqrt{\delta^2 - 4\delta \cos k + 4}. \tag{9}$$

We plot the eigenvalues for different δ and set $E_0 = 0$ to obtain the band structure. The blue graph is the conduction band and the orange graph is the valence band.



(a) $\delta = 0$ (b) $\delta = 1$

(c) $\delta = 3$ (d) $\delta = 8$

Figure 3: Band structure with different values of δ.

The band gap is the smallest difference between the conduction band and the valence band. For this Hamiltonian this is always at $k = 0$. The band gap is direct. Which means that the lowest energy of the conduction band and the highest energy of the valence band are at the same value of k. To give an example, the band gap for $\delta = 1$ is 2 t.

4 Magnetic Field

Since the Hamiltonian is Hermitian, we can write it as a linear combination of the Pauli matrices and the 2x2 unit matrix. To show the principle we use, we rename the components of the Hamiltonian to placeholder variables A, B and C. We simplify the matrix as follows

$$H = \begin{pmatrix} \text{A} & \text{iC} \\ \text{-iC} & \text{B} \end{pmatrix} = \begin{pmatrix} \frac{A+B}{2} + \frac{A-B}{2} & \text{iC} \\ \text{-iC} & \frac{A+B}{2} - \frac{A-B}{2} \end{pmatrix}. \tag{10}$$

If you subtract the constant from the eigenvalues in Equation 9 and then multiply by -1 you get the other eigenvalue. This is the same as the energy of a spin-up and spin-down particle in a magnetic field. This is exactly like the Hamiltonian of a Zeeman interaction. So we rewrite the Hamiltonian in this format

$$H = D\, I_2 + \vec{B} \cdot \vec{\sigma}. \tag{11}$$

Here, $\vec{\sigma}$ is the Pauli vector, which is defined as $\vec{\sigma} = \sigma_1 \hat{x} + \sigma_2 \hat{y} + \sigma_3 \hat{z}$. With $\sigma_{1,2,3}$ the Pauli matrices. With I_2 the 2x2 identity matrix and D a constant. We can read off the variables from the matrix in Equation 10 and write down the Hamiltonian in the correct form

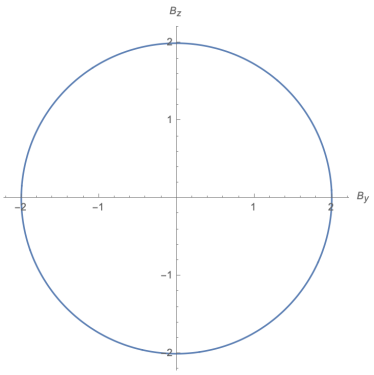
$$D = E_0, \vec{B} = \begin{pmatrix} 0 \\ -2\sin k \\ \delta - 2\cos k \end{pmatrix}, \tag{12}$$

$$H = E_0\, I_2 + \begin{pmatrix} 0 \\ -2\sin k \\ \delta - 2\cos k \end{pmatrix} \cdot \vec{\sigma}. \tag{13}$$

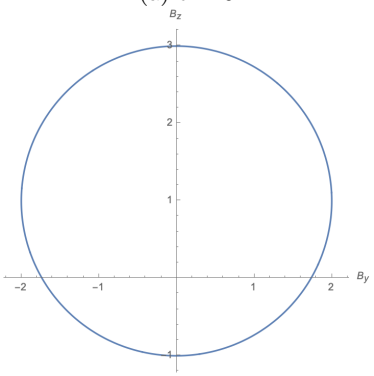
We can also rewrite this into matrix form

$$H = \begin{pmatrix} \text{E}_0 + \delta - 2\cos k & \text{2isin}\, k \\ \text{-2isin}\, k & \text{E}_0 - \delta + 2\cos k \end{pmatrix}. \tag{14}$$

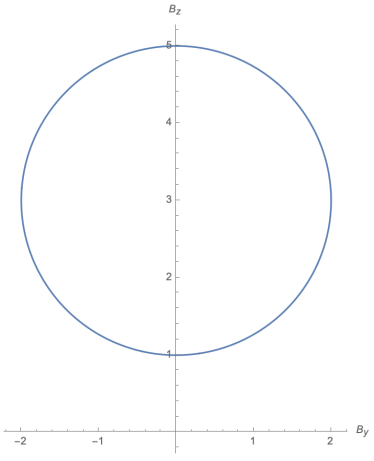
There is no magnetic field in the original problem, but we introduce this fictional magnetic field to make this problem easier to understand. We can plot $\vec{B}(k)$ for different values of δ. We plot the y- and z-component of the magnetic field for $k \in [-\pi, \pi]$ in Figure 4.



(a) $\delta = 0$



(b) $\delta = 1$



(c) $\delta = 3$

Figure 4: Fictional magnetic field with different values of δ.

For the first two cases, you can see that the origin is within the circle. And that for the last case the origin is outside of the circle. If you increase δ, the circle moves up the axis, as expected from $\vec{B}(k)$. There is a difference between whether the origin is within the circle or not. That is because if the origin is outside of the circle, we can smoothly deform the circle to a point. But if the origin is within the circle we cannot. Because the magnetic field cannot go through the origin because then it would not be an insulator anymore, as the band gap exactly closes. So there is an inherent difference between those two cases. In other words, the winding number of the magnetic field determines whether it is topological or not. The Hamiltonian describes a topological insulator for $0 \leq \delta < 2$ and a normal insulator for $\delta > 2$. Now we will elaborate on what happens at $\delta = 2$

4.1 Dirac point

If we choose $\delta = 2$, the fictional magnetic field passes through the origin, as you can see in Figure 5. That is called the Dirac point[3]. If $\delta = 2$ the Hamiltonian no longer describes an insulator. Because the band gap disappears. We can show this by plotting the band structure for $\delta = 2$ in Figure 6.

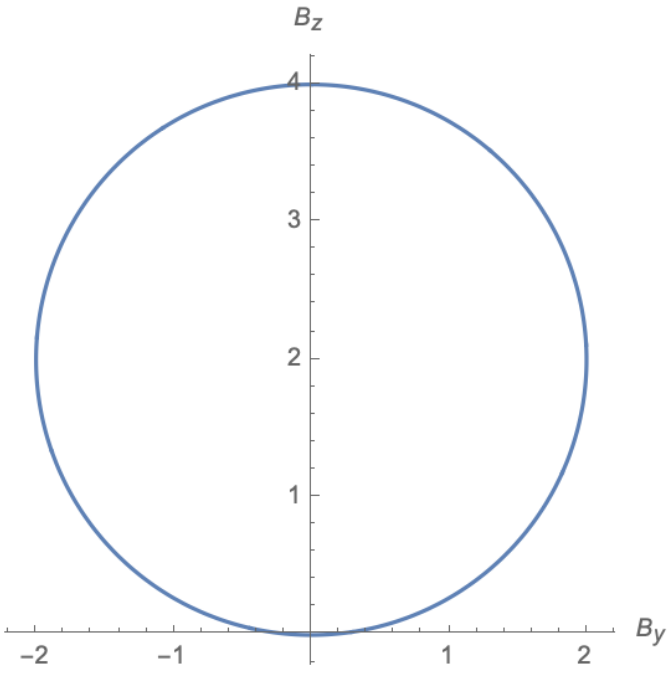


Figure 5: Magnetic field at the Dirac point($\delta = 2$).

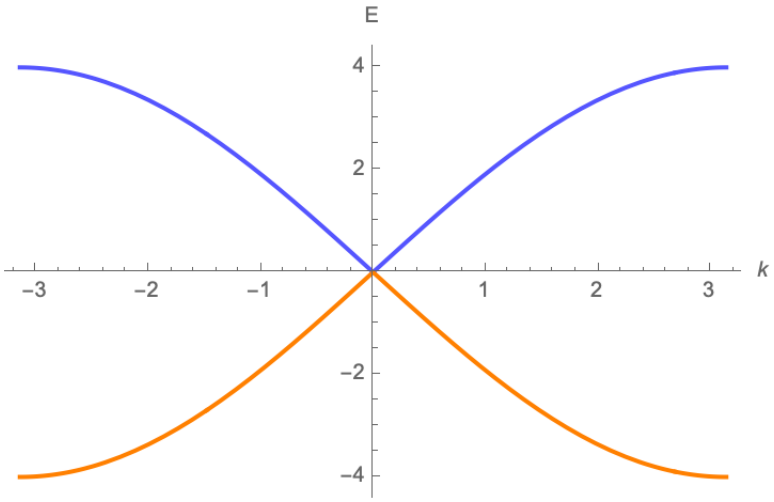


Figure 6: Band structure at the Dirac point (for $\delta = 2$).

The Dirac point is the transition between the topological case and the trivial case. Because for $\delta > 2$ you can smoothly deform the magnetic field to a point and for $0 \leq \delta < 2$ you cannot.

4.2 Band Structure

We have rewritten the Hamiltonian into that of Zeeman interactions. That means we can also plot the band structure by taking the length of the magnetic field times +1 and -1. We plot the length of the fictional magnetic field for $\delta = 3$ in Figure 7.

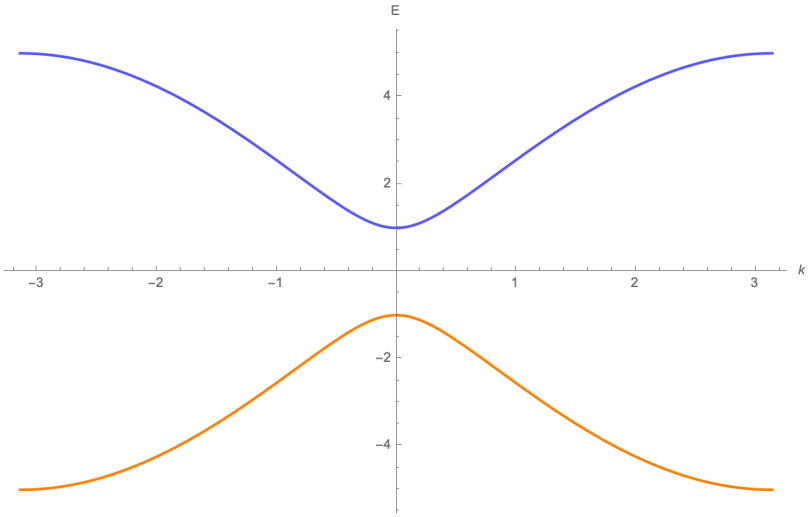


Figure 7: Length of the fictional magnetic field for $\delta = 3$.

4.3 Topology

The topology follows from a rule we set for the Hamiltonian. Namely that is has to describe an insulator. So that means that there has to be a band gap. And since for $\vec{B} = 0$, there is no band gap. We cannot allow $\vec{B}$ to be zero. So if the origin is enclosed by the magnetic field, we cannot smoothly deform the magnetic field to a point. Because we cannot go through the origin. But if the origin is not enclosed by the magnetic field, we can smoothly deform the magnetic field to a point. That means that whether the origin is enclosed by the magnetic field, determines the topological class.

5 Berry phase

We are now going to calculate the Berry phase[2]. This is the mathematical way of proving the difference between the topological and normal insulator. The Berry phase is defined by the following integral:

$$\nu = \frac{\mathrm{i}}{\pi} \int_{-\pi}^{\pi} \vec{u}^*(k) \cdot \frac{d\vec{u}(k)}{dk}\, dk \tag{15}$$

With $\vec{u}(k)$ an eigenvector of the Hamiltonian. We integrate over k from $-\pi$ to π. We multiply the integral by $\frac{i}{\pi}$. There is a Berry phase for the valence band and a Berry phase for the conduction band. Each eigenvector corresponds to either the valence or conduction band. To calculate the Berry phase we start of

with the Hamiltonian

$$H = \begin{pmatrix} \mathrm{E}_0 + \delta - 2\cos k & 2\mathrm{i}\sin k \\ \text{-}2\mathrm{i}\sin k & \mathrm{E}_0 - \delta + 2\cos k \end{pmatrix}. \tag{16}$$

Then, we calculate the eigenvectors

$$\vec{v}_1 = \begin{pmatrix} \frac{-i(-\delta+2\cos k+\sqrt{\delta^2-4\delta\cos k+4})}{2\sin k} \\ 1 \end{pmatrix}, \vec{v}_2 = \begin{pmatrix} \frac{i(\delta-2\cos k+\sqrt{\delta^2-4\delta*\cos k+4})}{2\sin k} \\ 1 \end{pmatrix}. \tag{17}$$

Then we normalize these eigenvectors by dividing by the length of the eigenvector. The lengths are

$$L_1 = \sqrt{1 + \frac{1}{4}(-\delta + 2\cos k + \sqrt{4 + \delta^2 - 4\delta\cos k})^2(\csc k)^2}, \tag{18}$$

$$L_2 = \sqrt{1 + \frac{1}{4}(\delta - 2\cos k + \sqrt{4 + \delta^2 - 4\delta\cos k})^2(\csc k)^2}. \tag{19}$$

Hence the normalized eigenvectors are

$$\vec{w}_1 = \begin{pmatrix} \frac{-i(-\delta+2\cos k+\sqrt{\delta^2-4\delta\cos k+4})}{2L_1\sin k} \\ \frac{1}{L_1} \end{pmatrix}, \vec{w}_2 = \begin{pmatrix} \frac{i(\delta-2\cos k+\sqrt{\delta^2-4\delta*\cos k+4})}{2L_2\sin k} \\ \frac{1}{L_2} \end{pmatrix}. \tag{20}$$

We name the components of these eigenvectors to simplify the calculation

$$\vec{w}_1 = \begin{pmatrix} w11 \\ w12 \end{pmatrix}, \vec{w}_2 = \begin{pmatrix} w21 \\ w22 \end{pmatrix}. \tag{21}$$

Now we apply a unitary transformation on the normalized eigenvectors. The current eigenvectors are in the y-z-plane. If we integrate from $-\pi$ to π with these eigenvectors the path will go trough the z-axis and not around it, since the basis is in the z-direction. The integral would just be zero. Because it ends up at the same point in the circle. If we apply this transformation the integrand moves around the z-axis. Thus ending up with a surface on the unit sphere. Which is exactly what the Berry phase is. Thus we apply the rotation

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{22}$$

$$U\vec{w}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} w11 + w12 \\ w11 - w12 \end{pmatrix}. \tag{23}$$

Then we divide the first eigenvector by their first component and the second eigenvector by the second component. If we don't carry out these divisions the

Berry phase calculation will not be correct. And finally, we divide both by $\sqrt{2}$. For the first eigenvector we obtain

$$\vec{u}_1 = U\vec{w}_1 \frac{1}{\sqrt{2}} \frac{\sqrt{2}}{w11 + w12} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{w11 - w12}{w11 + w12} \end{pmatrix}, \tag{24}$$

$$\vec{u}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{-2\mathrm{i} + 2\cot k + (-\delta + \sqrt{4 + \delta^2 - 4\delta\cos k})\csc k}{2\mathrm{i} + 2\cot k + (-\delta + \sqrt{4 + \delta^2 - 4\delta\cos k})\csc k} \end{pmatrix}. \tag{25}$$

And for the second eigenvector we obtain

$$\vec{u}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{-2\mathrm{i} - 2\cot k + (\delta + \sqrt{4 + \delta^2 - 4\delta\cos k})\csc k}{2\mathrm{i} - 2\cot k + (\delta + \sqrt{4 + \delta^2 - 4\delta\cos k})\csc k} \\ 1 \end{pmatrix}. \tag{26}$$

5.1 Integrand

We have calculated the eigenvectors in the correct form, now we can calculate the integrand. To calculate the integrand we have to compute the conjugate and the derivative of these eigenvectors, we obtain

$$\vec{u}_1^* = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{2\mathrm{i} + 2\cot k + (-\delta + \sqrt{4 + \delta^2 - 4\delta\cos k})\csc k}{-2\mathrm{i} + 2\cot k + (-\delta + \sqrt{4 + \delta^2 - 4\delta\cos k})\csc k} \end{pmatrix}, \tag{27}$$

$$\frac{d\vec{u}_1}{dk} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ \frac{2\mathrm{i}(-2 + \delta\cos k)}{(-2\mathrm{e}^{\mathrm{i}k} + \delta)\sqrt{4 + \delta - 4\delta\cos k}} \end{pmatrix}. \tag{28}$$

Now we calculate the integrand as

$$\vec{u}_1^* \cdot \frac{d\vec{u}_1}{dk} = \frac{(\delta\cos k - 2)(\mathrm{i}\cos k + \sin k)}{(2\mathrm{e}^{\mathrm{i}k} - \delta)(-2 + \delta\mathrm{e}^{\mathrm{i}k})}. \tag{29}$$

We do the same computation for $\vec{u}_2$:

$$\vec{u}_2^* \cdot \frac{d\vec{u}_2}{dk} = \frac{\mathrm{i}e^{\mathrm{i}k}(\delta\cos k - 2)}{(2\mathrm{e}^{\mathrm{i}k} - \delta)(-2 + \delta\mathrm{e}^{\mathrm{i}k})}. \tag{30}$$

5.2 Integral

And finally we integrate from $k = -\pi$ to $k = \pi$. For the conduction band, the first eigenvector, we obtain

$$\nu_c = \frac{\mathrm{i}}{\pi} \int_{-\pi}^{\pi} \frac{(\delta \cos k - 2)(\mathrm{i} \cos k + \sin k)}{(2\mathrm{e}^{\mathrm{i}k} - \delta)(-2 + \delta \mathrm{e}^{\mathrm{i}k})}\, dk. \tag{31}$$

The Berry phase is not the same for both eigenvectors. The Berry phase for the conduction band and for the valence band add up to 0

$$\nu_c + \nu_v = 0 \quad \forall\, \delta. \tag{32}$$

We can compute the Berry phase for different values of δ. For example, the Berry phase for $\delta > 2$ is always zero. At the Dirac point, $\delta = 2$, $\nu_c = \frac{1}{2}$,$\nu_v = -\frac{1}{2}$. If we look at $0 \leq \delta < 2$, $\nu_c = 1$ and $\nu_v = -1$.
We have now mathematically defined the difference between a topological case and a trivial case. The difference is the Berry phase. This also means that the Berry phase and winding number of the fictional magnetic field are the same. Because the winding number also made a distinction between the topological and normal insulator. Thus, if the winding number is 0, the Berry phase is 0. And if the winding number is 1, the Berry phase is either +1 or -1. At the Dirac point, the winding number is $\frac{1}{2}$ and the Berry phase is either $\frac{1}{2}$ or $-\frac{1}{2}$. So the absolute value of the Berry phase and the winding number of the fictional magnetic field are exactly the same for all values of δ.

6 Edge states

We now assume that we have 2 half infinite 1D chains. We connect these chains at $x = 0$. This means we now have two sides. We can assign a certain δ value for the right side and a different δ value for the left side. We want to connect the wave functions from either sides. So we have to write up the wave functions and then set them equal at the edge, $x = 0$. We also set as a condition that the derivatives are the same at $x = 0$. This way we will have four coupled equations. First we have to simplify the Hamiltonian. We assume $E_0 = 0$ and we also approximate the trigonometric functions by $\sin k \approx k$ and $\cos k \approx 1 - \frac{k^2}{2}$. We enter the approximations in to the Hamiltonian, to obtain

$$H = \begin{pmatrix} \mathrm{E}_0 + \delta - 2\cos k & 2\mathrm{i}\sin k \\ \text{-}2\mathrm{i}\sin k & \mathrm{E}_0 - \delta + 2\cos k \end{pmatrix} \approx \begin{pmatrix} \delta - 2 + k^2 & 2\mathrm{ik} \\ \text{-}2\mathrm{ik} & \text{-}\delta + 2 - k^2 \end{pmatrix}. \tag{33}$$

We want to obtain a wave function that describes a bound state. That means that we do not allow plane wave functions as solutions. We need a wave function that approaches zero as x goes to infinity, for the right side. And a wave

function that approaches zero as x goes to minus infinity, for the left side. Only in the band gap do we have exponentially decaying wave functions. Outside of the band gap there will just be plane wave functions. That is why we transform $k \rightarrow \mathrm{i}\kappa$, because the eigenvalues of the Hamiltonian will be in the band gap. After the transformation we obtain the Hamiltonian

$$H = \begin{pmatrix} \delta - 2 - \kappa^2 & \text{-}2\kappa \\ 2\kappa & \text{-}\delta + 2 + \kappa^2 \end{pmatrix}. \tag{34}$$

6.1 The wave function

We will now define two wave functions for either sides of $x = 0$. The wave functions are a superposition of the two eigenvectors multiplied by the corresponding exponential functions. A singe solution takes the form of

$$\vec{v}_n e^{\mathrm{i}k_n x}. \tag{35}$$

We carry out the transformation $k \rightarrow \mathrm{i}\kappa$ and remove the minus sign because there always is a positive and negative value for κ as a solution. Since we know that the band structure is symmetric around $E = 0$ t. The wave function for the left side is

$$\Psi = c_1 \vec{v}_1 e^{\kappa_1 x} + c_2 \vec{v}_2 e^{\kappa_2 x} \quad for \quad x \in (-\infty, 0]. \tag{36}$$

The wave function for the right side is

$$\Phi = c_3 \vec{w}_1 e^{\kappa_3 x} + c_4 \vec{w}_2 e^{\kappa_4 x} \quad for \quad x \in [0, \infty). \tag{37}$$

The vectors $\vec{v}_{1,2}$ are the eigenvectors for the left side and $\vec{w}_{1,2}$ are the eigenvectors of the right side. We define κ_n as the the transformed wave numbers that correspond to each eigenvector. They are calculated by setting the eigenvalue, in terms of κ_n, equal to energy E. And finally, c_n are constant coefficients.
We make sure that the wave functions approach zero as x goes to plus and minus infinity. That means that $\kappa_{1,2}$ have to be positive for the left-side wave functions. And $\kappa_{3,4}$ have to be negative for the right-side wave functions. Let κ_1 be the κ of the eigenvalue that corresponds to $\vec{v}_1$. For example

$$E = 1 - \kappa_1^2 \quad \Rightarrow \quad \kappa_1 = \sqrt{1 - E}. \tag{38}$$

We also substitute this formula for κ_1 in the corresponding eigenvector. And do the same procedure for all eigenvectors. That way we obtain wave functions in terms of energy only.

6.2 Coupled equations

We take the wave functions and define our boundary conditions. Namely, the wave functions and their derivatives with respect to x have to be equal at $x = 0$. We obtain

$$\Psi(E, x = 0) = \Phi(E, x = 0), \tag{39}$$

$$\frac{\partial}{\partial x}\Psi(E, x)\bigg|_{x=0} = \frac{\partial}{\partial x}\Phi(E, x)\bigg|_{x=0}. \tag{40}$$

We have 2 components per equation, so 4 equations in total

$$c_1\vec{v}_1 + c_2\vec{v}_2 - c_3\vec{w}_1 - c_4\vec{w}_2 = 0, \tag{41}$$

$$c_1\kappa_1\vec{v}_1 + c_2\kappa_2\vec{v}_2 - c_3\kappa_3\vec{w}_1 - c_4\kappa_4\vec{w}_2 = 0. \tag{42}$$

We define the components of $\vec{v}_1$ as v_{11} and v_{12}. And define the components of the other vectors in the same manner. Now we can write these equations into a 4x4 matrix equation, to obtain

$$\begin{pmatrix} v_{11} & v_{21} & -w_{11} & -w_{21} \\ v_{12} & v_{22} & -w_{12} & -w_{22} \\ \kappa_1 v_{11} & \kappa_2 v_{21} & -\kappa_3 w_{11} & -\kappa_4 w_{21} \\ \kappa_1 v_{12} & \kappa_2 v_{22} & -\kappa_3 w_{12} & -\kappa_4 w_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = 0. \tag{43}$$

We now have a matrix that only depends on energy. We want to know what energy solves this equation, so we calculate the determinant of the matrix for a specific value of δ. The resulting energy is plugged into the matrix and then we can solve for the coefficients. All coefficients being zero is a useless solution so we do not consider that solution. That is why we want to find the energy for which the determinant is zero.

7 Results

For example, let us choose $\delta = 1.5$ for the left side, $\delta = 3$ for the right side. That means we have the topological case on the left side and the trivial case on the right side. The eigenvectors are

$$\vec{v}_1 = \begin{pmatrix} -\frac{0.5(0.5+\kappa_1^2+\sqrt{0.25-3\kappa_1^2+\kappa_1^4})}{\kappa_1} \\ 1 \end{pmatrix}, \vec{v}_2 = \begin{pmatrix} -\frac{0.5(0.5+\kappa_1^2-\sqrt{0.25-3\kappa_1^2+\kappa_1^4})}{\kappa_1} \\ 1 \end{pmatrix}, \tag{44}$$

$$\vec{w}_1 = \begin{pmatrix} -\frac{-1+\kappa_3^2+\sqrt{1-6\kappa_3^2+\kappa_3^4}}{2\kappa_3} \\ 1 \end{pmatrix}, \vec{w}_2 = \begin{pmatrix} -\frac{-1+\kappa_4^2-\sqrt{1-6\kappa_4^2+\kappa_4^4}}{2\kappa_4} \\ 1 \end{pmatrix}. \quad (45)$$

We also calculate the eigenvalues to transform κ to energy as

$$\vec{v}_1 : E = -\sqrt{0.25 - 3\kappa_1^2 + \kappa_1^4}, \quad \vec{v}_2 : E = \sqrt{0.25 - 3\kappa_2^2 + \kappa_2^4}, \quad (46)$$

$$\vec{w}_1 : E = -\sqrt{1 - 6\kappa_3^2 + \kappa_3^4}, \quad \vec{w}_2 : E = \sqrt{1 - 6\kappa_4^2 + \kappa_4^4}. \quad (47)$$

We now rewrite each κ in terms of E, keeping in mind that $\kappa_{1,2}$ have to be positive, $\kappa_{3,4}$ have to be negative.

$$\kappa_1 = 0.5\sqrt{6 - 2\sqrt{9 + 4(E^2 - 0.25)}}, \kappa_2 = 0.5\sqrt{6 + 2\sqrt{9 + 4(E^2 - 0.25)}}, \quad (48)$$

$$\kappa_3 = -\sqrt{3 - \sqrt{8 + E^2}}, \kappa_4 = -\sqrt{3 + \sqrt{8 + E^2}}. \quad (49)$$

We now fill in these values and calculate the determinant of the matrix. We now plot the determinant for all energies within the smallest of the two band gaps, so for $E \in (-\frac{1}{2}, \frac{1}{2})$. The band gap can be found by plugging in $\kappa = 0$ in to the eigenvalues.

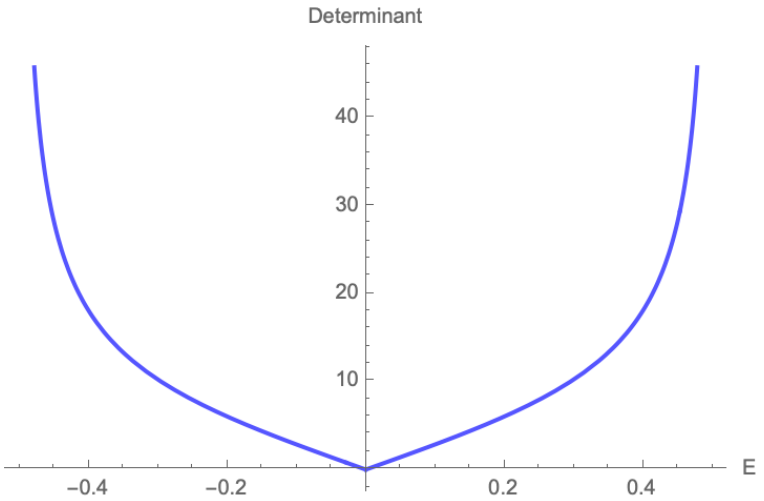


Figure 8: The determinant of the coupled equations matrix plotted in the band gap.

As you can see in Figure 8, the determinant is zero for $E = 0$. So we plug this energy in to the matrix and solve for the coefficients. We first define $c_1 = 1$ without loss of generality. And then solve for the other three coefficients:

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{1}{3} \\ 0 \\ \frac{2}{3} \end{pmatrix}. \tag{50}$$

As you can see $c_3 = 0$, that means that the first eigenvector of the right side is not taken into account. That is because both $\vec{v}_{1,2}$ are (-1,1) and $\vec{w}_2$ is also (-1,1). But $\vec{w}_1$ is (1,1), so that can never work. That means c_3 has to be zero. We then fill the coefficients into the wave functions and plot both components in Figures 9 and 10.

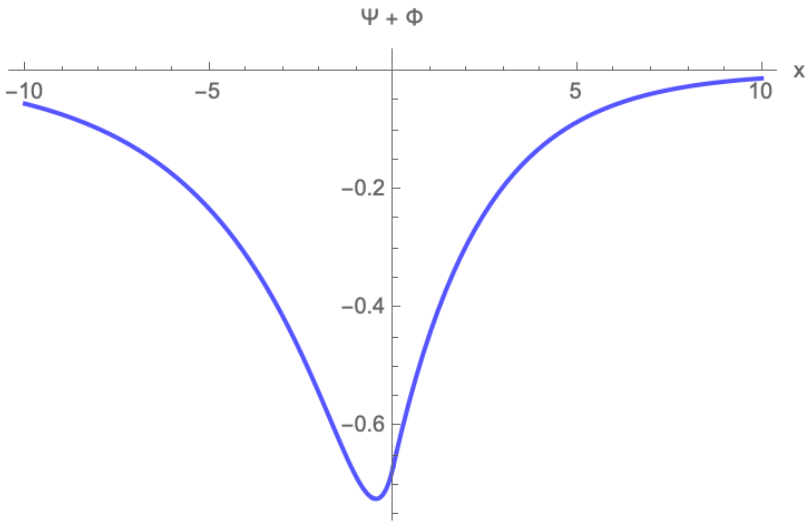


Figure 9: First component of the wave functions.

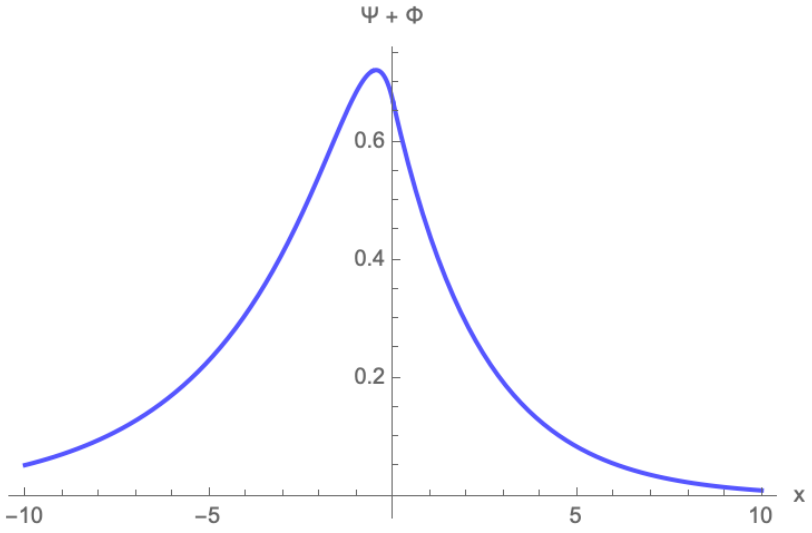


Figure 10: Second component of the wave functions.

What we can see from these figures, is that the first component is the same as the second component but times -1. In other words, the eigenvector is (-1,1), as explained in the previous paragraph. Furthermore, we can see that the maximum of the wave function is slightly to the left side. So that means it is slightly towards the side with $\delta = 1.5$. We can explain that by looking at the wave functions. Since $c_3 = 0$, the trivial side only has one exponential function. And there can never be a peak in that wave function other than at $x = 0$. So that is why the maximum of the wave function has to be on the topological side. You cannot connect two trivial sides because both sides only have one exponential function, as seen in the calculation above. So the boundary conditions can never be met. We tried connecting two topological insulators. But this is not possible. This is not obvious from looking at the exponential functions. Since there are two on each side. But the determinant of the coupled equations matrix is never zero. That means that there cannot be a solution.

For $\delta = 1$ and $\delta = 0$ something interesting happens. You cannot connect these values of δ to a normal insulator. Even if the determinant of the coupled equations matrix is zero somewhere inside the band gap. The problem arises when calculating $\kappa_{1,2}$. For example, let us set $\delta = 1$ for the left side and $\delta = 3$ for the right side. The determinant is zero when $E = 0$. Then when we calculate $\kappa_{1,2}$, we only obtain 1 and -1 as solutions. Since they both have to be positive, $\kappa_1 = \kappa_2 = 1$. This means that there is only one exponent in the wave function. If we enter the respective values for κ_1 and κ_2 into the eigenvectors, they become the same as well. So the wave function on the left side now consists of one term. And the wave function on the right side as well, as shown in the previous

paragraph. That means the boundary conditions cannot be met, since we don't allow the wave functions to be zero everywhere as a solution. So for $\delta = 1$ and $\delta = 0$ the eigenvectors and values of κ become equal making it impossible to meet the boundary conditions.

7.1 Energy

Now we go back to the initial edge state of two connected chains. If we look at the magnetic field from the left side and from the right side, we know that there is a difference regarding their winding number. That means that the edge, which is at $x = 0$, has to cross that difference. The bridge between those points must therefore happen at the Dirac point, since the magnetic field touches the origin at that point. That means the magnetic field is zero at $k = 0$. So that means the energy is also zero. Which is defined as the energy halfway the band gap. So the topology explains the energy of the edge states.

7.2 Solution of edge state against wall

We can also impose different boundary conditions onto the wave function. We define a wall at $x = 0$. So that means we only have one wave function this time. The boundary condition is that the wave function has to equal zero for $x \geq 0$. We write the boundary condition as an equation, to obtain

$$\Psi(E, x = 0) = 0. \tag{51}$$

We write down the wave function

$$\Psi = c_1 \vec{v}_1 e^{\kappa_1 x} + c_2 \vec{v}_2 e^{\kappa_2 x} \quad for \quad x \in (-\infty, 0]. \tag{52}$$

And apply the boundary conditions to obtain the value of the coefficients:

$$\Psi(E, x)\Big|_{x=0} = c_1 \vec{v}_1 e^{\kappa_1 x} + c_2 \vec{v}_2 e^{\kappa_2 x}\Big|_{x=0} = 0. \tag{53}$$

We calculate the eigenvalues and eigenvectors. Then we calculate the values of $\kappa_{1,2}$ for $E = 0$. As x goes to negative infinity, $\kappa_{1,2}$ have to be positive. Since we know $E = 0$ is the solution, from the boundary conditions of the previous chapter. Now we plug these values of κ into the eigenvectors. We also define $c1 = 1$ without loss of generality. As an example, we calculate the wave function for $\delta = 1.5$, to obtain

$$\Psi(0, x)\Big|_{x=0} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} + c_2 \begin{pmatrix} 1 \\ -1 \end{pmatrix} = 0. \tag{54}$$

We see that c_2 has to be -1. Now we can plot the wave function in Figures 11 and 12.

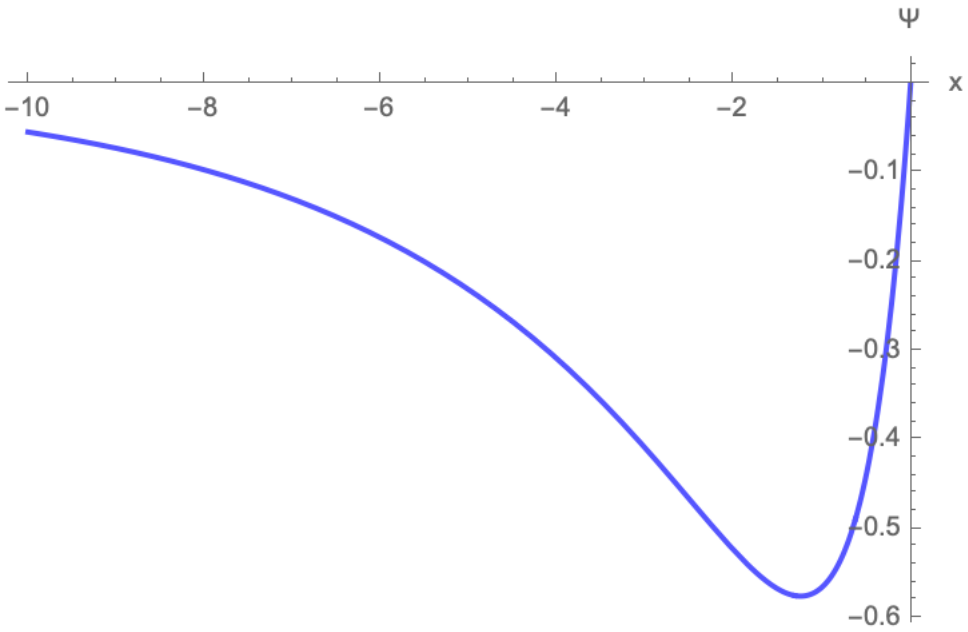


Figure 11: First component of wave function ($\delta = 1.5$).

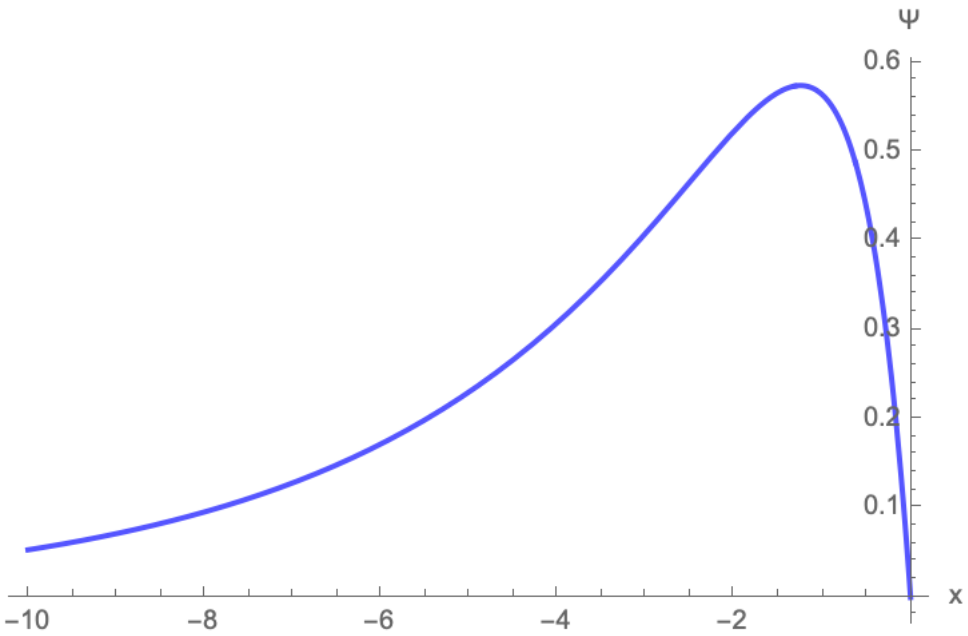


Figure 12: Second component of wave function ($\delta = 1.5$).

We can see that for these boundary conditions, there is no solution possible for a normal insulator. This is because in that case the two eigenvectors are not a multiple of each other, as mentioned in Chapter 7. That means that they cannot be added up together to become 0. That is needed for this boundary condition to hold. This shows that the topology is not a consequence of the specific boundary conditions. In other words it is topologically protected[4].
For $\delta = 1$ and $\delta = 0$ there is also no solution possible in this boundary condition. Since the real part of the values of κ_1 and κ_2 are equal, there is only one exponent again. Thus resulting in a wave function that is zero everywhere, which we do not allow.

8 Conclusion

In this thesis we researched the properties of the edge states of a 1D chain topological insulator. We constructed the wave functions of these edge states. Moreover, we found that the energy of the edge states are always at the energy halfway the band gap. We can explain why the edge state always this energy. This is because the connection between the trivial and topological case is at the Dirac point. Which is at $\vec{B} = 0$. And if $\vec{B}$ is zero then the energy is also zero. To show the difference between the topological insulator and the normal insulator, we plotted the fictional magnetic field to show the difference in winding number of the magnetic field. The winding number is zero for a normal insulator and one for the topological insulator. We calculated the Berry phase to show the mathematical difference between the normal and topological insulator. So the Berry phase and the winding number of the fictional magnetic field are zero for a normal insulator. For a topological insulator the Berry phase is -1 or +1 and the winding number is 1. While constructing the wave functions, we have made one approximation. Namely that k is small for the edge states. Therefore the trigonometric terms could be simplified. In future research, it is interesting to look at the edge states of excitons and the behaviour of excitons themselves as well.

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