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Topological effects in photonic lattices

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Περίληψη

Σε αυτή την μεταπτυχιακπή εργασία ασχολούμαστε με το οπτικό γραφένιο, το οποίο είναι το οπτικό ανάλογο του γραφενίου, ενός δισδιάστατου υλικού, αλλά αντί για άτομα έχουμε κυματοδηγούς. Μελετάμε τις συμμετρίες του οπτικού γραφενίου και υπολογίζουμε τις ιδιοτιμές τις ενέργειας. Στην συνέχεια σπάμε κάποιες συμμετρίες, και παρατηρούμε πως μεταβάλλονται οι ενεργειακές ιδιοκαταστάσεις. Η παρούσα μεταπτυχιακή εργασία ασχολείτε αρχικά με το άπειρο γραφένειο, στη συνέχεια θεωρούμε περιοδικές συνοριακές συνθήκες στην μία διάσταση και πεπερασμένες στην άλλη. Αυτό το κάνουμε για τέσσερεις διαφορετικές περιοδικές συνθήκες. Τέλος λύνουμε το πρόβλημα του πεπερασμένου γραφενίου, για τρία διαφορετικά είδη. Όλα τα προβλήματα λύνονται με την μέθοδο της διαγωνιοποίησης ώστε να βρεθούν οι ιδιοτιμές τις ενέργειας, και όπου υπάρχει περιοδικότητα, χρησιμοποιούμε την Χαμιλτονιανή του Bloch.

Abstract

In this master thesis, we solve the problem of optical graphene.This problem is the analogue of graphene but instead of atoms we have waveguides. First we study the symmetries of optical graphene. And calculate the eigenvalues. Then we break the time reversal symmetry, and we see the change in energy eigenstate that this break of symmetry creates. In the beginning we solve the problem of infinite graphene, then we solve the problem of semi infinite graphene, for four different cases of boundary conditions. At the end we solve the problem of finite graphene. We do this for three different cases of finite graphene models. We solve these problems using the method of diagonalization and when periodicity is present we use the Bloch Hamiltonian which is the Fourier transform of the original Hamiltonian, in order to account for periodicity.

Contents

Chapter 1

Defining the problem

In this thesis, we study two-dimensional photonic graphene lattices. In this first chapter, we begin by explaining what photonic graphene and honeycomb lattice are. Furthermore, we discuss the concept of coupling, which we use in the whole thesis, and we will introduce the notion of waveguides. We will also talk about graphene as a solid due to its intriguing properties, applications and importance in solid state physics and material science.

1.1 Honeycomb lattice structure properties

The graphene's lattice is called honeycomb lattice and is a special case of hexagonal lattice whose unit cell consists of two kinds of atoms[1]. Honeycomb lattice is shown in figure 1.1a. Observe in figure 1.1a that every waveguide connects to three neighbour waveguides. Furthermore, there are only two kinds of waveguides in the lattice. These waveguides are called A and B waveguides. The difference between these two is that A waveguides are connected to two B waveguides below and one B waveguide above, while B waveguides are with two A waveguides above and one A waveguide below. Namely, the coupling's orientation gives A waveguides and B waveguides different properties.

The experimental structure consists of waveguides, which distributes as a honeycomb lattice imposes. Then we choose the initial conditions we decide by using a laser of the desired intensity, pointing at the waveguides that the initial conditions demand. After the light reaches the wave guides, since they are coupled, the light will move in the neighbour waveguides and eventually will spread in the whole lattice. The main difference between this experiment and the study of graphene is that we cannot put waveguides at the same length as carbon atoms are on graphene so that the final system is some order of magnitudes larger than graphene is.

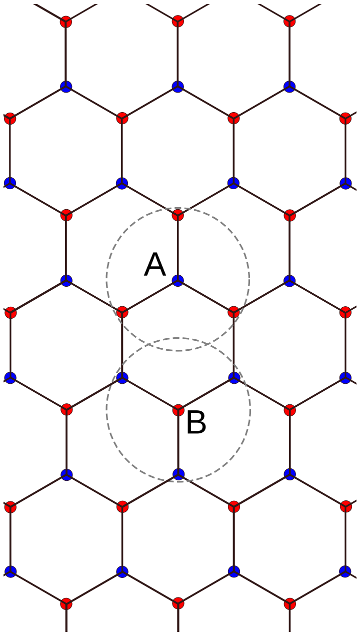

Figure 1.1a: An infinite honeycomb lattice. A waveguides are represented in blue, while B waveguides in red. The grey circles represent the area of the nearest atoms of A and B waveguides. Remark that every nearest waveguide of A is a B, and every nearest waveguide of B is an A.

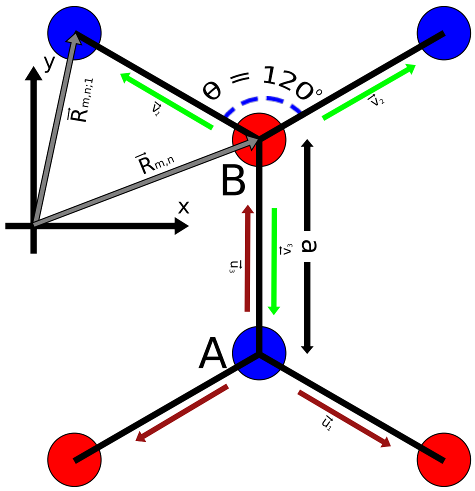

Figure 1.1b: Caption.

We can study this system both theoretically and experimentally. In addition, graphene lattice can be also studied as an arrangement of atoms, having the same properties discussed above. The main difference between the atomic structure and the structure we deal with, is that when you study atoms you need to consider all the atomic states, that all principal quantum numbers n, all angular momentum numbers l, and all projections of angular momentum m_l. As we will see in section 1.2.1, in the case of a photonic lattice, this is not the case, and we can make reasonable and almost necessary simplifications, to only consider the first mode of our system. The other difference with the atomic graphene, is that the propagation of the system is happening in time, while, in the case of photonic graphene, the system propagates in the direction of the waveguides.

We can also study graphene theoretically by assuming that we have a Hamiltonian where the diagonal elements represent the energy of the carbon atoms when no interaction between them is present. The non-diagonal elements represent the coupling of each other. Since experimentally we measure energy differences, there is no point in writing the exact energy of a Carbon atom. We can set the energy of a free carbon atom to zero, and measure any other energy difference with respect to that. That was the process we mostly do in this thesis. The non-diagonal elements are given by calculating the coupling between the atoms. We will see this explicitly below. By diagonalizing this matrix, we can get the spectrum of graphene, and thus we can calculate

Graphene as an atomic structure, was explicitly studied in the previous two decades, and it continues to study it. It has some intriguing properties that we should discuss, even if this thesis deals with photonic graphene. But atomic graphene, also mentioned as just graphene, is one of the most important solids in the material science, so we should discuss its properties before we move on to our problem.

Graphene is a two-dimensional structure consisting of carbon atoms arranged in a honeycomb lattice. The distance between carbon atoms in the Bravoir lattice is $a = 1.42$Å [2], and it is only 3.4Å thick. It is a material with high mobility of approximately $\mu = 2 \times 10^5 cm^2/V$ at room temperature, which also gives a high conductivity of around 35% higher than copper. These properties make Graphene a semi-metal, which means that it is not metal though it behaves like one. A property that distinguishes graphene from metals is its optical properties. Most conductors are optically opaque due to the screening effect in atoms which alters electrons' absorption frequencies from UV to optical. In addition, its transparency is roughly independent of the wavelength of light. Also, graphene is an excellent thermal conductor. The thermal conductivity is larger than 3000 W/mK at room temperature, which is the highest along all metals. Even higher than a diamond. Its thermal conductivity is isomorphic. Graphene is chemical rather stable. The sp^2 bonds in graphene are one of the strongest in nature. The bond energy is 607 KJ/mol, even higher than the diamond (347 KJ/mol). Due to the bond strength, it cannot easily break the bonds using acids and basis, although very strong acids and basis; do modify graphene properties to some extent. At room temperature, it is also rather stable with oxygen, but at high temperatures of about 700 ℃ graphene reacts with oxygen into CO_2. On the other hand, the surface of graphene is relatively easy to modify with oxygen or nitrogen containing functional groups. Finally, we mention the high breaking strength of graphene, which is as high as 130 GPa, about 100 times greater than steel.

Graphene was first produced by Andre Geim and Konstantin Novoselov in 2005 using a mechanical exfoliated method[1], and especially, by rubbing graphite in another surface and studying the second surface to find graphene mono-layers [3]. Today this method is performed by sticking graphite into a tape and then sticking the tape on another surface, so part of the graphite will move to the other surface due to van der Walls force between the graphite on the tape, the surface, and the tape itself. After this process has been repeated a desirable number of times, so that a lot of monolayers remain on the tape, we finally stick the tape into a substrate and remove it, in which we will study the graphite remain on this tape, which is expected to have a few graphene monolayers. In general, graphene is widely studied so that a great number of properties is known [4].

Due to the sp^2 hybridization in graphene states of principal quantum number $n = 2$, and since graphene consists only of carbon atoms, no direction is preferable, and thus we have exactly $120°$ angles. Furthermore, due to the same reasoning as before, there would be no difference in the length of the bonds, so we define that the distance of the bond is a. a was experimentally calculated, as we have discussed above, but we will not use the experimental value. We will denote it just as a. These figures can be seen in figures 1.1a and 1.1b. Using these properties, we conclude that the vectors between atom A and its three neighbour atoms are given by

$$\vec{u}_1 = a(\sqrt{3}/2, -1/2), \quad \vec{u}_2 = -a(\sqrt{3}/2, 1/2), \quad \vec{u}_3 = a(0, 1). \tag{1.1a}$$

In addition, the vector between B atoms and the nearest neighbour A atoms are given by

$$\vec{v}_1 = -a(\sqrt{3}/2, -1/2), \quad \vec{v}_2 = a(\sqrt{3}/2, 1/2), \quad \vec{v}_3 = -a(0, 1). \tag{1.1b}$$

Vectors $\vec{u}_1$, $\vec{u}_2$, $\vec{u}_3$; $\vec{v}_1$, $\vec{v}_2$ and $\vec{v}_3$ are represented in figure 1.1b.

Next, we define the concept of coupled quantum states. Two quantum states $|\psi_1\rangle$, $|\psi_2\rangle$, in the presence of a potential V are called coupled if $\langle\psi_1|V|\psi_2\rangle \neq 0$. When two states are coupled, it means that one affects the other.Maybe we should explain this concept a little bit more We notate the wave function of the A atoms as Ψ and the wave function of the B atoms as Φ. In the system we study, each atom is coupled only to the three neighbour atoms, namely the atoms it is connected with. This hypothesis is called "nearest neighbour approximation", and is compatible with the exponentially decaying of the wave functions in atoms. This assumption can be mathematically formed by

$$\langle\Psi|V|\Phi_i\rangle = \langle\Psi|H|\Phi_i\rangle \equiv t_i, \tag{1.2a}$$

where the Hamiltonian in the second equality appeared because we assumed that $\langle\psi_1|\psi_2\rangle = 0$, so we can have a complete base. The i index represents any of the atoms in the direction $\vec{u}_i$ with respect to the A atom we assumed. The variable t_i is called coupling constant between the A and the B atom in the direction of $\vec{u}_i$. Note that by defining the coupling constant of $\langle\Psi|V|\Phi\rangle$, we have also defined the coupling constant of B in the direction of $\vec{v}_i$ this time, since

$$\langle\Phi|V|\Psi_i\rangle = \overline{\langle\Phi_i|V|\Psi\rangle} = \overline{\langle\Psi|V|\Phi_i\rangle} = \bar{t}_i, \tag{1.2b}$$

where $\bar{z}$ denotes the complex conjugate of a complex number z, and the index i, has to be the same index as in Eq. (1.2a), or else Eq. (1.2b) would not be the same. So in the graphene system by the assumption of nearest neighbour atom approximation, three coupling terms exist. We call them t_1, t_2, t_3, which correspond to A atoms and the set of $\vec{u}$ vectors, namely $\vec{u}_1$, $\vec{u}_2$ and $\vec{u}_3$, and their complex conjugates will correspond to B atoms and to the set of $\vec{v}$ vectors.

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[1] Mechanical exfoliated method is a method which uses mechanical forces in order to separate one surface from another.

Furthermore, we consider loss of probability for A atoms and gain of probability for B atoms. That is, as the total wave function propagates in time or space in the case of waveguides, or waveguides type A lose photons while B atoms gain photons. The model we define experience gain and losses is linearly in the probability by a factor γ. We can solve this problem using two methods. The first one is by solving Schröndinger equation, and then diagonalising the Hamiltonian to get the solution. The other is by using the second quantization formalism to define the Hamiltonian using creation and annihilation operators to describe coupling. The coupling can be measured experimentally [5], and one can see that the second neigbour term will play much less of a role.

1.2 The physics of waveguides

1.2.1 Introduction to waveguides

We will now derive the equations for waveguides. Since this focuses more on the attention of engineers than physicists we will show analytically how the equations of waveguides are derived. We will also show explicitly that the problem of graphene is identical to the problem of waveguides in a honeycomb lattice.

Waveguides are used for directing electromagnetic waves in a certain direction. They use Snell's law [6] and particularly the fact that light experiences full reflection when we move from a larger refractive index to a medium with a smaller refractive index, and the incident angle is larger than the critical angle. The critical angle is defined as the smaller angle where all light is reflected. This is defined mathematically as

$$n_1 \sin\theta_1 = n_2 \sin\theta_2 \Rightarrow \sin\theta_{crit} = n_1/n_2 \Rightarrow \theta_{crit} = \arcsin(n_1/n_2)$$

Notice that for the equation above to make sense we need $n_2 > n_1$ as we established before. In that case, the light is trapped inside the medium. One example of waveguides is optical fibres.

In order to talk about waveguides, we need an equation describing the motion of electrons in a waveguide. This is going to be the so-called "paraxial approximation" equation that describes the electric field. The paraxial equation has the form

$$i\frac{\partial A(\vec{r},t)}{\partial z} + \frac{\partial^2 A(\vec{r},t)}{\partial x^2} + \frac{\partial^2 A(\vec{r},t)}{\partial y^2} + U(x,y)A(\vec{r},t). \tag{1.3}$$

We prove paraxial equation on appendix A.

The paraxial equation seems a lot to Schröndinger equation. The differences are the following. Firstly, in this case, we do not have a wave function, but we have a field describing the electric field of light. Furthermore, the potential is the opposite of the potential of Schröndinger equation. This means that photonic states become more localized as potential increases, while in quantum mechanics the opposide is true. States become more localized when potential is very low.

1.2.2 Proprties of waveguides

Now we will prove some properties of the waveguides that are going to be very useful for understanding the difference between photonic lattices and atom lattices. The general solution of the paraxial equation gives a linear combination of all the modes in the system as we know from the theory of PDEs. Furthermore, the higher the eigenvalue of the mode, the higher the energy needed to provide for the system to reach that eigenvalue. In addtition, waveguides do not always support all modes in the system. The frequency of the mode should be higher from a certain frequency called cut-off frequency. This makes total sense when a waveguide has a specific shape, because not all wavelengths have modes in a specific distance, but only certain of them. In our case, we assume that the laser has enough energy that the lowest mode has enough frequency to be supported by the wave guide.

Another property that is usually seen in PDE is what we call node theorem. The first mode of the system has no modes, the second mode has one mode, the third mode has three etc. Even if this theorem is true only in one dimension, this is observed in more dimensions as well[2]. So, we will have that the first mode of the problem will have no nodes.

Since the light emitted by laser has a Gaussian form, and since waveguides support as a first mode, an envelope with no nodes, we can easily see that the higher coefficient, will be the one that correspond to the first mode of the waveguide, because it is a lot alike the Gaussian. All the other coefficients will be sufficiently smaller. Furthermore, we can change the shape and the dielectric constant of the waveguide as we please, so that the first mode of the waveguide will be almost identical (or identical) with the Gaussian form of the envelope. This makes the first mode of the system as the only mode that there is. These makes things much more simple, because we do not need to study the coupling between different modes of the system, we can just restrict ourselves on the first mode. This is what we will do on the rest of this thesis.

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[2] For example when we have spherical symmetry in a system, we know that the solution of the angular part of the system will be given by the spherical Harmonics, so the only unknown part is the radial part of the PDE, which using separation of variables have turn into an ODE, so indeed the node theorem will apply in this case as well

Chapter 2

Methodologies for solving the problem

2.1 Methodology for solving the problem

In this section, we will introduce the methodologies that we use to solve each problem. As we will see, the methodology we use differs in the infinite and the finite case.

2.1.1 Diagonalization of Hamiltonian

First, we talk about the method of diagonalizing the system. This method is useful when we have finite dimensional systems. We can also use it when we have periodic boundary conditions by putting some elements into the write rows and columns of the matrix[1].

We start by defining the wave function of our system. We can see in figure 1.1a, our system is constructed by a two-dimensional array of atoms. Each of these atoms will have its probability density for the electron, so its wave function. The total wave function, that is the envelope of all the waveguides will be a superposition of the wave functions of all these atoms. So the wave function would have the form,

$$|\psi\rangle = \sum_{i,j} c_{A;i,j} |\Psi\rangle + \sum_{i,j} c_{B;i,j} |\Phi\rangle , \tag{2.1}$$

where the index A correspond to the wave functions belonging to A atoms, and correspondingly to index B. The two indexes i and j represent the exact position of the atom. Since we have a two-dimensional lattice, the degree of freedom of each atom is two, and so we need two indexes to fully describe their positions. Lastly, $c_{i,j}$ are some complex coefficients whose norm squared corresponds to the probability of finding the wave function at i, j position. Coefficients $c_{A;i,j}$ correspond to A atoms, while coefficients $c_{B;i,j}$ correspond to B atoms.

The solution of the system is obtained by the diagonalization of the Schröndinger equation. The Schröndinger equation states that by acting with the Hamiltonian operator in the total wave function of the problem, we get the time evolution of the total wave function and it is summarized in the equation

$$H |\psi\rangle = H \sum_{i,j} c_{A,i,j} |\Psi\rangle + H \sum_{i,j} c_{B,i,j} |\Phi\rangle \Rightarrow i\frac{\partial\psi}{\partial t} = H \sum_{i,j} c_{A,i,j} |\Psi\rangle + H \sum_{i,j} c_{B,i,j} |\Phi\rangle . \tag{2.2}$$

By separation of variables, we can split Schröndinger equation in the so-called "time independent Schröndinger equation", and on the time evolution of each state. By doing this we turn the

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[1] We will discuss this part explicitly below

Schröndinger equation into the eigenvalue problem

$$H\left|\psi\right\rangle = E\left|\psi\right\rangle \tag{2.3}$$

where $\left|\psi\right\rangle$ is given by Eq. (2.1). The solution to this equation can be obtained by acting with every bra state from the left. If we act with one bra state, then on the right-hand side, we get just the energy with the coefficient of the states we acted since we assumed perfect completeness in our model. On the left-hand side, we would have the energy of the left-acted state, as well as the states that couple to the bra state. If we do it for every state in our Hilbert space, that is for every possible atom, we would get a system of the equation that needs to be satisfied. If we write the system into a matrix form, we get

$$\begin{bmatrix} E_0 & & & & & \\ & \ddots & & & & \\ & & E_0 & & & \\ & & & E_0 & & \mathrm{C} \\ \bar{C} & & & & \ddots & \\ & & & & & E_0 \end{bmatrix} \begin{bmatrix} c_{A;1,1} \\ c_{B;1,1} \\ c_{A;2,1} \\ \vdots \\ \\ c_{A;n,m} \\ c_{B;n,m} \end{bmatrix} = E \begin{bmatrix} c_{A;1,1} \\ c_{B;1,1} \\ c_{A;2,1} \\ \vdots \\ \\ c_{A;n,m} \\ c_{B;n,m} \end{bmatrix} \tag{2.4}$$

where the unperturbed energies of the atoms are in the diagonal elements of the matrix, and the reason that we have chosen these specific elements for the coupling terms will be specified in chapter 4. So in order to solve this problem we have to solve this diagonalization problem, that is, we have to diagonalize the matrix and obtain the eigenvalues and eigenvectors of the system. The eigenvalues give us the energy spectrum, and the eigenvectors give the exact form of the total wave function for every energy eigenstate.

Hamiltonian (2.4) is correct but does not accurately describe graphene. As we will see in section 3.1, graphene has the property that the Fermi energy is exactly zero. So to describe graphene accurately, we will approximate this matrix into the form

$$\begin{bmatrix} 0 & & & & & \\ & \ddots & & & & \\ & & 0 & & & \\ & & & 0 & & \mathrm{C} \\ \bar{C} & & & & \ddots & \\ & & & & & 0 \end{bmatrix} \begin{bmatrix} c_{A;1,1} \\ c_{B;1,1} \\ c_{A;2,1} \\ \vdots \\ \\ c_{A;n,m} \\ c_{B;n,m} \end{bmatrix} = E \begin{bmatrix} c_{A;1,1} \\ c_{B;1,1} \\ c_{A;2,1} \\ \vdots \\ \\ c_{A;n,m} \\ c_{B;n,m} \end{bmatrix} \tag{2.5}$$

As we can see from Eq. (2.4), this method is effective when we have a finite system, since we solve it by diagonalization of the Hamiltonian, which can be obtained computationally. This process however is not able to solve the infinite system because we cannot. In order to solve the infinite problem we have to use another method which is obtained by the definition of creation and annihilation operators, and by using the second quantization approach.

2.1.2 Bloch Hamiltonian

We have seen in section 2.1.1 how to solve any finite problem. In this section, we will study how to solve the infinite problem.

$$
\begin{aligned}
H_{A;m,n} &= -i\gamma + \sum_{NN} \left(t_{NN}\, b^{\dagger}_{NN;m,n} a_{m,n} + h.c \right), \\
H_{B;m,n} &= i\gamma + \sum_{NN} \left(t_{NN}\, a^{\dagger}_{NN;m,n} b_{m,n} + h.c \right),
\end{aligned}
\tag{2.6}
$$

where the first term is responsible for the gain and loss of probability[2], and the second term corresponds to the coupling of atoms with the nearest neighbour atoms. The quantity t_{NN} in the second term expresses the coupling constant of the state with all NN atoms and b, a; $b^{\dagger}$, $a^{\dagger}$ are operators act in B or A atoms respectively, which annihilate or create atoms respectively. In general, every atomic bond will have a different coupling constant, so we have denoted t with the subscript NN so that it depends on the exact NN atom[3]. The two operators in the second term; express the probability of annihilation of the electron from the atom and the creation of the electron to the NN atoms, and the hermitian conjugate part expresses the inverse process. Particularly the operator $a^{\dagger}_{NN;n,m} b_{n,m}$ reads "the electron is annihilated from the B atom and goes to the NN atom B".

So the operators in the sum are local operators since they only act on each atom and have the property to create or annihilate particles. These operators are known to be constructed in the second quantization formalism, which we describe in appendix B, and the exact form of these operators, as it is proven in the appendix, has the form of Eq. (B.2). This expression depends on the position of the atoms on the lattice, so the exact form of the second term of Eq. (2.6) is needed. That is, we have to know the position of the particles. Using figure 1.1b we see that we have three coupled states both for A and B, so, by substituting (B.2), we get

$$
\begin{cases}
H_{A;m,n} = -i\gamma + \left(t_1 b^{\dagger}_{m,n;1} a_{m,n} + t_2 b^{\dagger}_{m,n;2} a_{m,n} + t_3 b^{\dagger}_{m.n;3} a_{m,n} + h.c \right) \\
H_{B;m,n} = i\gamma + \left(t_1 a^{\dagger}_{m,n;1} b_{m,n} + t_2 a^{\dagger}_{m,n;2} b_{m,n} + t_3 a^{\dagger}_{m,n;3} b_{m,n} + h.c \right)
\end{cases}
\quad \xRightarrow{(B.2)}
$$

$$
\Rightarrow
\begin{cases}
H_{A;m,n} = -i\gamma + \left(t_1 + \sum_{\vec{k}} e^{-i\vec{k}\vec{u}_1} + t_2 \sum_{\vec{k}} e^{-i\vec{k}\vec{u}_2} + t_3 \sum_{\vec{k}} e^{-i\vec{k}\vec{u}_3} \right) \\
H_{B;m,n} = i\gamma + \left(t_1 \sum_{\vec{k}} e^{-i\vec{k}\vec{v}_1} + t_2 \sum_{\vec{k}} e^{-i\vec{k}\vec{v}_2} + t_3 \sum_{\vec{k}} e^{-i\vec{k}\vec{v}_3} \right).
\end{cases}
\tag{2.7a}
$$

Where the last equality is a consequence of

$$
\begin{aligned}
b_{m,n;i}\, a_{m,n} &= \frac{1}{\sqrt{V}} \sum_{\vec{q}} a_{\vec{q}} \dagger\, e^{-i\vec{q}\vec{R}_{m,n;i}} \frac{1}{\sqrt{V}} \sum_{\vec{k}} a_k e^{i\vec{k}\vec{R}_{m,n}} = \frac{1}{V} \sum_{\vec{q},\vec{k}} e^{i(\vec{q}-\vec{k})\vec{R}_{m,n}} e^{-i\vec{q}\vec{u}_i} = \\
&= \sum_{\vec{q},\vec{k}} \delta_{\vec{q},\vec{p}} e^{-i\vec{q}\vec{u}_i} = \sum_{\vec{k}} e^{-i\vec{k}\vec{u}_i}.
\end{aligned}
$$

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[2] The reason it represents the gain and loss of probability can be seen by setting the coupling constant to be zero. Then we have only $H = i\gamma\ Rightarrow H \left|\psi\right\rangle = i\gamma \left|\psi\right\rangle \Rightarrow \left|\psi\right\rangle = e^{\gamma t} \left|\psi\right\rangle$. So we see that for $\gamma > 0$, we have gain of probability, and for $\gamma < 0$ we have loss of probability.

[3] Notice that this is not physically correct. Since we have the same atoms and at the same distance, the coupling constants cannot be different. But we can always generalize that one bond can be stronger than the other. In the case of waveguides, however, we can always choose one bond to have a stronger coupling than the others. Also, it has theoretical interest since we can see how the change of a coupling would affect the whole system

In the derivation above we used the identity $1/V \sum_{\vec{q}} e^{i(\vec{k}-\vec{q})\vec{r}_{n,m}} = \delta_{\vec{k},\vec{q}}$SAY ONE WORD FOR THIS IDENTITY. By substituting Eqs. (1.1a) and (1.1b), we get

$$H_{A;m,n} = -i\gamma + \left(t_1 \sum_{\vec{k}} e^{-i\sqrt{3}/2ak_x + ia/2k_y} + t_2 \sum_{\vec{k}} e^{i\sqrt{3}/2ak_x + i/2\cdot ak_y} + t_3 \sum_{\vec{k}} e^{-iak_y} \right) \tag{2.7b}$$

$$H_{B;m,n} = -i\gamma + \left(t_1 \sum_{\vec{k}} e^{i\sqrt{3}/2ak_x + i/2\cdot ak_y} + t_2 e^{-i\sqrt{3}/2ak_x - i/2\cdot ak_y} + t_3 \sum_{\vec{k}} e^{iak_y} \right) \tag{2.7c}$$

As we can see, from Eqs. (2.7b) and (2.7c), the Hamiltonian of the system is summed in all allowed momenta. To make the Hamiltonian simpler, we will write it in a matrix form where the first row and column will correspond to the A atom, and the second row and column will correspond to the B atom, and also we will write from one allowed momentum. So we define a new quantity which is the Hamiltonian for one momentum.

$$H_{\vec{k}} = \begin{bmatrix} -i\gamma & t_1 e^{-i\sqrt{3}/2ak_x + ia/2k_y} + t_2 e^{-i\sqrt{3}/2ak_x - i/2\cdot ak_y} + t_3 e^{-iak_y} \\ t_1 e^{i\sqrt{3}/2ak_x + i/2\cdot ak_y} + t_2 e^{-i\sqrt{3}/2ak_x - i/2\cdot ak_y} + t_3 e^{iak_y} & i\gamma \end{bmatrix} \tag{2.8}$$

and the total Hamiltonian is given by

$$H = \sum_{\vec{k}} H_{\vec{k}}. \tag{2.9}$$

The matrix above can be written in the following simpler form.

$$\begin{gathered} H_{\vec{k}} = \begin{bmatrix} H_{\vec{k};AA} & H_{\vec{k};AB} \\ H_{\vec{k};BA} & H_{\vec{k};BB} \end{bmatrix}, \\ H_{\vec{k};AA} = -i\gamma, \quad H_{\vec{k};AB} = t_1 e^{-i\sqrt{3}/2ak_x + ia/2k_y} + t_2 e^{i\sqrt{3}/2ak_x + i/2\cdot ak_y} + t_3 e^{-iak_y} \\ H_{\vec{k};BA} = t_1 e^{i\sqrt{3}/2ak_x + i/2\cdot ak_y} + t_2 e^{-i\sqrt{3}/2ak_x - i/2\cdot ak_y} + t_3 e^{iak_y}, \quad H_{\vec{k};BB} = i\gamma. \end{gathered} \tag{2.10}$$

In the case of graphene, the diagonal terms are zero as we said in section 2.1.1, so the Hamiltonian will be given by

$$H_{\vec{k}} = \begin{bmatrix} 0 & H_{\vec{k};AB} \\ H_{\vec{k};BA} & 0 \end{bmatrix} \tag{2.11}$$

where $H_{\vec{k};AB}$ and $H_{\vec{k};BA}$ will be given by Eq. (2.10).

2.2 Approximations of total Hamiltonian

As we have seen in the previous sections, Hamiltonian given by Eqs. (2.6), or(2.8) is a complicated Hamiltonian. Nevertheless, it is a Hamiltonian that we can solve analytically, and it is the most general Hamiltonian one can write for honeycomb lattices. But there is one disadvantage. This system rarely appears in any physical problems. This has mostly to do with the difference between the coupling constants. As we said, the system of graphene consists of individual atoms, so it is reasonable that no difference in the coupling constants exists, which is exactly what experiments show as we described in section refMethodology for solving the problem.

In this section, we will divide our problem into three levels of difficulty. The first one is when all coupling constants are different. This is the most general problem, and it is not very applicable in nature. We will call them the "hard" problem. The second is when two coupling constants are identical. This is a problem that is much more encountered in physics EXPALIN WHY THIS IS THE CASE. We call them "medium difficulty" problems. The third case is when all coupling constants are identical. This is the problem in which the graphene structure appears, which makes it the most important and applicable of these cases. We will call it the "easy" problem.

The hard problem has already been established in the previous section. It is described by Hamiltonian (2.8) for the finite system and Hamiltonian (2.6) for the infinite system. We have no approximations in this Hamiltonian, so every other level of difficulty is a special case of this problem.

The medium difficulty problem is a special case of the hard problem when

In the first level of difficulty, we assume that all couplings are equal one another: $t_1 = t_2 = t_3 = t$. When this applies Eq. (2.8), using Euler's formula $e^{i\theta} = \cos\theta + i\sin\theta$, the Hamiltonian gets the form

$$H_{\vec{k}} = \begin{bmatrix} -i\gamma & 2te^{i/2\cdot ak_y}\cdot\cos\left(\sqrt{3}/2ak_x\right) + te^{-iak_y} \\ 2te^{-i/2\cdot ak_y}\cdot\cos\left(\sqrt{3}/2ak_x\right) + te^{iak_y} & i\gamma \end{bmatrix} \tag{2.12}$$

$$\begin{cases} i\partial_z a_{m,n} = -i\gamma a_{m,n} + t(b_{m-1,n} + b_{m,n+1} + b_{m,n-1}) \\ i\partial_z b_{m,n} = i\gamma b_{m,n} + t(a_{m+1,n} + a_{m,n+1} + a_{m,n-1}) \end{cases} \tag{2.13a}$$

where γ is a real number which denotes the amplitude of gain and loss and t expresses the coupling of each atom with its neighbour atoms. We can generalize the system even more by assuming γ as a complex number $\tilde{\gamma}$. If we do this the system at Eq. (2.13a) can be written in the form

$$\begin{cases} i\partial_z a_{m,n} = -(\Delta + i\gamma)a_{m,n} + t(b_{m-1,n} + b_{m,n+1} + b_{m,n-1}) \\ i\partial_z b_{m,n} = (\Delta + i\gamma)b_{m,n} + t(a_{m+1,n} + a_{m,n+1} + a_{m,n-1}) \end{cases} \quad ,\tilde{\gamma} = \gamma - i\Delta, \tag{2.13b}$$

and Eq. (2.13b) comes from Eq. (2.13a) by the substitution $\gamma \to \tilde{\gamma}$. The solution of this system highly depends on the edges of the problem, since the solution will diffuse until it reaches the boundaries where it will be reflected since it cannot propagate away from the boundary due to the absence of atoms for the wave function to couple to. So to solve this system, we assume different geometries in the edges, and we will solve the system (2.13b) at all these cases.

Chapter 3

Solving the system of infinite graphene

In the previous chapter we defined the equations of the model of graphene. These equations connect every state with the three nearest states of the problem. This is however not satisfied by the states at the edge of the sample. These states, the so called “edge states”, are affected only by atoms inside the sample. That is, the equations we showed in the previous chapter are not satisfied by these states, so the energy band will be affected by edge states. On he other hand, all the other states satisfy Eq. (2.5), so their energy spectrum will not differ as much[1]. Due to this observation, we can split our system into two pieces. The edge states of the system, and the bulk states of the system.

In this chapter we will focus on the bulk states of the system. As we will see in section 4, the further we get inside the bulk, the more edge states become less important. So states deep in the bulk, see an infinite periodic structure of atoms which extend to infinite. So by solving the infinite honeycomb lattice, we get an approximate solution for the behavior of the center of the bulk. This is useful to compare with the solution when edges are far away. Some work in this are has been done by [7], [8]

3.1 General Hamiltonian for graphene

In the previous part we settled the general Hamiltonian that we will solve. We also explained the similarities with the graphene problem as well as with an arrangement of wave guides. In this section we will explain this concept with detail to see how we can experimentally create this Hamiltonian. In this section, the symmetrical structure of graphene will be of great importance. In an experiment, we measure properties on the bulk of graphene, where edge states play little to no role.

3.1.1 Definition of d vector

In the previous chapter we explained that graphene is an arrangement of atoms where each particle is affected by the three neighbour atoms giving the Hamiltonian of the form Eq. (2.5), or in an infinite system which we will study, from Eq. (2.12). The energies we will measure in experiment have to be real, so the Hamiltonian have to be hermitian, and also, since graphene forms a solid, it has to be momentum dependent. The most general 2×2 hermitian Hamiltonian is written as

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[1] As we will see in section 4, these states are still affected by the edge states, because they coupled to the edge states of the system, or they couple to other states that they couple to the edge states of the system.

a linear combination of four matrices. The three Pauli matrices, and the unitary matrix. In the case where the Hamiltonian is dependent in a certain parameter, as here where the Hamiltonian depends on momentum, the coefficients in front of Pauli and unitary matrices should be momentum dependent, so the Hamiltonian can be written as a linear combination of $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, the Pauli matrix vector and σ_0 the identity matrix. If we notate the four coefficients as d_i's, then we get,

$$H_{\vec{k}} = \vec{d}(\vec{k}) \cdot \vec{\sigma} + d_0(\vec{k})\sigma_0 = \begin{bmatrix} d_0(\vec{k}) + d_z(\vec{k}) & dx(\vec{k}) - id_y(\vec{k}) \\ dx(\vec{k}) + id_y(\vec{k}) & d_0(\vec{k}) - d_z(\vec{k}) \end{bmatrix} \tag{3.1}$$

Since we know that the momentum Hamiltonian for graphene is given by Eq. (2.12), we can split the Hamiltonian into the form of Pauli matrices. First of all since Eq. (2.12) has no components on the diagonals, we infer that $d_0(\vec{k}) = d_z(\vec{k}) = 0$. For the non diagonal points, we get for the element $H_{\vec{k};B,A}$ that $d_x(\vec{k})$ would be its real part, and $d_y(\vec{k})$ would be its imaginary part, so we have

$$d_x(\vec{k}) = t\cos(ak_y) + 2t\cos\left(\frac{ak_y}{2}\right)\cos\left(\sqrt{3}/2 \cdot ak_x\right) \tag{3.2a}$$

$$d_y(\vec{k}) = t\sin(ak_y) - 2t\sin\left(\frac{ak_y}{2}\right)\cos\left(\sqrt{3}/2 \cdot ak_y\right) \tag{3.2b}$$

The equations above represent a mapping from momentum space, to the space of vector $\vec{d}(\vec{k})$ as you can see on figure ref. Since we have the Hamiltonian from Eq. (3.1), as a function of the d vector, we can diagonalize the Hamiltonian, and find the energies and the wave functions as a function of the d vector. We start with the energy eigenvalues which ae given by

$$\det\begin{bmatrix} d_0(\vec{k}) + d_z(\vec{k}) - E & d_x(\vec{k}) - id_y(\vec{k}) & \\ d_x(\vec{k}) + id_y(\vec{k}) & d_0(\vec{k}) - d_z(\vec{k}) - E & d_x(\vec{k}) \end{bmatrix} = 0 \Rightarrow \left(E - d_0(\vec{k})\right)^2 - d_z^2(\vec{k}) = d_x^2(\vec{k}) + d_y^2(\vec{k}),$$

So we get that the energies of the system, are

$$E_{\pm} = \pm\sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k}) + d_z^2(\vec{k})} + d_0(\vec{k}) \tag{3.3}$$

Having the energies, we can see into what eigenvectors correspond to. We can easily see[2] that the eigenvectors corresponding to $E_{\pm}$ are

$$u_{\vec{k};\pm} = \frac{1}{\sqrt{2d(d \pm d_z}}\begin{bmatrix} d_z \pm d \\ d_x + id_y \end{bmatrix}, \quad \text{where} \quad d = \sqrt{d_x^2 + d_y^2 + d_z^2}. \tag{3.4}$$

In the case of graphene, where $d_z = 0$ the eigenvalues have the form

$$u_{\vec{k};\pm} = \frac{1}{\sqrt{2}}\begin{bmatrix} \pm 1 \\ e^{i\theta} \end{bmatrix} \tag{3.5}$$

3.1.2 Graphene symmetries

We saw previously that the z component of the d vector vanishes. We will see now that this is a fact of the symmetries that graphene has. More precisely we will see that the graphene has two symmetries. The first that we will study is called C_2 symmetry or inversion symmetry, and the other is called time reversal symmetry. The combination of these symmetries is forcing graphene to have Dirac points.

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[2] In order to prove it, we can make the dot product of the vector with the matrix of $H_{\vec{k}} - E_{\pm}$ where $E_{\pm}$ is the eigenvalue we found. Indeed, the dot product is zero since $(d_z \mp d, d_x + id_y) \cdot (d_z \pm d, d_x - id_y) = (d_z \mp d)(d \pm d_z) + d_x^2 + d_y^2 = -(d - d_z)(d + d_z) + d_x^2 + d_y^2 = -d^2 + d_z^2 + d_y^2 + d_x^2 = 0$, where we cover just the case of the up sign because $(d_z - d)(d + d_z) = (d_z + d)(d - d_z)$, so it does not matter which sign will I pick, I will have the same result for both of these. So we have found that indeed that vector on Eq. (3.4) is indeed an eigenvector of the system.

Inversion symmetry

Graphene has two symmetries. The one symmetry is called inversion symmetry, and it is defined such that, at any point $\vec{r} = (x, y, z)$ in the unit cell, there is an indistinguishable point $-\vec{r} = (-x, -y, -z)$. The other is called C_2 symmetry, and it states that if I rotate my system with angle π in respect to the z axis, then the system will not change, it is symmetric under π rotations. Notice that the two symmetries above are different because they behave differently on the z axis. At inversion symmetry, every z is mapped to a $-z$, while at C_2 symmetry, the z axis remains intact.

We can easily prove that rotations by π are identical with the inversion symmetry in two-dimensions. In order to see it take a general two-dimensional vector and we rotate it by an angle π using the rotation matrix $R(\theta = \pi)$.

$$\vec{v} \equiv \begin{bmatrix} x \\ y \end{bmatrix}, \vec{v}' = R(\pi)\vec{v} = \begin{bmatrix} \cos\pi & -\sin\pi \\ \sin\pi & \sin\pi \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = -\begin{bmatrix} x \\ y \end{bmatrix} = -\vec{v} \Rightarrow$$
$$\Rightarrow \vec{v}' = -\vec{v}$$

So indeed inversion symmetry and C_2 symmetry give us the same result in two dimensions. So, from now on, we will refer to both these symmetries as inversion symmetry.

Let us now see how inversion symmetry will affect the Hamiltonian. We start with how the vector c_j will be affected.

$$Ic_{j,A}I^{-1} = c_{-j,B}, \quad Ic_{j,B}I^{-1} = c_{-j,A} \tag{3.6}$$

$$Ic_jI^{-1} = \sigma_x c_{-j} \tag{3.7}$$

$$Ic_{\vec{k}}I^{-1} = \sigma_x c_{-\vec{k}} \tag{3.8}$$

So the total Hamiltonian will be affected like

$$\sigma_x H_{\vec{k}} \sigma_x = H_{-\vec{k}} \tag{3.9}$$

Since we can write the Hamiltonian in the form of Eq. (3.1) we can find how exactly the inversion symmetry would affect the Hamiltonian.

$$H_{-\vec{k}} = \sigma_x \left(\vec{d}(\vec{k}) \cdot \vec{\sigma} + \sigma_0 d_0(\vec{k}) \right) \sigma_x$$

Since Pauli matrices anticommute with each other, and because $\sigma_i^2 = 1$ for every Pauli matrix, we pass σ_y and σ_z from σ_x with the cost of a minus sign, and we pass σ_x and the identity matrix, and get

$$\sigma_0 d_0(-\vec{k}) + \sigma_x d_x(-\vec{k}) + \sigma_y d_y(-\vec{k}) + \sigma_z d_z(-\vec{k}) = \sigma_0 d_0(\vec{k}) - \sigma_x d_x(-\vec{k}) - \sigma_y d(-\vec{k}) + \sigma_z d(-\vec{k})$$

Since all of Pauli matrices, taking also into account the identity, are linear independent, we get that the coefficients in the RHS should be equal to the corresponding coefficients in the LHS. So, we get that the inversion symmetry is described by

$$d_0(\vec{k}) = d_0(-\vec{k}), \quad d_x(\vec{k}) = d_x(-\vec{k}), \quad d_y(\vec{k}) = -d_y(-\vec{k}), \quad d_z(\vec{k}) = -d_z(-\vec{k}), \tag{3.10}$$

Time reversal symmetry

Now we will define the time reversal symmetry[3]. Time reversal symmetry transforms the imaginary unity i into $-i$, or in a mathematical form,

$$TiT^{-1} = -i \tag{3.11a}$$

This operator also has effect on the momentum. This is because the momentum is given by an imaginary exponential, so when time acts on the momentum, it shifts the imaginary unit in the factor e^{ikx}, which is equivalent as the shift in momentum

$$Tc_iT^{-1} = c_i, \quad Tc_{\vec{k}}T^{-1} = c_{-\vec{k}} \tag{3.11b}$$

The transformation of the Hamiltonian, is given by

$$H_{\vec{k}} = \bar{H}_{-\vec{k}} \tag{3.12}$$

which gives

$$d_0(\vec{k}) = d_0(-\vec{k}), \quad d_x(\vec{k}) = d_x(-\vec{k}), \quad d_y(\vec{k}) = -d_y(-\vec{k}), \quad d_z(\vec{k}) = d_z(-\vec{k}), \tag{3.13}$$

Results and breaking of Symmetry

We discussed how the two symmetries affect the d vector. We see that these two constraints that the symmetries give us a strong constrain for the z component of the d vector. From Eqs. (3.10) and (3.13) we get

$$d_z(\vec{k}) = 0 \tag{3.14}$$

3.2 Solving the infinite system

Now we will solve the system by assuming gain and losses on A and B atoms respectively. In the beginning we assume that honeycomb lattice has no edges and it extends to infinite in both dimensions. This is called “the infinite system” and it is described in figure 1.1a. We will solve it both analytically and computationally, since the analytic approach and solution is simple enough. As we will see the steps for solving the system using the computational approach does not differ significantly with the analytic approach. At this system every state is affected by the neighbour states, and we have no edge states, so we can just use a two by two Hamiltonian to describe every unit cell in our system. Since we only want to calculate the first Brillouin zone, and because the Brillouin zone is the Fourier transform of the unit cell of the system, it is enough to stick to this two by two matrix. The Hamiltonian of the unit cell is given by

$$H = \begin{bmatrix} -\Delta - i\gamma & 2te^{i/2\cdot ak_y}\cos(\sqrt{3}/2\cdot ak_x) + te^{-iak_y} \\ 2te^{-i/2\cdot ak_y}\cos(\sqrt{3}/2\cdot ak_x) + te^{iak_y} & \Delta + i\gamma \end{bmatrix} \tag{3.15}$$

We can find analytically the energies if the sample by diagonalization as you can see below

$$\det\begin{bmatrix} -\Delta - i\gamma - E & 2te^{i/2\cdot ak_y}\cos(\sqrt{3}/2\cdot ak_x) + te^{-iak_y} \\ 2te^{-i/2\cdot ak_y}\cos(\sqrt{3}/2\cdot ak_x) + te^{iak_y} & \Delta + i\gamma - E \end{bmatrix} = 0$$

$$(E + \Delta + i\gamma)(E - \Delta - i\gamma) = t^2\left|2e^{i/2\cdot ak_y}\cos(\sqrt{3}/2\cdot ak_x) + e^{-iak_y}\right|^2$$

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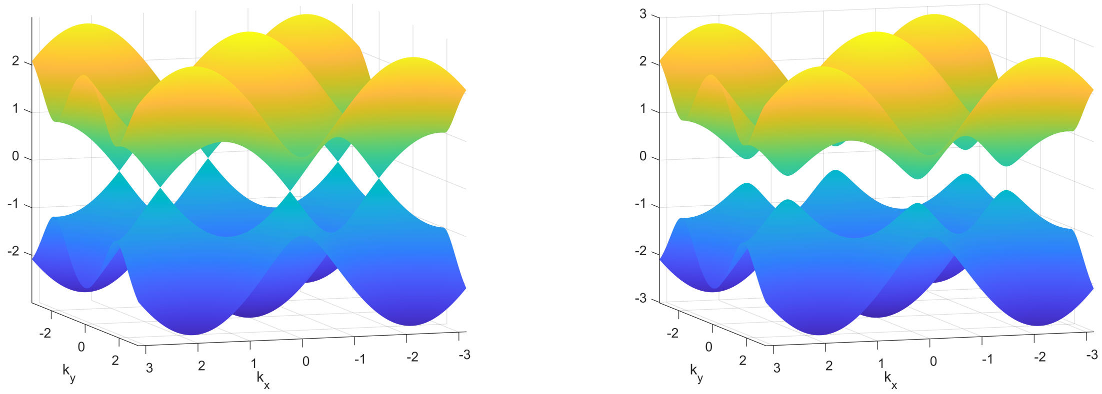
[3] Or spinless time reversal symmetry



(a) Caption 1 (b) Caption 2

Figure 3.1: Solution of the infinite Hamiltonian for different values of Δ. These figures shows that the larger the parameter Δ, the larger the splitting.

Where in the last equality we have the complex conjugate because the non diagonal terms are complex conjugates one another, which is the definition of norm squared. Also when we multiply a number by a phase, his norm does not change, so we multiply the norm with $e^{-i/2 \cdot ak_y}$, to simplify the expression, and get

$$E^2 = \Delta^2 + 2i\gamma\Delta - \gamma^2 + t^2 \left[\left(2\cos(\sqrt{3}/2 \cdot ak_x) + \cos(3/2 \cdot ak_y) \right)^2 + \sin^2(3/2ak_y) \right]$$

$$E = \pm\sqrt{\Delta^2 + 2i\Delta\gamma - \gamma^2 + 4t^2\cos^2(\sqrt{3}/2 \cdot ak_x) + 4t^2\cos(\sqrt{3}/2 \cdot ak_x)\cos(3/2 \cdot ak_y) + t^2} \tag{3.16}$$

We see that the energies of the system are in general complex, despite the PT symmetry of the Hamiltonian. That is, we have exceptional points in the system where the eigenvalues of Hamiltonian become complex. These exceptional points appear when the two energy eigenvalues vanish, namely when

$$E = 0 \Rightarrow \sqrt{\Delta^2 + 2i\Delta\gamma - \gamma^2 + 4t^2\cos(\sqrt{3}/2ak_x) + 4t^2\cos(\sqrt{3}/2ak_x)\cos(3/2ak_y) + t^2} = 0.$$

The imaginary value $2i\Delta\gamma$ vanishes if $\Delta = 0$ or if $\gamma = 0$. If the imaginary part of a function is non zero, then the real part of the square root of the function will be non zero[4]. That means that the exceptional points...

We can also find computationally the energies by using diagonalization for different values for γ or $\tilde{\gamma}$. This helps us understand how $\tilde{\gamma}$, namely how Δ and γ affects the energies of the system. First let us see how Δ affects the system. We can do it analytically by simply setting $\gamma = 0$ at Eq. (3.16), and see that the equation gives

$$E_{\pm} = \pm\sqrt{\Delta^2 + 4t^2\left(\cos^2(\sqrt{3}/2 \cdot ak_x) + \cos(\sqrt{3}/2ak_x)\cos(3/2ak_y)\right) + t^2} \tag{3.17}$$

The expression Δ^2 is always positive since we assume that Δ is a real number. So the expression totally depends on the expression $4t^2\left(\cos^2(\sqrt{3}/2 \cdot ak_x) + \cos(\sqrt{3}/2ak_x)\cos(3/2ak_y)\right) + t^2$. This

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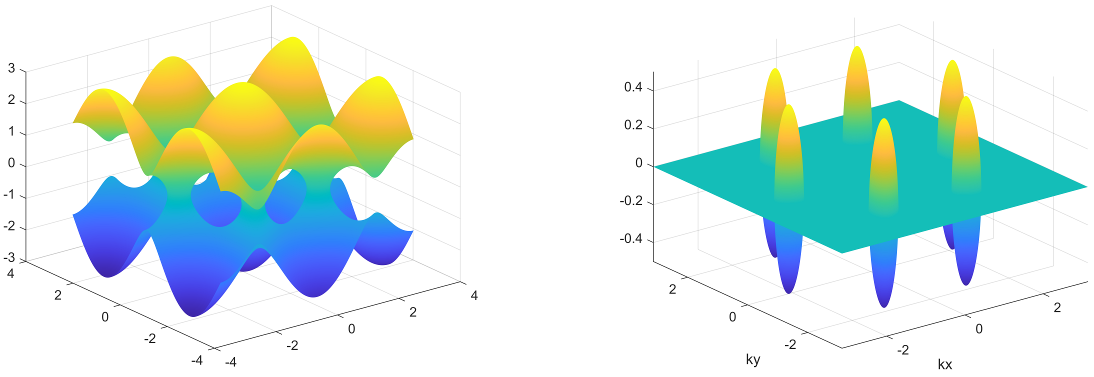
[4] This is easily proved, since any complex number can be written in the form $z = re^{i\theta} = \sqrt{x^2+y^2}e^{i\arctan(y/x)}$ so its square can be written as $\sqrt{z} = (x^2+y^2)^{1/4}e^{1/2i\arctan(y/x)}$ which always have a non zero imaginary part, which vanishes as $x \to \infty$.



(a) Caption 1

(b) Caption 2

Figure 3.2: Solution of the infinite Hamiltonian for different values of Δ. These figures shows that the larger the parameter Δ, the larger the splitting.

expression this expression is always positive or zero since it is equal to the eigenvalues of a Hermitian operator. More precisely, its minimum value is zero and can be found on points $(), (), \ldots$. So we see that in the case of $\gamma = 0$, the property of Δ is to split the two bands. The larger the value of Δ, the larger the gap between the bands.

This becomes more obvious by plotting the solution, but instead of this, we will solve it computationally. We use the values $\Delta = 0$ and for $\Delta = 0.25$ and we plot the results on figure 3.1. The value of γ at these figures is zero. We see that in the case of $\Delta = 0$ valence band touches just one point of the conduction band. This point is called Dirac point. As we increasing the parameter Δ the two bands split. The more we increase Δ the more the band will split.

Now we see how γ affects the solution. For the study of this case, we set the value of Δ to be zero. We will generalize it even more later.

We have plotted our results for $\gamma = 0$ and for $\gamma = 0.5$. Th difference in this case is that the existance of γ forces the energy band to extend to the complex plane, so we plot both the real and the imaginary part of the energy to get the whole information of the system.

Chapter 4

Solving the semi finite problem

In the previous chapter we solved the infinite problem. In experiments however, no infinite sample is possible. We can only use finite samples. At this kind of problems, we have to take into account the boundary conditions of the system. In this section we will see all the possible boundary conditions that we can have in graphene structures, and we will solve them computationally.

As we will see, the Bloch Hamiltonian will be given by (2.8), but with the exception that we will have two neighbour atoms at the edge states. A lot of work has been done for the solution of the semi infinite lattice, like for example [9], [10], [11], [8], [12]. A nice detailed paper for graphene and semi infinite graphene is given by [13].

4.1 Splitting the positions

It is essential, at any finite problem, to be able to give each waveguide a certain value corresponding to the element of the matrix it belongs. In this section we will give each waveguide a natural number which correspond to the position of the waveguide in the system. This process is not unique, and in principle you can give the elements any place in the matrix (2.5) assuming that coupling terms are in agreement. In this section, we will talk about both the notation that we use when we are talking about the states at the edges, and what happens when we talk about a finite graphene sample. Let us start with the finite graphene sample seen on figure 4.1. Since we are in two dimensions, every space is characterized by two degrees of freedom. So, we will notate the wave functions Ψ and Φ with two natural numbers, i and j, indicating the atom's position. The variable i describe the position on the x axis of graphene as we can see on figure 4.1, and the j variable describes the y axis position. Every atom will be characterized by a unique doublet of i and j as you can see on the same figure.

However, this cannot help us build the Hamiltonian of every problem. We will use this numbering only for semi infinite states. When we deal with finite photonic graphene lattices, we will use a different way of numbering the waveguides of each problem.

Since we have a finite graphene lattice in one specific dimension, we have a finite number of waveguides in this direction which we will calculate explicitly on section 5 for different models. For now we will assume that the total number of waveguides on the photonic graphene structure is N. For the Hamiltonian to be build, we need each electron to represent a specific row of the Hamiltonian. This means that the whole Hamiltonian will have the same dimension as the total number of particles, that is the Hamiltonian will be a $N \times N$ matrix. This makes sense because after the diagonalization, we will get the same number of energy eigenstates as the number of atoms, and the states will eventually be a linear combination of the first mode of all the waveguides.

Next is the case of a semi finite sample which we study in this section, we will have a different way of numbering the states of the system because we treat the system like a one-dimensional array

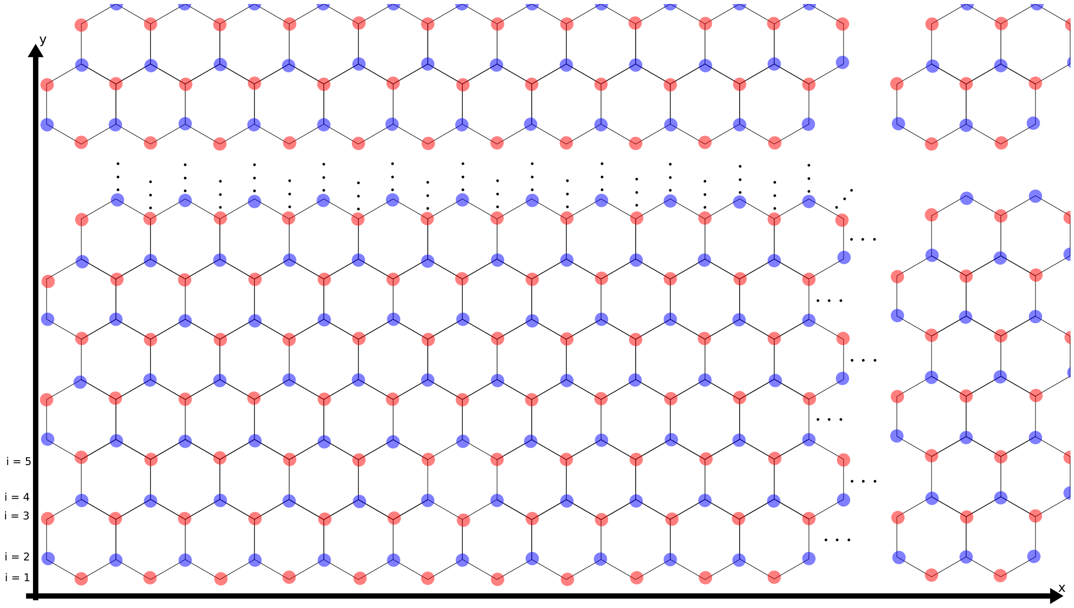


Figure 4.1: Caption

of atoms. So we cannot have two variables, but only one variable. There are two way to assume periodic boundary conditions[1]. The first is by assuming periodic boundary conditions in x and that the photonic graphene is finite in the y direction, and the other way is to assume that we have periodic boundary conditions in y direction and finity in x direction. In both cases we can describe the electrons using as a number its position of the direction that graphene is finite. That is we start from the left, and we go to the right when photonic graphene is finite on the x direction, and we will start from the bottom, and we will go to the top when graphene is finite in the y direction.

4.2 Armchair edge

Firstly we will assume finite sample only on one axis and infinite sample on the other axis. This is called “the semi finite-problem”. The reason we make this assumption is in order to see all the possible boundary conditions that we can have in graphene. Furthermore, this is not an unrealistic scenario for experiments. We can create experimental structures that have the same properties. These kind of structures are atomic structures and not photonic. This is because we can create cylindrical samples. We know that cylindrical samples have periodic boundary conditions in one axis and they are finite in the other axis. These structures are called nanotubes, and they have the form of figure SAY MORE THINGS ABOUT THEM. We will begin by writing the general equation for a unit cell of the system, that is, for now we will not consider the effects of the edge. This equation can be obtained by using Eq. (2.5) in the easy case, namely by assuming that all coupling constants are equal. Due to the aforementioned, we get the system

$$\begin{cases} -t\Psi_{n-1,m} - t\Psi_{n+1,m+1} - t\Psi_{n+1,m-1} = E\Phi_{n,m} \\ -t\Phi_{n+1,m} - t\Phi_{n-1,m-1} - t\Phi_{n-1,m+1} = E\Psi_{n,m}. \end{cases} \tag{4.1a}$$

Here let me explain how this equation came from. This is exactly the same equation as (2.1), or equivalent Eq. (2.1.1), with the exception that we have only picked the energy component of n, m

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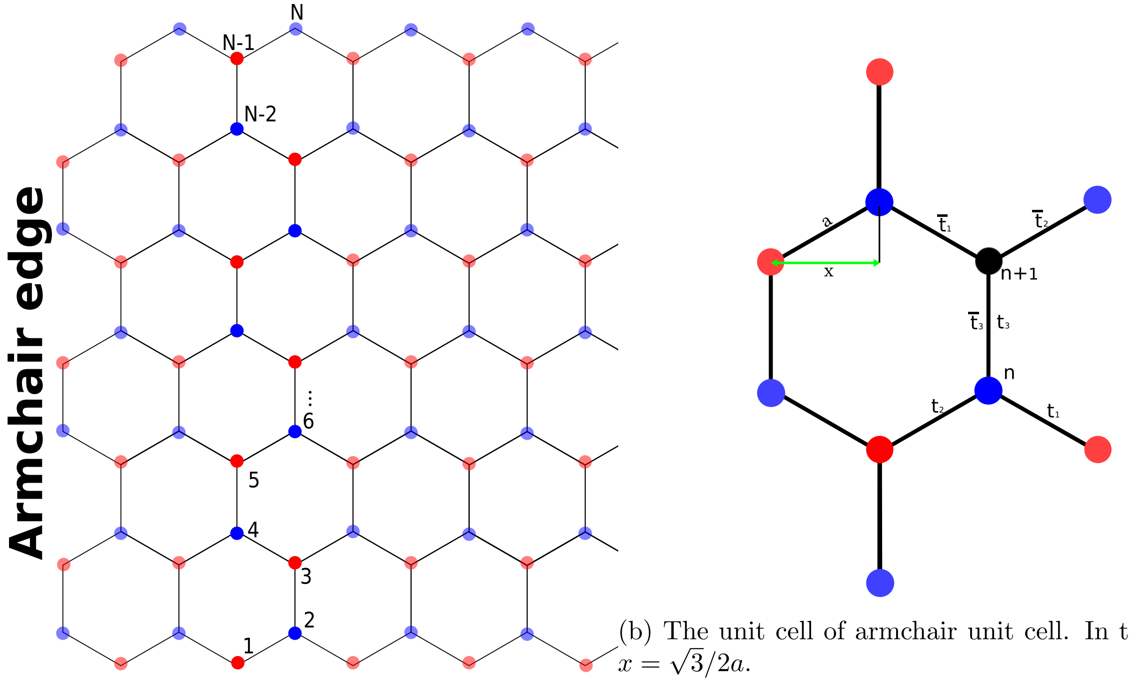
[1] Actually there are more, and we will see this in this chapter



(a) Caption 1

(b) The unit cell of armchair unit cell. In this figure, $x = \sqrt{3}/2a$.

Figure 4.2: In figure 4.2a, you see the armchair edge. Every waveguide on the bottom edge corresponds to number one. Note that all the bottom atoms in this case are B atoms. Every waveguide to the second chain corresponds to number two waveguides. These waveguides are A atoms. This goes on until the final chain of atoms, the N atoms. The reason we assume that all waveguides corresponding to the same value j, that is are on the same y, are equivalent is because of thbe periodic boundary conditions. Since we have periodicity on the x axis, we have translational symmetry, so all waveguides at the same y are equivalent.

eigenstate, and we have done that both for an A atom and for a B atom. This is why we have a 2×2 system. It is reminded that $\Psi_{i,j}$ and $\Phi_{i,j}$ are not wave function, but coefficients.

Furthermore, we will also solve the medium difficulty problem which is given by

So, the finding of the solution of the semi infinite problem is equivalent with the solution of the above system with the appropriate boundary conditions. Since the system is semi finite, we will assume periodic boundary conditions in one dimension. If we choose the system periodic in respect to the x direction, then the wave functions take the form

$$\Psi_{n,m} = e^{ik_x x}\Psi_n, \quad \Phi_{n,m} = e^{ik_x x}\Phi_n, \quad x = x_m = \sqrt{3}/2ma, \tag{4.2a}$$

where the last equality show the possible values of x since x is a discrete variable which is increased by a constant length $\sqrt{3}a$ as you can see on figure 4.2b, since the value x is $\sqrt{3}/2a$. Furthermore, we have to see after which value the momentum k, starts to repeat its values. We know that in real space this is happening at every 2 a distance. Using that, we can find what is the lattice constant on momentum space in the y direction. We have

$$e^{ik_x x} = e^{ik_x(x+\sqrt{3}a)} \Rightarrow e^{i\sqrt{3}k_x a} = 1 = e^{i2n\pi} \Rightarrow k_x = \frac{2n\pi}{\sqrt{3}a} \tag{4.2b}$$

So, k_x repeats its self after every

$$k_x = \frac{2\pi}{\sqrt{3}a} \tag{4.2c}$$

Eq. (4.2b) gives us the values that k_x can take. Of course, we can give k_x a larger value, but it will have the same exact energy with a previous value. So, we will plot the values of k_x given by the equation above.

4.2.1 Original Armchair edge

First we will talk about the armchair edge. The armchair edge has the form seen in figure 4.2a, where we use the same numbering discussed in section 4.1. Since it is a finite system, to solve it, we need to write the Hamiltonian describing this system as we did in section 2.1.1. Furthermore, since we have periodicity in the x direction, we expect to have exponentials of k_x in the Hamiltonian, and as we will see, this is indeed the case.

In order to solve this system, we use the system of Eqs. (4.1a) with the boundary conditions (4.2a). This gives us the system,

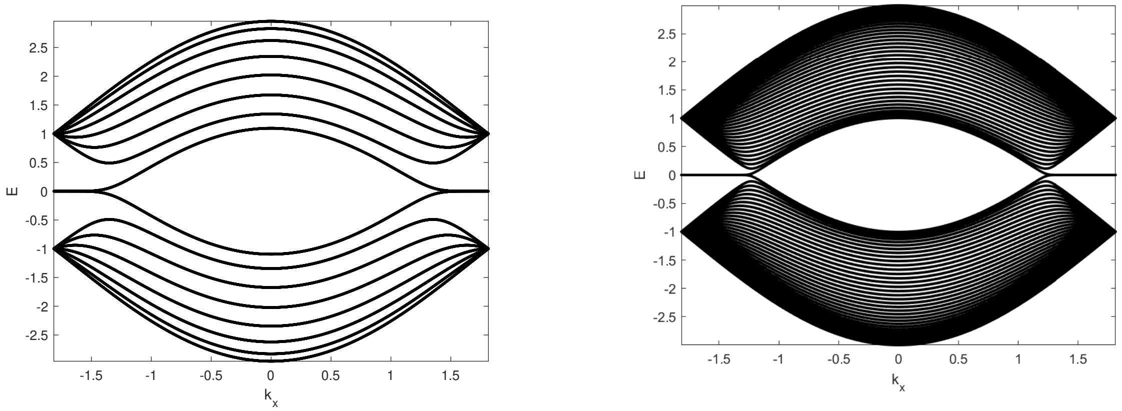
$$\begin{cases} -te^{ik_y\sqrt{3}/2ma}\Psi_{n-1} - te^{ik_y\sqrt{3}/2(m+1)a}\Psi_{n+1} - te^{ik_y\sqrt{3}/2(m-1)a}\Psi_{n+1} = Ee^{ik_y\sqrt{3}/2ma}\Phi_n \\ -te^{-ik_y\sqrt{3}/2ma}\Phi_{n+1} - te^{ik_y(m-1)a}\Phi_{n-1} - te^{i\sqrt{3}/2k_y(m+1)a}\Phi_{n-1} = E\Phi_n \end{cases} \Rightarrow$$

$$\Rightarrow \begin{cases} -t\Psi_{n-1} - te^{i\sqrt{3}/2k_y a}\Psi_{n+1} - te^{-i\sqrt{3}/2k_y a}\Psi_{n+1} = E\Phi_n \\ -t\Phi_{n+1} - te^{-i\sqrt{3}/2k_y a}\Phi_{n-1} - te^{i\sqrt{3}/2k_y a}\Phi_{n-1} = E\Psi_n \end{cases}$$

Using Euler's formula for exponential, we can write it in the final and elegant form

$$\begin{cases} -t\Psi_{n-1} - 2t\cos(\sqrt{3}/2k_x a)\Psi_{n+1} = E\Phi_n \\ -t\Phi_{n+1} - 2t\cos(\sqrt{3}/2k_x a)\Phi_{n-1} = E\Psi_n \end{cases} \tag{4.3}$$

Now, we have to take into account the boundary conditions. We assume that we have N waveguides in total in one chain, so that the waveguide at $n = 1$ and the waveguide at $n = N$ will be coupled only with one waveguide. More specifically, the waveguide at $n = 1$ will only be



(a) Four unit cells. So there are 16 energy eigenstates.

(b) Twenty unit cells. So there are 80 energy eigenstates.

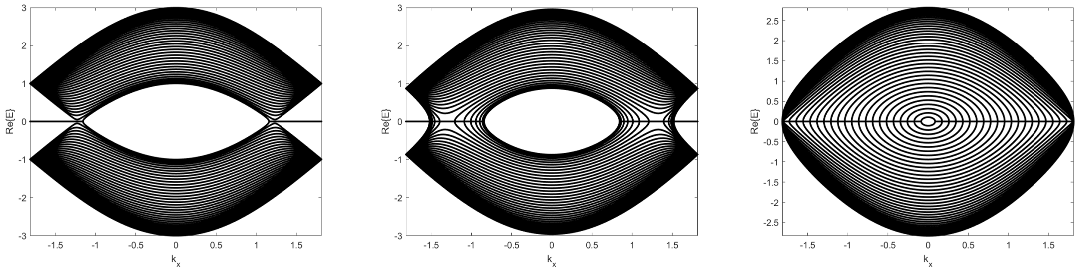
Figure 4.3: Energy momentum bands for different number of unit cells for value $a = 1$ and $t = t_1 = t_2 = t_3 = 1$. The k_x axis starts from value $-\pi/\sqrt{3}$ and ends at $\pi/\sqrt{3}$

connected with the waveguide $n = 2$ (notice that there are two waveguides of the form $n = 2$ connected to $n = 1$, so we will have a t_2 coupling as you see on equation (4.4)). In other words we can say that $\Phi_0 = \Psi_{N+1} = 0$ which in quantum mechanical terms express the absence of probability in finding the electron at atom $n = 0$ and $n = N + 1$. In photonic term, this corresponds to the probability amplitude of finding the photon at waveguide $n = 0$ and $n = N + 1$. By doing this, the Bloch Hamiltonian will have the form

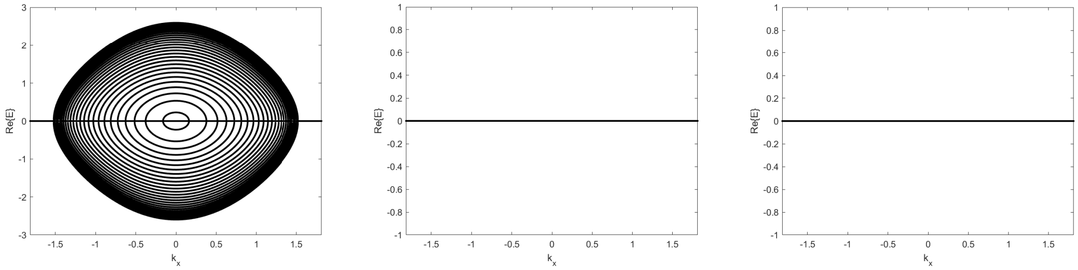
$$H = \begin{bmatrix} 0 & -t_2 & & & & & \\ -t_2 & 0 & -t_1 & & & & \\ & -t_1 & 0 & -t_2 & & & \\ & & -t_2 & 0 & & & \\ & & & & & & \\ & & & & \ddots & & \\ & & & & & & -t_2 \\ & & & & & -t_2 & 0 \end{bmatrix}, \tag{4.4}$$

where $t_1 = t$ and $t_2 = 2t\cos(\sqrt{3}/2 \cdot ak_x)$. We wrote them as t_1 and t_2 for elegance, so that the Bloch Hamiltonian look nice. As we see, the t_2 coupling depends on the wavelength k_x, that is $t_2 = t_2(k_x)$, as it should, since we have periodicity on the x axis.

Here we will explain why Hamiltonian given by Eq. (4.4) has this exact form. Let us first use figure 4.2a. Each row represent one waveguide in the Hamiltonian. So the first row of the Hamiltonian correspond to the waveguide number one in figure 4.2a. We see from the same figure that this waveguide is coupled to two waveguides of type two. Since these two waveguides are equivalent, we sum their coupling as we explained when we solved the system (4.11), and we write it us the coupling t_2. Since it is represented with number two on figure 4.2a, we put the t_2 on the element H_{12} of the Hamiltonian, that is $H_{12} = -t_2$. So in the first row, we just have a t_2 coupling in the second column. Now we go to the waveguide corresponding to number 2 in figure 4.2a. This is an A atom. As we can see, this waveguide is coupled to two waveguide of corresponding number 1, that is coupling t_2, and one waveguide corresponding to number three, which is coupling t_1 according to Eq. (4.7a). So in the second row we put t_1 in the first collumn, and t_2 in the third collumn. The third row corresponds to the waveguides of $j = 3$, which in figure 4.2a are coupled



(a) $\gamma = 0.1$.	(b) $\gamma = 0.5$.	(c) $\gamma = 1$.



(d) $\gamma = 1.5$.	(e) $\gamma = 3$.	(f) $\gamma = 5$.

Figure 4.4: Energy momentum bands. We plot the real part of energies in the case of twenty unit cells for the values $a = 1$ and $t = t_1 = t_2 = t_3 = 1$. The k_x axis starts from value $-\pi/\sqrt{3}$ and ends at $\pi/\sqrt{3}$.

with one waveguide on the y axis at $y = 2$, so t_1 at H_{32}, and two waveguides corresponding to number four, so $H_{34} = t_2$. We can continue like this and built the whole Hamiltonian.

One faster way to do this is to observe that every A atom which as we see in figure 4.2a, is conneted with a t_2 coupling with the previous number atom, and t_1 with the next number. This means that every element in the Hamiltonian, corresponding to A atoms will have as the only non zero elemetns, the elements

$$H_{ii+1} = -t_1 \quad \text{and} \quad H_{ii-1} = -t_2. \tag{4.5a}$$

Furthermore, we can see from figure 4.2a, that A atoms correspond to even numbers. So all even number of the Hamiltonian will have the form of Eq. (4.5a), with the exception of the final atom in the armchair edge, which is only coupled to the previous waveguide with t_2 coupling.

For B atoms we can see in figure 4.2a that all B waveguides are coupled to their previous waveguide with couplng t_1, and in the next with coupling t_2, and since the B waveguides are presented on the odd rows of Hamiltonian, in all odd rows except the first one which we only have a t_2 coupling with above, we have

$$H_{ii+1} = -t_2 \quad \text{and} \quad H_{ii-1} = -t_1. \tag{4.5b}$$

It is important to note that the unit cell of the armchair chain has four atoms. So the Hamiltonian must be a $4n \times 4n$ matrix where $n \in \mathbb{N}$. If this doesn't apply then the Hamiltonian does not describe an armchair edge. We have plotted the states on figure 4.3

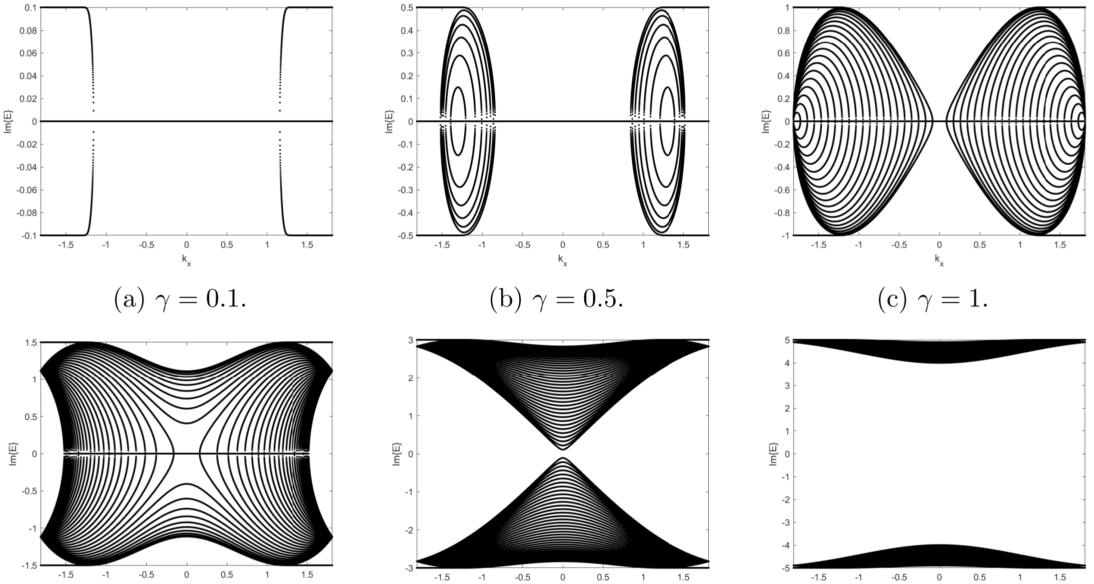
As we can see on figure 4.3, this is the shape that energy eigenstates have in the case of an armchair edge. The states that begin and end at zero energy are the edge states, that is the states correspond at waveguides $n = 1$ and $n = N$. As we see in the figures, the shape does not change as we put more and more unit cells, just the states becomes denser.

4.2.2 Armchair edge with gain and losses

Now we will put gain and losses on the system. This is trivial to do. As we said previously, we put on the diagonal elements the term $i\gamma$ in order to put losses, and the term $-i\gamma$ in order to put gains. If we do this, the Hamiltonian takes the form

$$H_{k_x} = \begin{bmatrix} -i\gamma & -t_2 & & & & \\ -t_2 & i\gamma & -t_1 & & & \\ & -t_1 & -i\gamma & -t_2 & & \\ & & -t_2 & 0 & & \\ & & & & & \\ & & & & \ddots & \\ & & & & & -t_2 \\ & & & & -t_2 & i\gamma \end{bmatrix}. \tag{4.6}$$

The solution of this Hamiltonian can be found by diagonalization, but now, we can have complex values for the eigenstates. We assume twenty unit cells for the solution, and that $t_1 = t_2 = t_3 = 1$. Finally we put the value of the distance a between two waveguides to be $a = 1$. The results for the real part of energy are represented at figure 4.4



(a) $\gamma = 0.1$.

(b) $\gamma = 0.5$.

(c) $\gamma = 1$.

(d) $\gamma = 1.5$.

(e) $\gamma = 3$.

(f) $\gamma = 5$.

Figure 4.5: Energy momentum bands for different number of unit cells for value $a = 1$ and $t = t_1 = t_2 = t_3 = 1$. The k_x axis starts from value $-\pi/\sqrt{3}$ and ends at $\pi/\sqrt{3}$.

We now discuss, how the real part of energy eigenstates of the Bloch Hamiltonian changes as we increase gain and losses. We begin with $\gamma = 0$ where we have figure 4.3b (remember that we work for the case of $N = 4$ unit cells). As we increase gain and losses, we see that states expand going closer to zero since the energy gap for states close to $k_x = 0$ becomes smaller, and we also see that more states approach values close to $k_x = \pm\frac{\pi}{\sqrt{3}}$, so that the whole shape seems to take more the shape of a sphere. At $\gamma = 1$ is the value where the states are close to the values of $k_x = \pm\frac{\pi}{\sqrt{3}}$, so it seems most like a sphere shape (more like an eye shape actually). After the value of $\gamma = 1$, as we increase gain and losses more, the real part of energy eigenstates decrease more and more, as

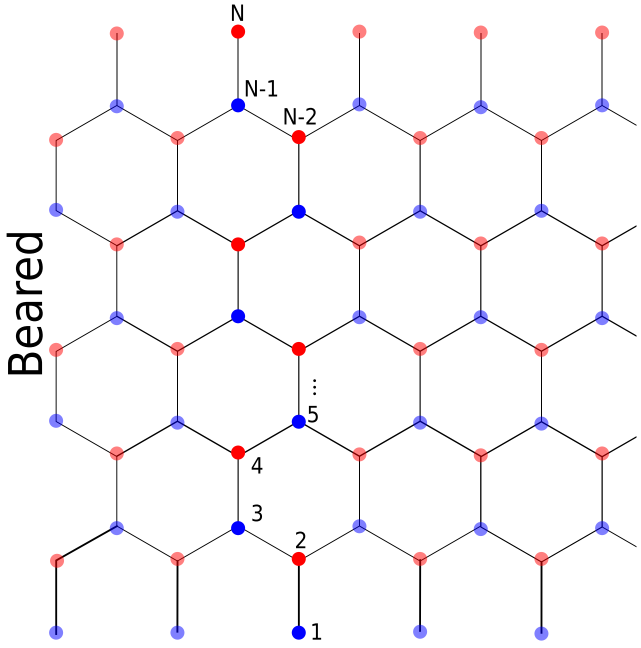


Figure 4.6: This is the definition of the beared edge. It is the same as the Armchair edge with the exception that the first B atom and the final A atom are missing. Each carbon atom is at distance a with every other carbon atom. The total number of atoms in a bearded chain is assumed to be N, which is an even number.

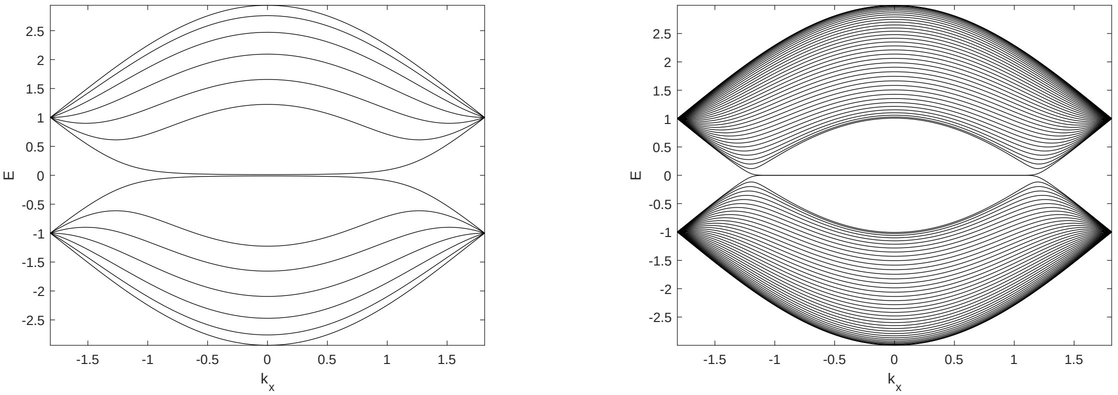
we see on figure 4.4d, and the circle starts to sring. After $\gamma = 3$, no real energies exists as we can see on figures 4.4e and 4.4f.

Now let use how the imaginary part of the energies is affected by gain and losses. You can see this on figure 4.5.

Now let us see what is going on with the imaginary part of the energy eigenstates. In the beginning there are no states with imaginary part. All states are real since the original Hamiltonian, given by Eq. (4.4), is hermitian. If we start putting gain and losses, we see that most states stays zero, but states smaller than the value of $k_x \approx -1.15$ and states larger than the value of $k_x \approx 1.15$, start to have a non zero imaginary part. This is true even for very small values of γ. The only thing that changes as we descrease γ is the value of the imaginary part of the energies which will be smaller. But the same exactly states will have a non zero imaginary part. As we increase gain and losses, we see that there are some ellipses that start appearing around point $k_x = 1.15$, and growing larger as γ increases. This can be seen in figure 4.5b. At value $\gamma = 1$, these ellipses almost tough each other (actually by a small change in the value of γ they will connect), and also imaginary values at $k_x = \pm\frac{\pi}{\sqrt{3}}$ start to appear as we can see on figure 4.5c. After this value, the ellipses have been connected, and also as we increase gain and losses more and more, no energies with zero imaginary part remain at valus near $k_x = \pm\frac{\pi}{\sqrt{3}}$ as you can see in figure 4.5d. As we continue increasing the value of γ, more and more states, closer to $k_x = 0$ start to get an imaginary part. At $\gamma = 3$ no states with non zero imaginary part remains, as you can see in figure 4.5e. Finally, for large gains and losses, all states go to the limit of the imaginary part as you can see in figure 4.5f.

4.3 Bearded edge

Another kind of boundary condition is the so called bearded boundary conditions which can be seen on figure 4.6. Namely it has the same form as an armchair chain, but we exclude the two atoms on the edges, that is the B waveguide on the bottom edge and the A waveguide to the top edge. Thus we change the boundary conditions of the model. The total number of waveguides (or



(a) Four unit cells and 14 energy states.

(b) Twenty unit cells and 78 energy states.

Figure 4.7: This is the solution of bearded edge. In the

atoms in the case of regular graphene) in this case, is the same as in the previous case studied on section 4.2, minus the two atoms that missing. So we have $4N-2$ waveguides in the case of the bearded edge.

The bulk of the problem is the same with the one we discussed on section 4.2, so it is given by the system (4.1a). This is why we expect that the bearded edge case, will give similar results for the bulk of the edges with the armchair edge. As we said, what will change is the edge states. Now the edge states are not the same, so we expect that the edge states will change, but the rest of the spectrum will mostly be the same. In this case, the Bloch Hamiltonian of the problem can be written on the matrix form

$$H = \begin{bmatrix} 0 & -t_1 & & & \\ -t_1 & 0 & -t_2 & & \\ & -t_2 & \ddots & & \\ & & & & -t_1 \\ & & & -t_1 & 0 \end{bmatrix}. \tag{4.7}$$

As we can see, the Bloch Hamiltonian is the same with out Hamiltonian is a $(4n-2)\times(4n-2)$. This is because we have subtracted the two atoms for he edges, so we have remained with $4n-2$ atoms as we said before.

In order to computationally calculate the energy eigenstates of this problem, we just diagonalize Hamiltonian (4.7) as we did for the previous problem at section 4.2.1. The result of the diagonalization can be seen on figure 4.7.

We see from this result that the two energy bands seem a lot alike. What is different are the edge states. All the other result is more or less the same. This makes sense because the system is exactly the same in the bulk, and the only thing that is different is the edge states. The edge states are now connected only with one state, so there is t_1 coupling, and not t_2 as in the previous case.

We could have put gains and losses in this system as well, but as we have seen the solution of the system is identical except of the edge states, we find that when we assume zero gain and losses, or in other words, we put zero γ, the solution is identical with figure 4.2. In the case of gain and

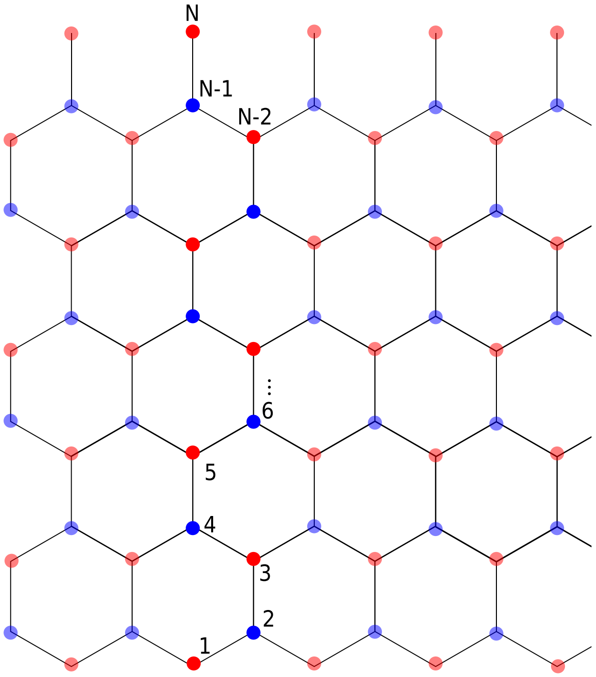


Figure 4.8: Here is the armchair bearded edge which is a combination of armchair edge (in the bottom) and bearded edge (in the top). We see that the waveguide in the top is only cpupled to one wave guide, while the waveguide on the bottom is coupled to two waveguides. In other words the B type waveguide in the upper edge experience a t_1 coupling, while the B type waveguide on the botton experience a t_2 coupling.

losses, the Hamiltonian will take the form

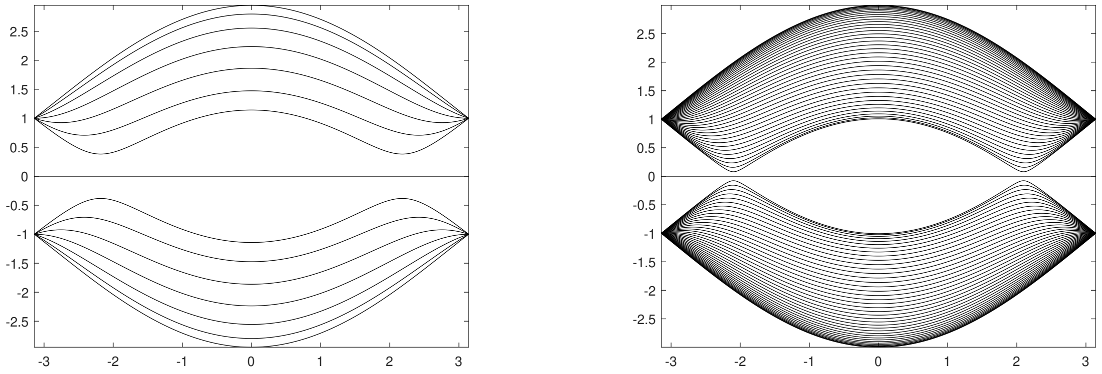
$$H = \begin{bmatrix} i\gamma & -t_1 & & & \\ -t_1 & -i\gamma & -t_2 & & \\ & -t_2 & i\gamma & & \\ & & & \ddots & \\ & & & & -t_1 \\ & & & -t_1 & -i\gamma \end{bmatrix}. \tag{4.8}$$

The results once again is almost identical with the results from the armchair edge, since the only thing that differs are the edge states. Particularly, in the real part that the edge states are zero inside the area as you can see in figure 4.7b. This does not change when we assume gain and losses. The edge states on the inside part will always be zero. Furthermore, the imaginary part of the states has an interesting property. As we said in section 4.2, values below $K_x = -1.15$ and above $k_x = 1.15$

4.4 Armchair bearded edge

Another kind of boundary conditions are the so called armchair bearded boundary condition. This is a chain of atoms which can be seen on figure 4.8. As you can see in this figure, it is a combination of armchair edge and bearded edge. In the bottom edge it has armchair edge, while in the top edge, it has bearded edge.

Once again the bulk of the system is the same and given by Eq. (4.11), so the Bloch Hamiltonian will be the same. The difference once again lie on the edge states. As you see in figure 4.8, in this case, the bottom wave guide, placed at position $n = 1$ experience a t_2 coupling, while the top waveguide, placed in position $n = N$ experience a t_1 coupling. So, in this case, the Hamiltonian



(a) Four unit cells

(b) Twenty unit cells

Figure 4.9: Solution of the zig-zag bearded Hamiltonian for two different numbers of unit cells.

takes the form,

$$H = \begin{bmatrix} 0 & -t_2 & & & \\ -t_2 & 0 & -t_1 & & \\ & -t_1 & \ddots & & \\ & & & & -t_1 \\ & & & -t_1 & 0 \end{bmatrix}, \tag{4.9}$$

where in this case the Hamiltonian is a $(4n-1)\times(4n-1)$ matrix since we have $4N-1$ waveguides. This can be proved trivially, because we have the same number as in the armchair edge case which is $4N$, but we exclude one waveguide on the top, so indeed we remain with $4N-1$ waveguides.

The computational results from the diagonalization of the Hamiltonian (4.9), are given in the figure 4.9. As we see, the characteristic property of the zig-zag bearded energy spectrum are the edge states since they are always zero in this case.

We can put in this case too gains and losses in the system. If we do this, by putting gain on A atoms and losses on B atoms, the Hamiltonain will take the form

$$H = \begin{bmatrix} -i\gamma & -t_2 & & & \\ -t_2 & i\gamma & -t_1 & & \\ & -t_1 & -i\gamma & & \\ & & & \ddots & \\ & & & & -t_1 \\ & & & -t_1 & -i\gamma \end{bmatrix}, \tag{4.10}$$

In this case, the figures of the real part of the energy is exactly the same, with the exception of the edge states, as in the bearded system as well. The edge states in the armchair bearded are always zero, as in the hermitian case where no gains and losses exist in the sample. Furthermore, the imaginary part of the energy eigenstates has a constant non zero part for every k_x. You can see this on figure 4.7a.

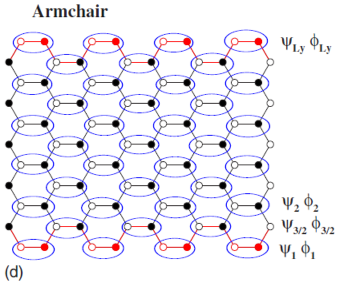


Figure 4.10: Armchair edge

4.5 Zig-zag edge

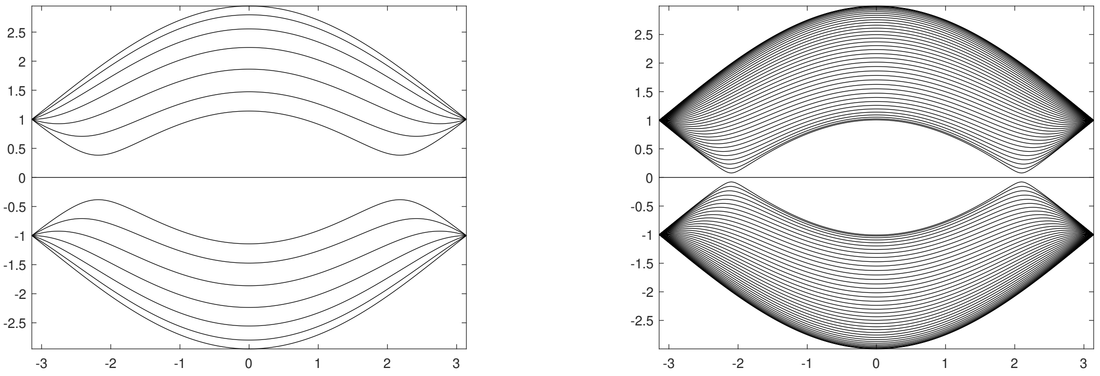
The zig-zag edge is one of the two edges that graphene is usually seen to have. It is different from the armchair edge and it can be seen on figure 4.2. As we will see it has a very different behaviour from the case of armchair edge. We will just solve this system computationally for two different cases of unit cells, as we did in the previous sections.

Now we will count the number of waveguides we have in this problem. In this case, we will measure the hexagons that we put. The first hexagon gives 3 atoms. The second one gives other two atoms since the last of the previous hexagon is equivalent with the first of the new hexagon. So every new hexagon puts two electrons in the Hamiltonian. That is, then order of the matrix of the Hamiltonian will be $(4N-2)\times(4N-2)$. The system of this problem is given by

$$\begin{cases} -e^{-ik/2}\Phi_m - \Phi_{m-1} - \Phi_{m+1} = E\Phi_m \\ -e^{ik/2}\Phi_m - \Psi_{m-1} - \Psi_{m-1} = E\Phi_m \end{cases} \tag{4.11}$$

And the Hamiltonian corresponding to system (4.11) is given by

$$H = \begin{bmatrix} 0 & -t_2 & 0 & -t_1 & & \\ -t_2 & 0 & -t_1 & & & \\ 0 & -t_1 & 0 & -t_2 & 0 & -t_1 \\ -t_1 & 0 & -t_2 & 0 & -t_1 & \\ & & & & & \ddots \end{bmatrix} \tag{4.12}$$



(a) Four unit cells

(b) Twenty unit cells

Figure 4.11: Solution of the zig-zag bearded Hamiltonian for two different numbers of unit cells.

Chapter 5

Solving the finite problem

In this chapter, we will solve the finite problem of photonic graphene lattice. As we will see, this is not a particular problem, but we can choose the two dimensional lattice as we please in order to solve the problem. In this thesis, we will define a couple of different problems concerning two dimensional lattices, and we will solve each one of them. Finally, we will discuss our results.

5.1 Two dimensional graphene of type 1

5.1.1 Defining the problem of type 1 graphene

Here we define the first problem of two dimensional graphene that we will solve. We will call it "type 1 graphene". This problem is the same as the one seen on figure 4.1. That is we build it by putting hexagons one of top of the other. The way we define it is by giving the number of hexagons we put on the x axis, and the hexagons we put in the y axis. Suppose that the number of hexagons in the x axis is N_x and the number of hexagons in the y axis is N_y. We assume that each problem is defined by the two natural number N_x and N_y. We call the problem that it is of the form $N_x \times N_y$.

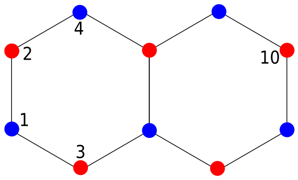
In figure 5.1 we present some kind of problems to be more clear. As we said in chapter 5, the first thing we need to do in order to computationally solve the problem is to give each waveguide, a certain numerical value corresponding to the position of the waveguide, or more importantly, in the row of the Hamiltonian that this waveguide corresponds to. In the figure below the numbering is written.

As you can see, we use the same numbering discussed in section 4.1. That is we begin with the atom with $i = 1$, and we increase the number j, or in other word, we count all the waveguides corresponding to smallest x, starting from lower to larger. After we end this counting, we start counting the second smallest value for x,and we continue like that until the end.

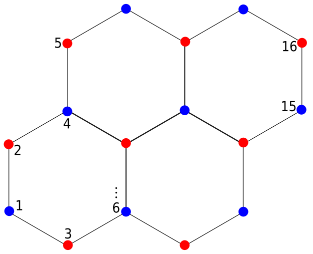
The waveguide number one will correspond to the first row, the waveguide corresponding to number two will correspond to the second row and second column of the Hamiltonian and so on. So that the diagonal terms correspond to the energy eigenstates, and the non diagonal terms represent the coupling between the waveguides correspond to the rows and columns of this term. That is the term H_{12} corresponds to the coupling between the waveguides number one and two.

5.1.2 Solution of the finite system of type 1

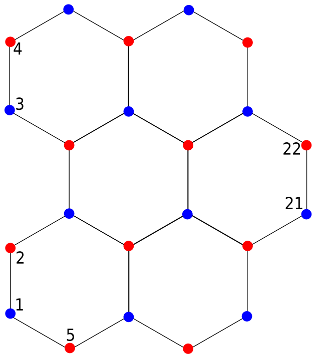
As we said in chapter 2.1, the way we solve the finite problem is the diagonalization method. In this case, there is no periodicity, so we expect that the Hamiltonian that we diagonalize will be independent of momentum, that is we will not have a Bloch Hamiltonian to diagonalize, but a regular Hamiltonian that we need to diagonalize.



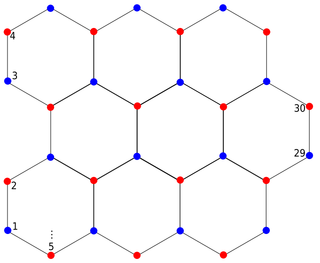
(a) $2x1$ problem.



(b) 2×2 problem.



(c) 2×3 problem.



(d) 3×3 problem.

Figure 5.1: Caption

When the Hamiltonian does not depend on momentum, we expect to find the eigenstates and the eigenvalues corresponding to the problem. This is our goal in this section. First we write the Hamiltonian of the problem. In this section we will solve the 2×2 problem which is the easier problem we will deal with, the 2×3 problem, the 3×3 problem and the 10×10 problem which is the most difficult problem we deal with.

We will not write the Hamiltonian for every problem, for elegance, but we will only write a part of the Hamiltonian of the 2×2 problem, and explain why it has the form that it has. The Hamiltonian of the 2×2 problem can be written as

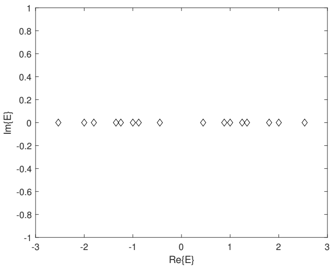
$$H = \begin{bmatrix} 0 & -t_3 & -t_2 & & & \\ -t_3 & 0 & 0 & -t_1 & & \\ -t_2 & 0 & 0 & 0 & 0-t_1 & \\ & & & & & \ddots \end{bmatrix} \tag{5.1}$$

Now let us explain why the Hamiltonian above corresponds indeed to the Hamiltonian of the 2×2 problem. First we begin with the first waveguide, which we know that corresponds to the first row of the Hamiltonian. We see that the waveguide number one in figure 5.1b is coupled to the two waveguides next to it. That is waveguides number two and number three. So we put as only non zero terms in the first row of the Hamiltonian the elements H_{12} and H_{13}. Now we begin with the second row of the Hamiltonian, or in other words the waveguide number two. We see that the neigbour waveguides of this waveguide are the waveguides number one and number four. This means that the only non zero elements will be H_{21} and H_{24}. For the waveguide number three, we see that it couples to waveguides one and six, so have that the only non zero terms are in the third row of the Hamiltonian are H_{31} and H_{36}. So this is why the Hamiltonian has these non zero elements. If we continue with the waveguide number four, we can see that the only non-zero elements are the elements H_{42}, H_{45} and H_{47}. We can now choose, if it is a t_1, a t_2 or a t_3 coupling according to figure 1.1b. We see if we have an A or a B atom. If we have an A atom, then we will put the coupling

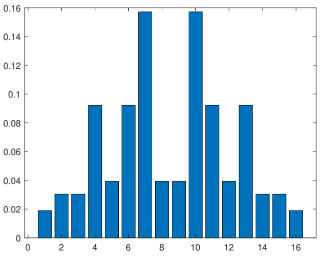
t_1 or t_2 or t_3, as it is. If ir is a B atom, we have to put its complex conjugate. Since we chose the coupling to be real, we do not need to care about complex conjugation. It is just mentioned for completeness.

The results of the energy eigenstates as well as the probability amplitude of the ground state, can be seen on figure 5.2a. For the plotting of these states, we used for the coupling the values $t_1 = t_2 = t_3 = 1$. We will discuss these results below.

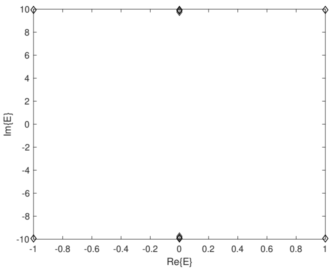
We start from the 2×2 system. In this system, where 16 waveguides, and thus 16 energy eigenstates in total states exists, we get that the ground state energy is $E_g(2 \times 2) = -2.532088886237956$ and we see from figure 5.2b that the maximum probability amplitude is on the waveguides numbered seven and ten. By looking at figure 5.1b, we see that these waveguides are the waveguides that are in the middle of the sample. Furthermore these waveguides are connected with their three neigbour waveguides, that it, with the maximum number of the waveguides that we can connect them, so this is the maximum way that electrons can come to these two waveguides. The waveguides, that seven and ten waveguides are connected are the numbers four, six eleven and thirteen and all of these waveguides are also connected with three waveguides each, but this gives lower energy because some of the waveguides that numbers four, six, eleven and thirteen are connected, are coupled with waveguides with two other waveguides connected. So this gives in total smaller probability amplitude for the photon to be found in these waveguides. the next smaller energy eigenstates are the numbers five, eight, nine and twelve. These waveguides are only connected to two other waveguides, whose one of the other is a waveguide that couples three, and the other a waveguide that couples to two other[1]. The waveguides with a little bit less probability amplitude are the waveguides 2,3,14 and 15. These waveguides have exactly the same properties, but the reason that they have less enenrgy than the previous is because one of the state that these waveguide couples to are the waveguides 1 and 16 which are the only ones which ar econnected with two waveguide that couple only to

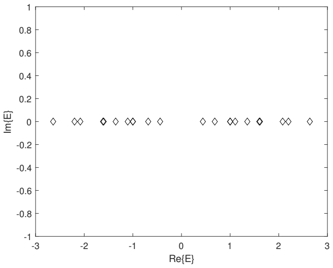


(a) Energy eigenstates, for 2×2 system for $\gamma = 0$.

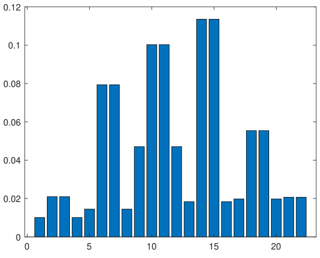


(b) Probability amplitude of 2×2 system.

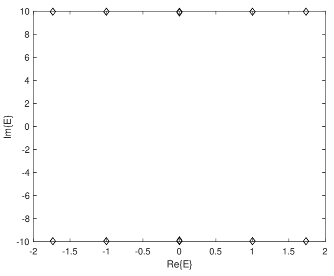




(c) Eigenstates of 2×3 system.



(d) Ground state of 2×3 problem.



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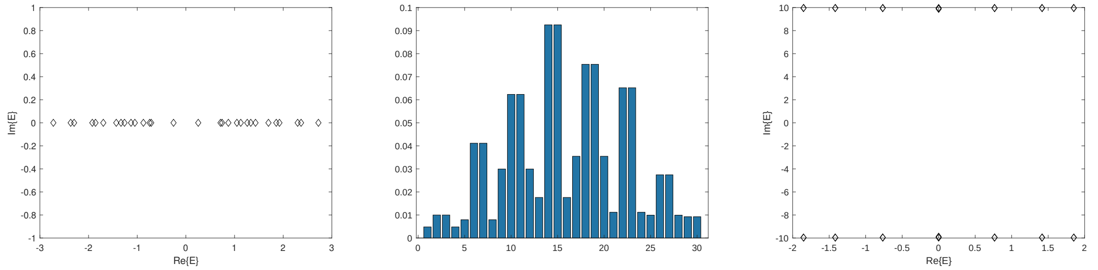
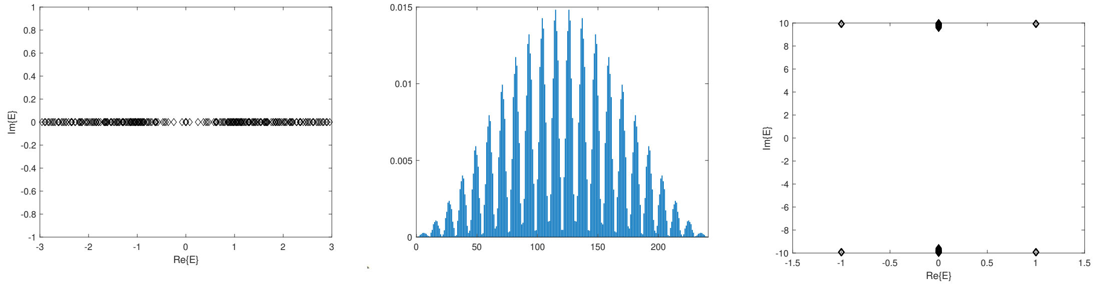
[1] For example, waveguide five couples to two wave guides. The first is waveguide number four, and the second is waveguide number 8. Waveguide number 8 couples only to two waveguides (5 and 11) and waveguide 4 couples to three waveguides (2,5 and 7).



(e) Energy eigenstates of 3 × 3 system.

(f) Probability amplitude of the ground state of 3 × 3 system.

(g) Energy eigenstate of 3 × 3 system for high gains and losses.



(h) Energy eigenstates for 10 × 10 system of type 1. No gains and losses.

(i) Probability amplitude of the ground state of 10 × 10 system of type 1 problem.

(j) Energy eigenstate of 10 × 10 system for high gains and losses.

Figure 5.2a: Above you see the solution of some systems of type 1 finite graphene problem. In the first column of figures, that is figures... you see the solution of energy eigenstates when no gain or losses are present in the system. Since the Hamiltonian is hermitian, we expect that all energy eigenstates are real. In the second column of figures, namely figures... we have notated the probability amplitude of ground state of each case. Finally the third column of figures, we presented the energy eigenstates of each case with high gain and losses. In that case we do not present the energy eigenstates of the ground state because, as you can see in these figures, there is high degeneracy, so you cannot pick a particular ground state.

two waveguides. So they should have less energy. And finally the two waveguides that have the least probability amplitude, are the waveguides 1 and 16, since, as we just said, they are the only waveguides that are connected with two waveguides that couple only to two waveguides, so there is the elast probability that the photon will found there.

Now let us move on to the 2 × 3 system. We will not discuss this system is such detail. We see that the larger probability amplitude can be seen in waveguides 14 and 15, then in waveguide 10 and 11, which are all waveguides that couples to three waveguides which are also connected with other three waveguides, and then, the next smaller energy is seen in waveguides 6 and 7 which are coupled to three waveguides, which two of them are connected to two. Furtheremore, there is higher probability amplitude for the photon to be found on the right edge, that is on waveguides 21 and 22, than on the waveguides 1 and 4. This is because the waveguides 1 and 4 are connected to two waveguides which couple to two, while in the right edge the waveguides are coupled to two which one of them is coupled to three. This is a very important fact, because it denotes that there is no inversion symmetry to our problem. We will talk later in more detail about that.

Most of the features discussed above are present to the 3 × 3 problem of type 1. We see that the maximum probability amplitude are on the waveguides 14 and 15 which we can see on figure 5.1d that they are in the middle of the sample. In general most of the probability amplitude is on waveguides that are more in the middle of the sample than the edges. And furthermore, the probability that you will find the photon on the left edge, is higher than the probability to find the photon on the right edge. As we will see later, this is in general a consequence of the problems where N_y is an odd number as we will see in section 5.2.

The last problem we solved on figure 5.2a, is the 10×10 problem which we have written the probability amplitude of the ground state on figure 5.2i. Here we see everything we discussed so far. Once again the probability amplitude is on the waveguides in the center, and as we leave the center and we go closer to the edge states, the probability amplitude gets lower and lower until we reach the waveguides number 1 and 240 where the probability amplitude is minimum. Furthermore, we see in the same figure a behavior like a beat. This is due to the way we counted the waveguides. As we said in section 5.1.1, we count all the states starting from the bottom edge, and moving through the upper edge. So it makes sense that the probability will start from low, it will reach a maximum when we will be in the middle of the chain of atoms, and it will reach again a minimum, when we reach on the top edge.

Another feature that we can see in figure 5.2a, is that when N_y is an even number, then all the energy eigenstates at high gain and losses become imaginary and are concentrated in six points. The value of N_x is not important, only the value of N_x has to be an even number. When N_y is an odd number, then this is not true. Actually, what happens in the case of an odd N_y is that now the energy eigenstates are concentrated into $2(2N_x + 1)$ points in the energy complex plane.

Before we move on, let us see how the energy eigenstates change as we increase the gains and losses of the system. On figure 5.3 we plot the real and imaginary part of energy eigenstates as a function of the gains and losses in the system, namely the variable γ.

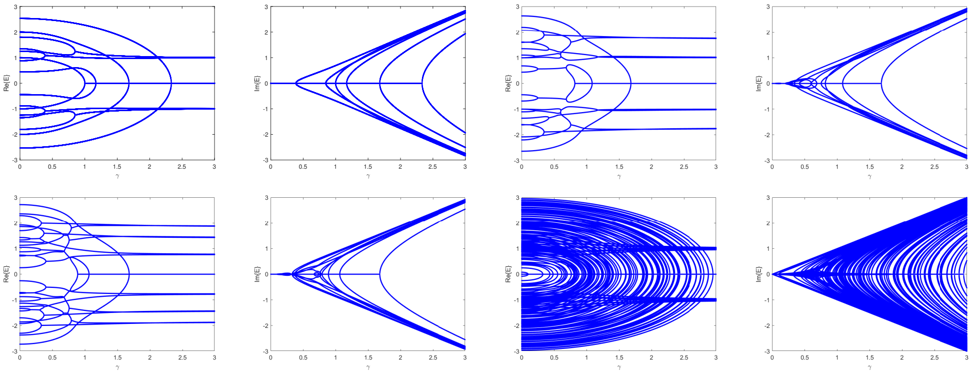


Figure 5.3: Caption

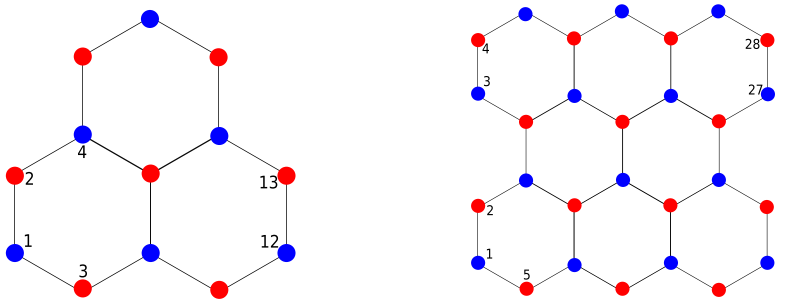
We see in the figure 5.3, that

5.2 Two dimensional graphene of type 2

5.2.1 Defining the problem of type 2 graphene

In order to test weather the reason of concentration in the six points is the inversion symmetry seen on the even values of N_y, we can define a model which has inversion symmetry on the odd values of N_y, but lacks C_2 symmetry for the even values. We call this new type of finite graphene "type 2 graphene". We represent some kinds of type 2 graphene lattices, in order to be more clear. You can see them on figure 5.4

So we see that the difference in this case is that we do not put the final hexagon at the even values of N_y. When we create for example a 4×4 problem using a type 2 graphene, we first put four hexagons on the bottom, since $N_x = 4$. On the top, we do not continue with four hexagons too,



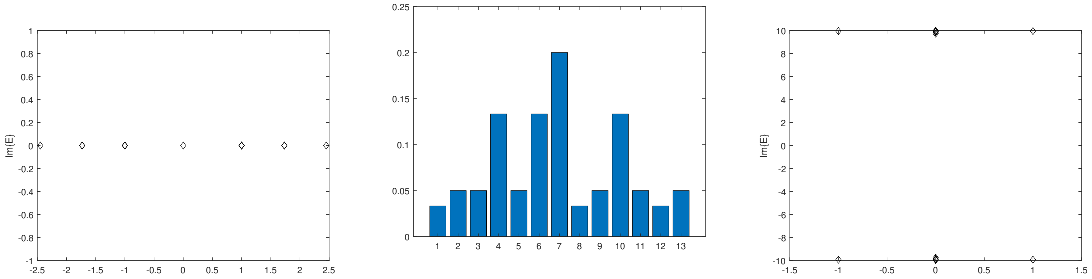
(a) 2 × 2 problem.
(b) 3 × 3 problem.

Figure 5.4: Different type 2 problems

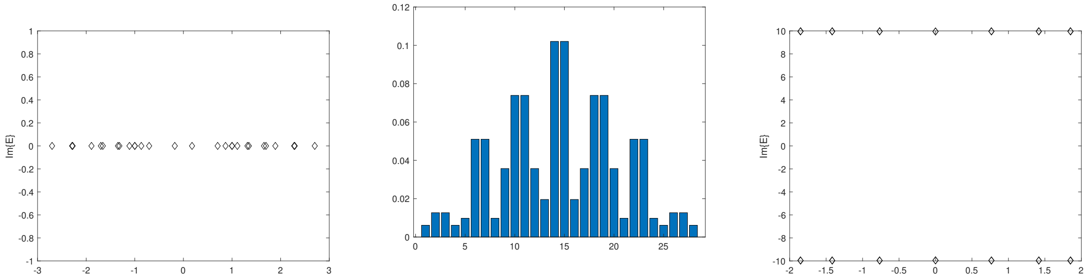
but we put three hexagons. After that, on the top of them we continue by putting four hexagons, and then again three hexagons. So what we really do is that we continue with N_x, on the top we put $N_x - 1$, then again N_x and $N_x - 1$, and so on. This shape we can easily observe that it has inversion symmetry for odd value of N_y. For example you can see that figure 5.4a does not have inversion symmetry, while figure 5.4b has.

We use the same method that we described to form the Hamiltonian in this case. As with type 1 graphene, we can find the solution via diagonalization. We will also find the solution for four problems. The 2 × 2 problem, the 3 × 3, the 5 × 5, and the 10 × 10 problem. The results are presented in figure 5.8a. Once again in order to plot the results we used $t_1 = t_2 = t_3 = 1$. Below we discuss the results.

In figure 5.8a, where we have the 2 × 2 system, we see that the waveguide with the larges probability to find the photon is the waveguide number 7. By looking on the figure 5.4a we see that this makes sense, because this waveguide is exactly on the middle of the sample. The less probable waveguides are numbers 4, 6 and 10, which are the waveguides that are coupled with the waveguide 7. The waveguides with less probability are the waveguides1,8 and 12, which once again makes sense because they are at the edges of the sample. As we clearly see from both figures 5.4a and 5.8a,



(a) Probability of 2 × 2 problem.



(b) Probability of 3 × 3 problem

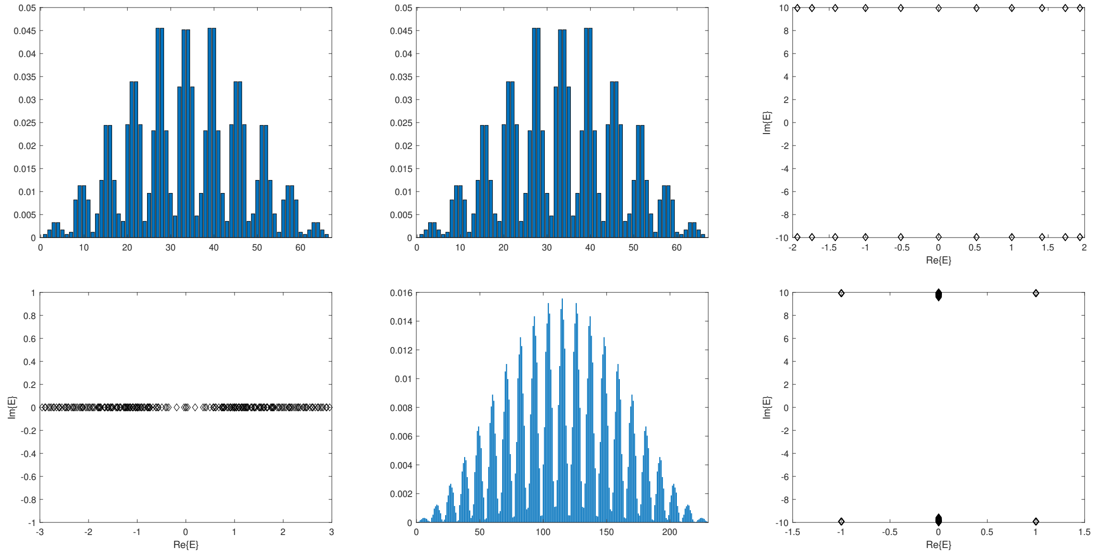


Figure 5.5a: Caption

there is no inversion symmetry in this case. On the other hand, we can easily see that there is C_3 symmetry in this case, and this is the reason that waveguides 1,8 an 12 have the same eigenvalue, as well as that the triplet of waveguides 3, 5, 13 and 2, 9 and 11 wave the same probability. In addition to C_3 symmetry, there are also mirror symmetries, but we will mostly talk about this in section 5.7.

At figure 5.8b we see indeed we have inversion symmetry in our system, since the histogram is symmetric, and that we have the same behaviour as we have seen in section 5.1, where we studied the type 1 graphene. That is, the maximum probability is in the center of our sample. We have a beating behavior because we count the atoms in y axis, so I expect to have low probability on the bottom and upper edge and maximum probability in the middle.

Then we see the 5 × 5 system which has inversion symmetry as we see, and the 10 × 10 system which does not, and the wave the same beating behavior.

Finally we see, that still the states with even N_y are concentrated into six point in the energy complex plane, while the problems with odd N_y are concentrated into $2(2N_x + 1)$ points, so we can see that the inversion symmetry was not the reason for this particular concentration.

Now let us see how the states change as we change γ.

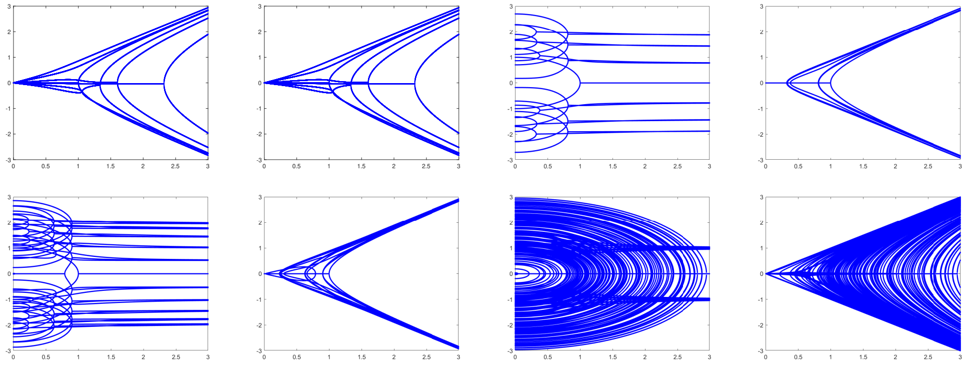
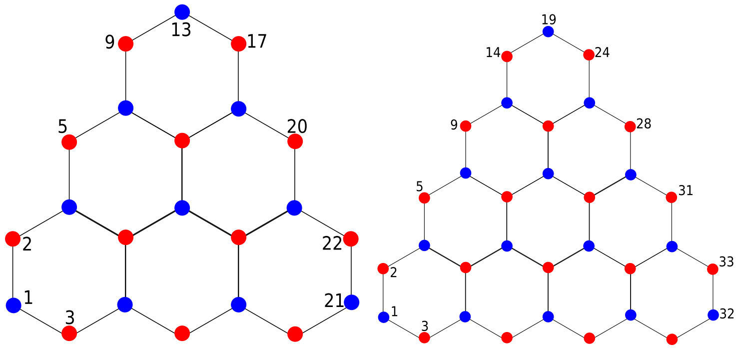


Figure 5.6: Caption



(a) $N = 3$ problem.

(b) $N = 4$ problem.

Figure 5.7: Type of 3 graphene problems.

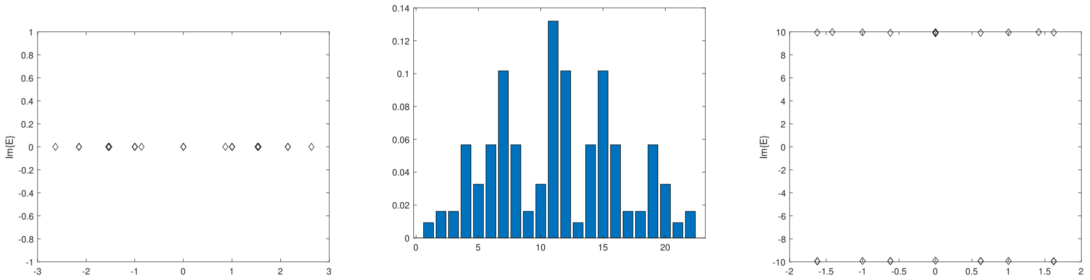
5.3 Two dimensional graphene of type 3

Now we will study a new type of problem, which we will call “type 3 graphene”. This has no real connection to the previous problems. It has its own philosophy. We note now that the following problem is a very famous problem.

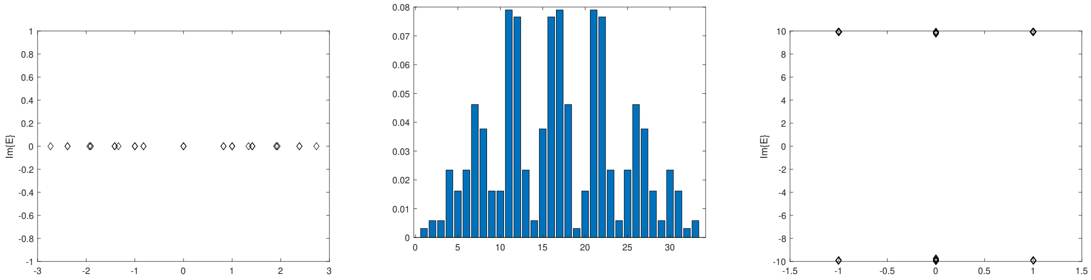
5.3.1 Defining the problem of type 3 graphene

In this part we will define the problem of type 3 graphene. This problem is defined just by one number. You just give the numbers of hexagons on the bottom which in this part of thesis we will call N for simplicity, and you obtain the whole picture of the problem.

The algorithm you need to make the graphene structure is the following. You begin by putting the first N hexagons in the bottom aligned with the x axis. Then, above this chain of hexagons you put another chain. This time you put $N-1$ atoms, as we did in section 5.2.1. When we go to the third row of hexagons, we put $N-2$, above that $N-3$ etc, until we put only one hexagon on the top. The type of finite graphene we have in this case can be seen in figure 5.7.



(a) Probability of 2×2 problem.



(b) Probability of 3×3 problem

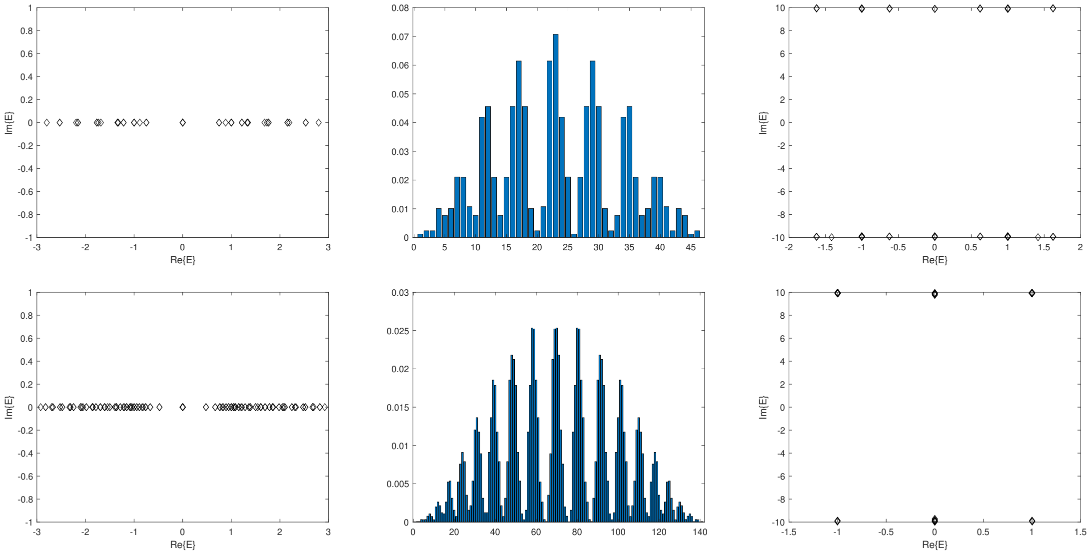


Figure 5.8a: Caption

Appendix A

Paraxial equation

In this Appendix we will solve Maxwell's equations inside matter, using the so called "paraxial approximation". By doing this we will prove Eq. (1.3), which is symmetric to the Schröndinger equation as we will see. In the first section we will prove what is the form of Maxwell's equation inside matter. Then we will solve these equations

A.1 Maxwell equations inside medium

Assume that you have light inside a waveguide. Our goal is to describe the propagation of light inside the waveguide. We assume that the waveguide can have a material with varying properties, that is with varying dielectric constant, in x and y directions, but the dielectric constant does not change in z direction. Maxwell's equations inside matter have the form

$$\begin{gathered}\vec{\nabla}\cdot\vec{\mathcal{E}}=\rho/\epsilon(x,y),\\ \vec{\nabla}\cdot\vec{B}=0,\\ \vec{\nabla}\times\vec{\mathcal{E}}=-\frac{\partial\vec{B}}{\partial t},\\ \vec{\nabla}\times\vec{B}=\mu_0\vec{J}+\mu_0\epsilon(x,y)\frac{\partial\mathcal{E}}{\partial t}.\end{gathered} \tag{A.1}$$

Inside dielectric materials, the charge density can be splitted into two parts. The first one is called "bound charge", and it describes the charge that stays on atoms. That is the charge that atoms has[1]. Furthermore, we can also have free charges. These are electrons that are not confined in an atom. These electrons can move from atom to atom, they are delocalized, so they belong to the conduction band of the solid. The way we put free charges to the material is via dopping. That is we put atoms that have one extra electron so that that they give one extra electron that can escape the atom even in relative small temperatures[2]. We should note that we cannot put electrons in the material to give the solid more free currents, because these currents would leave the material anytime it was in contact with another solid, which makes this way impractical. So we can write that the total charge is given by

$$\rho=\rho_b+\rho_f, \tag{A.2a}$$

---

[1] We should say here that usually we do not expect ions in the material, but what can happen is that atoms are polarized, namely that the electron cloud is has not the nucleus as its center, but it is a little bit translated as you can see in figure **??**. In this case, the molecule is affected by an applied electric field.

[2] The usual temperature for these electrons to escape from the atoms is given by...

where ρ_b represent the bound charges and ρ_f the free charges. In our case, we will not use dopping, so we will only consider bound charge in the medium. Bound charges are given by [**Griphits4.2**]

$$\rho_b = -\vec{\nabla} \cdot \vec{P}, \tag{A.2b}$$

where $\vec{P}$ is the polarization.

Now we will move on the current. The current inside a medium is given by

$$\vec{J} = \vec{J}_f + \vec{J}_M + \vec{J}_P.$$

As we can see above, the current is separated into three parts. J_f describes the current due to the motion of free charge. Since we assumed that there are no free charges, we do not have free current in our system. $\vec{J}_M$ represent the current produced by electronic motion due to induced magnetic field inside the material. This is usually tiny, so we consider it negligible. Finally, as we said before external elecric fields produce polarization in the material. The change in polarization can create current given by

$$\vec{J} = \vec{J}_P = \frac{\partial \vec{P}}{\partial t}. \tag{A.2c}$$

Due to Eqs. (A.2a) and (A.2c) Maxwell's equations take the form

$$\begin{cases} \vec{\nabla} \cdot \vec{\mathcal{E}} = \rho_b / \epsilon(x, y), \\ \vec{\nabla} \cdot B = 0, \\ \vec{\nabla} \times \vec{\mathcal{E}} = -\frac{\partial \vec{B}}{\partial t}, \\ \vec{\nabla} \times \vec{B} = \mu_0 \vec{J}_p \end{cases} \Rightarrow \begin{cases} \vec{\nabla} \cdot \left(\epsilon_0 \vec{\mathcal{E}} + \vec{P} \right) = 0, \\ \vec{\nabla} \cdot \vec{B} = 0, \\ \vec{\nabla} \times \vec{\mathcal{E}} = -\frac{\partial \vec{B}}{\partial t}, \\ \vec{\nabla} \times \left(\vec{B} / \mu_0 \right) = \frac{\partial}{\partial t} \left(\epsilon_0 \vec{\mathcal{E}} + \vec{P} \right) \end{cases} \tag{A.3}$$

By defining

$$\epsilon_0 \vec{\mathcal{E}} + \vec{P} \equiv \vec{D}, \quad \text{and} \quad \vec{B} / \mu_0 \equiv \vec{H} \tag{A.4}$$

Eq. (A.3) can be written in the form

$$\begin{aligned} \vec{\nabla} \cdot \vec{D} &= 0, \\ \vec{\nabla} \cdot \vec{B} &= 0, \\ \vec{\nabla} \times \vec{\mathcal{E}} &= -\frac{\partial \vec{B}}{\partial t}, \\ \vec{\nabla} \times \vec{H} &= \frac{\partial \vec{D}}{\partial t}. \end{aligned} \tag{A.5}$$

A.2 Wave equation inside a medium

Now we prove the wave equation inside a material. In order to do this we will use Eq. (A.5), but with an important difference. We assume that the material's dielectric constant vary in x and y direction, but it is constant on the z direction where light propagates. This requires

$$\epsilon_0 \to \epsilon = \epsilon(x, y). \tag{A.6}$$

We should also change the magnetic permeability of free space, with the magnetic permeability inside a medium. But experiments suggests that permeability stays almost intact, so we will keep the magnetic permeability of the vacuum. By plugging Eq (A.6) into Eqs. (A.5) we get

$$\vec{\nabla} \cdot \left(\epsilon(x, y) \vec{\mathcal{E}} \right) = 0 \tag{A.7a}$$

$$\vec{\nabla}\cdot\vec{B} = 0 \tag{A.7b}$$

$$\vec{\nabla}\times\vec{\mathcal{E}} = -\frac{\partial\vec{B}}{\partial t} \tag{A.7c}$$

$$\vec{\nabla}\times\vec{B} = \mu_0\epsilon(x,y)\frac{\partial\vec{\mathcal{E}}}{\partial t} \tag{A.7d}$$

We take equation (A.7c), and calculating its curl, we get

$$\vec{\nabla}\times\vec{\mathcal{E}} = -\frac{\partial\vec{B}}{\partial t} \Rightarrow \vec{\nabla}\times\left(\vec{\nabla}\times\vec{\mathcal{E}}\right) = -\frac{\partial}{\partial t}\left(\vec{\nabla}\times\vec{B}\right) \Rightarrow \epsilon_{ijk}\partial_i\epsilon_{klm}\partial_l\mathcal{E}_m = -\mu_0\epsilon(x,y)\frac{\partial^2\vec{\mathcal{E}}}{\partial t^2} \Rightarrow$$

$$\Rightarrow \epsilon_{ijk}\epsilon_{klm}\partial_i\partial_l\mathcal{E}_m = -\mu_0\epsilon(x,y)\frac{\partial^2\vec{\mathcal{E}}}{\partial t^2} \Rightarrow \left(\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl}\right)\partial_j\partial_l\mathcal{E}_m = \mu_0\epsilon(x,y)\frac{\partial^2\vec{\mathcal{E}}}{\partial t^2} \Rightarrow$$

$$\Rightarrow \vec{\nabla}\left(\vec{\nabla}\cdot\vec{\mathcal{E}}\right) - \vec{\nabla}^2\vec{\mathcal{E}} = -\mu_0\epsilon(x,y)\frac{\partial^2\vec{\mathcal{E}}}{\partial t^2} \tag{A.8}$$

Since we assume that we have no charge in the waveguide, we get

$$\vec{\nabla}\left(\epsilon(x,y)\cdot\vec{\mathcal{E}}\right) = \vec{\nabla}\epsilon(x,y)\cdot\vec{\mathcal{E}} + \epsilon(x,y)\vec{\nabla}\vec{\mathcal{E}} = 0 \Rightarrow \vec{\nabla}\cdot\vec{\mathcal{E}} = -\vec{\mathcal{E}}\frac{\vec{\nabla}\cdot\epsilon(\S,\dagger)}{\epsilon(x,y)}$$

By using this equation and substituting into Eq. (A.8), we get the final form of wave equation in matter, which is

$$\vec{\nabla}^2\vec{\mathcal{E}} - \mu_0\epsilon(x,y)\frac{\partial^2\vec{\mathcal{E}}}{\partial t^2} + \vec{\nabla}\left(\vec{\mathcal{E}}\frac{\vec{\nabla}\epsilon(x,y)}{\epsilon(x,y}\right) = 0 \tag{A.9}$$

A.3 Paraxial equation inside medium

In this section we will use the wave equation inside a medium, that is Eq. (A.9), in order to prove paraxial equation which describes the propagation of a beam of light inside a medium. We will assume that we have a waveguide, that is a medium with constant properties on the z direction but varying dielectric constant on the x and y direction, so that Eq. (A.9) is satisfied.

Firstly we assume weakly guiding approximation which is expressed by

$$\vec{\nabla}\left(\vec{\mathcal{E}}\cdot\frac{\vec{\nabla}\epsilon(x,y)}{\epsilon(x,y)}\right) \approx 0 \tag{A.10}$$

SAY ONE OR TWO THINGS ABOUT THIS EQUATION. Using Eq. (A.10) on Eq. (A.9), we get

$$\vec{\nabla}^2\vec{\mathcal{E}} - \mu_0\epsilon(x,y)\frac{\partial^2\vec{\mathcal{E}}}{\partial t^2}. \tag{A.11}$$

We assume, as we descussed previously on this appendix, propagation on the z axis. This means that the electric field will have the form,

$$\vec{\mathcal{E}} = \hat{k}\Phi(x,y,z)e^{i(kz-\omega t)} \tag{A.12}$$

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Phi(x,y,z)e^{i(kz-\omega t)} + \frac{\partial^2\Phi}{\partial z^2} + 2ik\frac{\partial\Phi}{\partial z}e^{i(kz-\omega t)}$$
$$-k^2\Phi(x,y,z)e^{i(kz-\omega t)} + \frac{n^2(x,y)}{c^2}\omega^2\Phi(x,y,z)e^{i(kz-\omega t)} = 0$$

$$\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} + 2ik\frac{\partial\Phi}{\partial z} + k_0^2\left((n^+(x,y))^2 - n^2(x,y)\right)$$

$$i\frac{\partial\Phi}{\partial z} + \frac{1}{2k}\left(\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2}\right) + k_0 V(x,y,z)$$

Appendix B

Second quantization

Second quantization is called the fact that wave like phenomena, for example electric field in an interaction with an atom, behave like particles. It is not a "new" quantization, but more like a new way to think about wave phenomena in quantum mechanics. An example of second quantization is the description of the momentum of the particles which can be described by a momentum wave function in an atomic description which is called Fock space. Fock space obeys the same algebra as the Harmonic oscillator[1]. A general state in Fock space is written as

$$|n_1, n_2, \cdots\rangle = \prod_{i=1} \frac{(a^\dagger_{p_i})^{n_i}}{\sqrt{(n_i)!}} |\{0\}\rangle. \tag{B.1}$$

Also using the formalism of second quantization, we can write local operators that create or annihilate particles at a certain position $\vec{r}$. In order to construct these operator we use a linear combination of all momentum eigenstates. We work in the case where momentum is discrete, since in a periodic lattice, the eigenvalues of momentum are always discrete. We claim that these states have the form,

$$\psi(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{i\vec{p}\vec{r}} a_{\vec{p}}, \quad \psi(\vec{r})^\dagger = \frac{1}{V} e^{-i\vec{p}\vec{r}} a^\dagger_{\vec{p}}, \tag{B.2}$$

where the first annihilates a particle which is at position $\vec{r}$, and the second creates a particle at position $\vec{r}$. We prove that claim below by acting with state $\langle \vec{r}'|$ from the write to infer the probability amplitude to be at any point in space. Suppose that you act with $\psi(\vec{r})^\dagger$ on the vacuum. Then you create a state which we define as $|\psi\rangle$

$$|\psi\rangle = \psi^\dagger(\vec{r})\,|0\rangle = \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{-i\vec{p}\vec{r}} a^\dagger_{\vec{p}} |0\rangle$$

We claim that the state above has created a particle at position $\vec{r}$. We act with state $\langle \vec{r}'$ to get the probability amplitude of being at position $\vec{r}'$. This probability amplitude is given by

$$\langle \vec{r}'|\psi^\dagger(\vec{r})|0\rangle = \frac{1}{\sqrt{V}} \langle \vec{r}'|\,|\sum_{\vec{p}} e^{-i\vec{p}\vec{r}'} a_{\vec{p}^\dagger}\,|0\rangle = \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{-i\vec{p}\vec{r}'}\,\langle \vec{r}|\vec{p}\rangle \tag{B.3a}$$

---

[1] For example suppose that we can only have a system with three different momenta: p_1, p_2, p_3. Then, the state $|1,0,0\rangle = a^\dagger_{p_1}|0\rangle$ in Fock space describes just one particle with momentum p_1, and nothing else. The state $|1,1,0\rangle = a^\dagger_{p_1}a^\dagger_{p_2}|0\rangle$ represents a Fock state with two particles, one with momentum p_1, and one with momentum p_2, and finally the state $|2,1,1\rangle = 1/\sqrt{2}\ (a^\dagger_{p_1})^2 a^\dagger_{p_2} a^\dagger_{p_3}|0\rangle$ has 4 particles in total, two with momenta p_1, one with p_2, and one with p_3. We see that in order to describe it we use the harmonic oscillator formalism, where $a^\dagger$ creates a particle with a certain momentum, and a annihilates a particle with a certain momentum, just like a and $a^\dagger$ create and annihilate particles

And since we know,

$$\langle \vec{r} | \vec{p} \rangle = \frac{1}{\sqrt{V}} e^{i\vec{p}\vec{r}}, \tag{B.3b}$$

we can substitute Eq. (B.3b) in Eq. (B.3a) and we get

$$\langle \vec{r}' | \psi \rangle = \frac{1}{V} \sum_{\vec{p}} e^{i\vec{p}(\vec{r}-\vec{r}')} \Rightarrow$$

$$\Rightarrow \langle \vec{r}' | \psi \rangle = \delta(\vec{r} - \vec{r}'), \tag{B.3c}$$

where the last equation comes from the identity,

$$\frac{1}{V} \sum_{\vec{p}} e^{i\vec{p}\vec{r}} = \delta(\vec{r}). \tag{B.3d}$$

The reason Eq. (B.3d) is satisfied is easy to understood in the continuous case, since then you have the definition of δ function in the form of the integral of the exponential. In the discrete case, the reason Eq. (B.3d) applies is because in the case where $\vec{r} \neq \vec{r}'$, we have the sum of roots of the unity which are zero. Remember that in discrete case the position vector $\vec{r}$ is also discrete. And in the case of $\vec{r} = \vec{r}'$, the exponential is equal to one for any momentum, and since we have infinitely many momentum states, the expression is infinite in this case, which is the definition of δ function.

The probability amplitude of being at any point in space given by Eq. (B.3c). It is zero at every point with the exception of $\vec{r}' = \vec{r}$. Then the probability is one, so we have showed that Eq. (B.2) creates a particle in position $\vec{r}$.

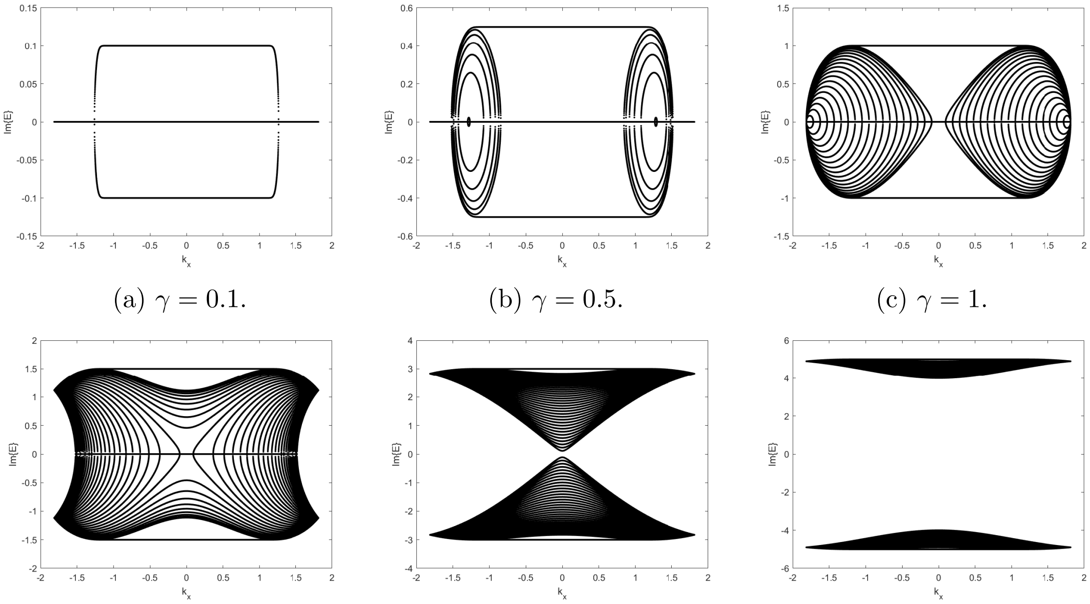
The second thing we need to show is that in that case there is one and only one electron in that point in space. In order to show that we act with the number operator which as we said has the same form as the harmonic oscillator number operator.

Appendix C

Supplementary figures

In this appendix, we will give the figures that do not fit in the thesis, and furthermore, because they are not crucial for describing the solution of the Hamiltonian for particular problems. The main reason of this appendix is to make the thesis more elegant, so that we do not have a lot of figures together.

C.1 Bearded edge Imaginary part of the solution of the energies

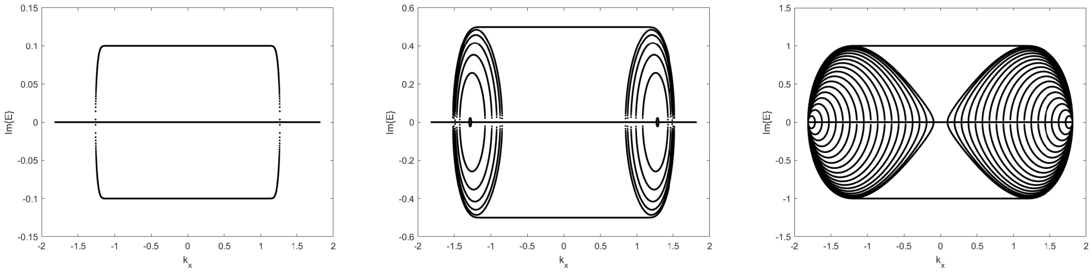


(a) $\gamma = 0.1$. (b) $\gamma = 0.5$. (c) $\gamma = 1$.

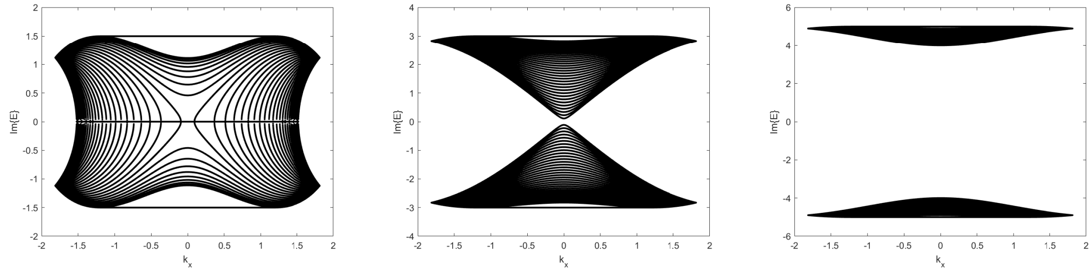
(d) $\gamma = 1.5$. (e) $\gamma = 3$. (f) $\gamma = 5$.

Figure C.1: Energy momentum bands for different number of unit cells for value $a = 1$ and $t = t_1 = t_2 = t_3 = 1$. The k_x axis starts from value $-\pi/\sqrt{3}$ and ends at $\pi/\sqrt{3}$.

C.2 Bearded armchair edge Imaginary part of the energy eigenstates



(a) $\gamma = 0.1$. (b) $\gamma = 0.5$. (c) $\gamma = 1$.



(d) $\gamma = 1.5$. (e) $\gamma = 3$. (f) $\gamma = 5$.

Figure C.2: Energy momentum bands for different number of unit cells for value $a = 1$ and $t = t_1 = t_2 = t_3 = 1$. The k_x axis starts from value $-\pi/\sqrt{3}$ and ends at $\pi/\sqrt{3}$.

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