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Relativistic Fermions in Graphene

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Submission date: December 2012
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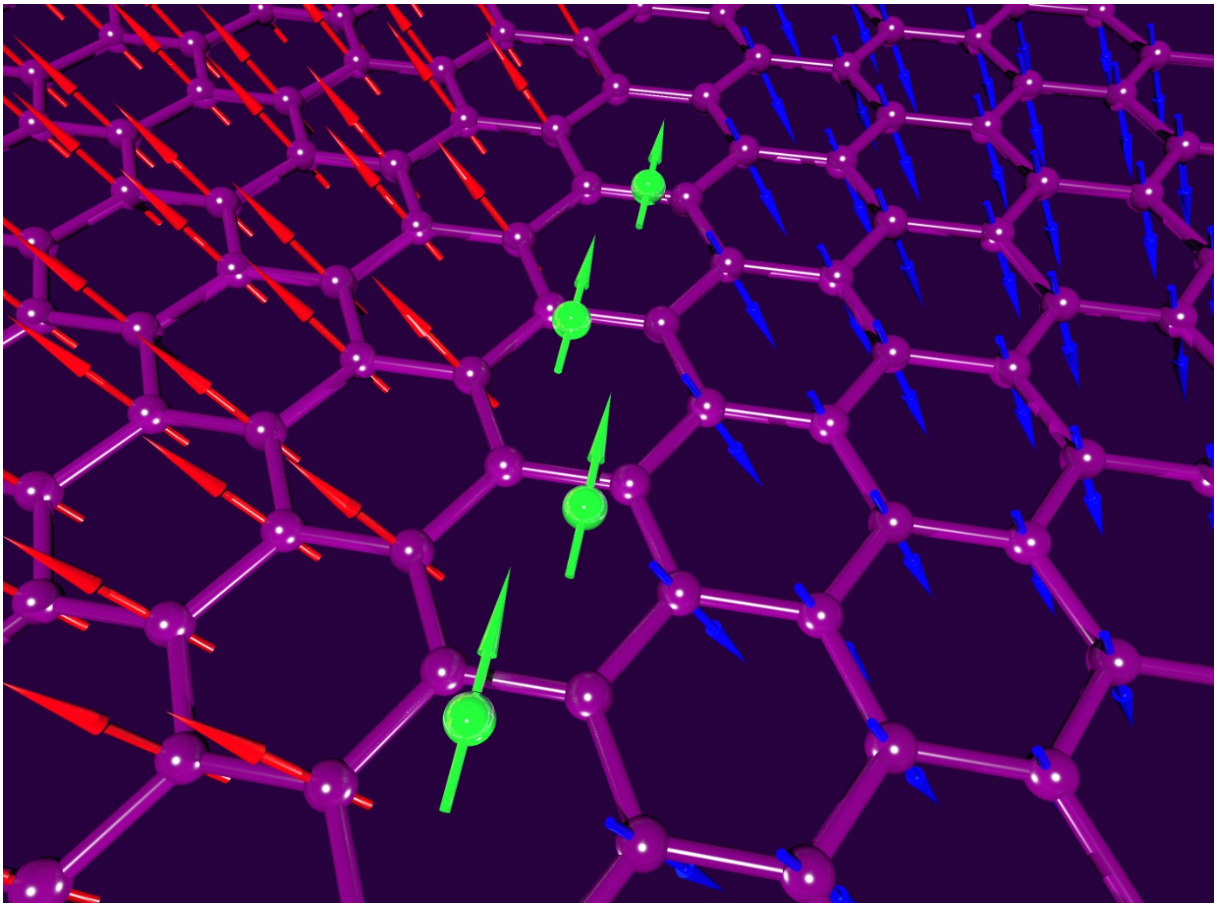
Desember 2012

Abstract:

The Fermi surface of graphene contains points where the connection between excitation energy and crystal momentum is linear, similar to massless or ultrarelativistic fermions. This is important for the physical properties of this material. In this thesis we have combined a study the theoretical and experimental literature with our own calculations of the excitation spectra of monolayer, bilayer and multilayer graphene.

Graphene



Acknowledgements:

I would like to thank my supervisor Kåre Olaussen for his guidance during the work with this master thesis and for many interesting discussions about the thesis and many topics in physics. I also thank him for his patience with my work through several different circumstances; I will cherish the fond memories working with an intelligent and charismatic person.

I would also like to thank my Parents; my father for showing me the beauty of science and the laws of nature and my mother for showing me the importance of education and hard work. I thank my parents generally for supporting me unconditionally my whole life and providing me, my brother and sister with all we needed.

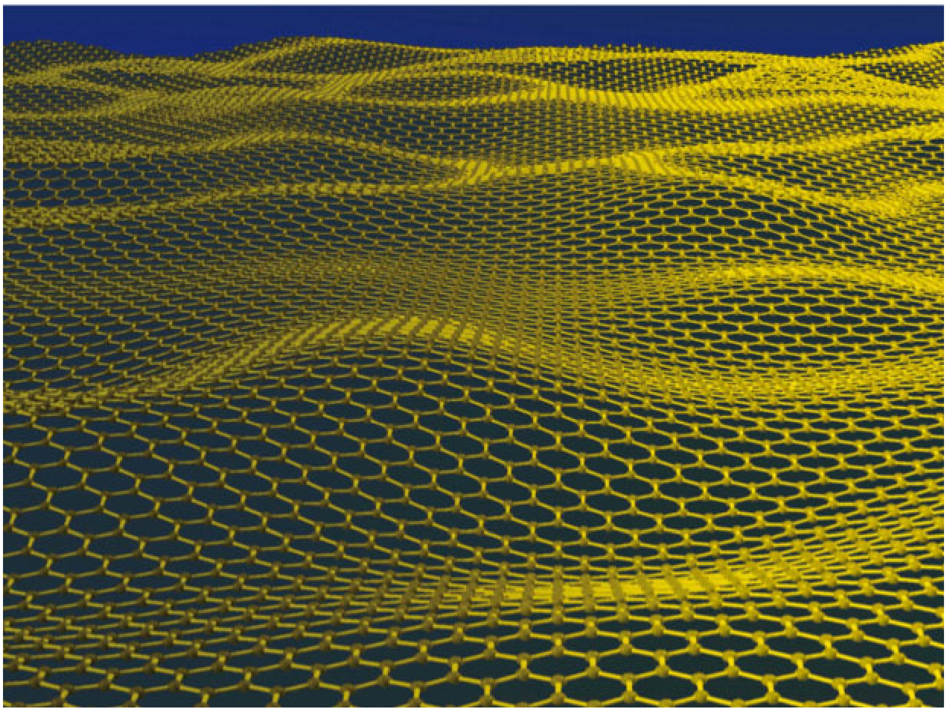
Contents

Introduction

Graphene is the basic structural element of some carbon allotropes including graphite, charcoal, carbon nano-tubes and fullerenes; it is a two dimensional collection of carbon atoms with thickness of only one atom, with each six atoms forming the hexagonal shape, a plane of atoms forms a sheet that looks like a honey comb.

Graphene has unique properties; a thin graphene sheet has high strength; about 200 times stronger than Steele, flexibility and highest electrical conductivity of all materials in room temperature, it has opened new fields of research on it both theoretically and also application in high technology and could be very useful several different technological aspects in the future **[1]**.

The 2010 Nobel Prize in physics was awarded for works on graphene to Andre Geim and Konstantin Novoselov for their pioneering research on graphene. The theory behind graphene was first studied by the theoretical physicist Philip Russell Wallace and published a pioneering paper in 1947 on the band structure of graphite **[2]**.



. *Figure (0): example 1 of a Graphene sheet*

Electrons can move with a very high speed through graphene sheets, which leads to relativistic description of their dynamics, their behavior is described by the two-dimensional Dirac equation and it might be possible to do high-energetic particle experiments on a graphene sheet because of their very little resistance, the electrons lose very little energy moving through the material and it makes graphene applicable for electronics on nano-scales and also among many other applications, graphene could be used for making very small transistors and replace silicon transistors, making high-power high frequency electronic devises, it might be possible to build circuits that are smaller and faster than what one can build in silicon.

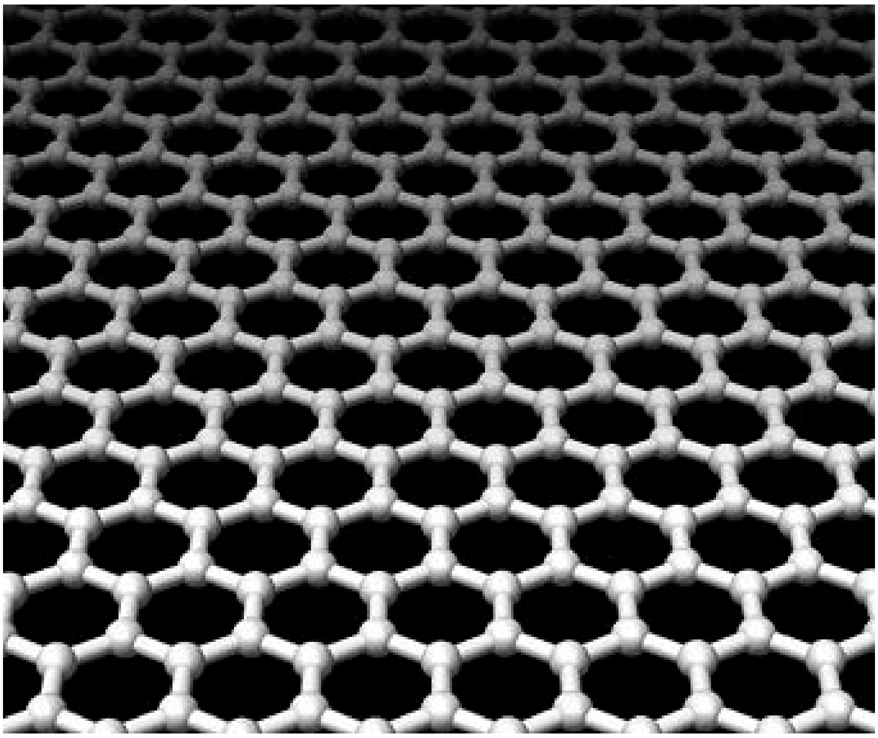


Figure (1): Example 2 of a graphene sheet

The Manchester team in 2008 created a 1-nanometer graphene transistor, only one atom thick and 10 atoms across. This is not only smaller than the smallest possible silicon transistor; Novoselov claimed that it could very well represent the absolute physical limit of Moore’s Law governing the shrinking size and growing speed of computer processors(Kaku, 2010).

Nobel Prize winner Andre Geim said in *New Scientist*. “Graphene is stronger and stiffer than diamond, yet can be stretched by a quarter of its length, like rubber. Its surface area is the largest known for its weight. ». The experimental results of the quantum Hall Effect in graphene are very interesting, such as higher values of measurements, measurements that can be observed in room temperature whereas in most materials it could only be observed in low temperature and finally there have been observations of the fractional quantum Hall conductivity.

Part I: the Physics and Mathematics behind the work on Graphene:

1. Mathematics

In this chapter we develop the mathematics needed for the project, we do so very quickly and write only the necessary tools we need and keep the details to a minimum, however some mathematics is needed to work with this project.

1.1 Eigenvalue equations:

When a random vector u in a vector space is multiplied by a square matrix A; the result generally gives a new vector v:

$$\mathrm{Au} = \mathrm{v} \tag{1}$$

Let us take an example; the matrix R defined as:

$$\mathrm{R} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{2}$$

When the matrix R acts on a random vector $\mathrm{r} = \begin{pmatrix} \mathrm{x} \\ \mathrm{y} \end{pmatrix}$ in the two dimensional space, it gives a new vector which is equal to the original vector rotated by 90 degrees:

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \mathrm{x} \\ \mathrm{y} \end{pmatrix} = \begin{pmatrix} -\mathrm{y} \\ \mathrm{x} \end{pmatrix} \tag{3}$$

Generally a matrix multiplied by a vector is an operation; a matrix is an **operator** when acted on some vector u gives a new vector v as previously mentioned. However there are a set of vectors $\mathrm{x_n}$ in the vector space under study that when the matrix A is operated on them, it gives back the vectors themselves, the only difference the new vector has from the original vector is a multiplication scalar λ_n :

$$\mathrm{Ax_n} = \lambda_\mathrm{n} \mathrm{x_n} \tag{4}$$

$$\left(\mathrm{A} - \lambda_\mathrm{n} \mathrm{I}\right)\mathrm{x_n} = 0 \tag{5}$$

The non-trivial solution where $\mathrm{x_n} \neq 0$; requires that:

$$\det\left(\mathrm{A} - \lambda_\mathrm{n} \mathrm{I}\right) = 0 \tag{6}$$

The set of vectors $\mathrm{x_n}$ that have this property are called the **eigenvectors** of the operator (matrix) A and the multiplication scalars λ_n are called the **eigenvalues** of A. If each eigenvalue λ_n has only one eigenvector $\mathrm{x_n}$ corresponding to it (or getting the eigenvalues when acted on by the operator A); then we call the system **non-degenerate**. If the eigenvalues λ_n of the system have more than one eigenvector $\mathrm{x_n}, \tilde{\mathrm{x}}_\mathrm{n}, ..., \mathrm{etc.}$ corresponding to it; then the system is called **degenerate** **[3]**. .

1.2 Basis vectors:

Let W be a vector space of dimension N over a Field F (real numbers, complex numbers etc.; a basis $U=\{\vec{u}_1,\vec{u}_2,.....,\vec{u}_N\}$ for W is a set of vectors with the following properties:

1-If we have the following equation:

$$\sum_{n=1}^{N} a_n\vec{u}_n = 0 \tag{7}$$

The coefficients $a_n \in F$, they are simply scalar multiplications; then it requires that:

$$a_1 = a_2 = ... = a_N = 0 \tag{8}$$

The above equation simply means that the vectors $\vec{u}_n$ are independent; that each vector cannot be expressed as linear combination of the others [4]. .

2- For every vector $\vec{V} \in W$; we can express it in terms of a linear combination of the basis vectors:

$$\vec{V} = \sum_{n}^{N} c_n\vec{u}_n \tag{9}$$

Where in the above equation; $c_1, c_2, ..., c_N \in F$.

An **Orthonormal** basis $E=\{\vec{e}_1,\vec{e}_2,.....,\vec{e}_N\}$ for W is a basis vector that has the following extra properties; the scalar multiplication between two vectors in E:

$$\vec{e}_n \bullet \vec{e}_m = \delta_{mn} \tag{10}$$

Where in the above equation; the symbol δ_{mn} is called the kronecker delta; it is zero if $m \neq n$ and 1 if $m = n$. In this case every vector $\vec{V} \in W$ can be expressed in the following way:

$$\vec{V} = \sum_{n=1}^{N} \left(\vec{V} \bullet \vec{e}_n\right)\vec{e}_n \tag{11}$$

The inner products

$$\vec{V} \bullet \vec{e}_n \tag{12}$$

Each one of them is the **projection** of $\vec{V}$ onto the basis vector $\vec{e}_n$; so the sum of all projections gives you the vector $\vec{V}$ in that space.

For example in Cartesian coordinates, the three dimension real space has a basis $X=\{\hat{x},\hat{y},\hat{z}\}$, we can write the vector potential $\vec{A}$ from Electromagnetic theory in terms of the basis X :

$$\begin{aligned}&\vec{A}=\left(\vec{A}\bullet\hat{x}\right)\hat{x}+\left(\vec{A}\bullet\hat{y}\right)\hat{y}+\left(\vec{A}\bullet\hat{z}\right)\hat{z}\\&\equiv A_x\hat{x}+A_y\hat{y}+A_z\hat{z}\\&\equiv\left(A_x,A_y,A_z\right)\end{aligned}\qquad\textbf{(13)}$$

1.3 The space of functions:

There are similar notions for the eigenvalue equations in the continuous case, for example in the real space an operator depending on x; L(x) can have the following equation:

$$L(x)g_\lambda(x)=\lambda g_\lambda(x)\qquad\textbf{(14)}$$

Where λ in the above equation is the eigenvalue for the operator $L(x)$ in this continues real space. The momentum operator in real space has the eigenvalue equation:

$$\hat{p}g_p(x)=-i\hbar\frac{d}{dx}g_p(x)=pg_p(x)\qquad\textbf{(15)}$$

The above equation has a simple normalized solution which is the exponential function:

$$g_p(x)=\frac{1}{\sqrt{2\pi\hbar}}e^{i\frac{p}{\hbar}x}\qquad\textbf{(16)}$$

The factor $1/\sqrt{2\pi\hbar}$ is just a normalization factor. The inner product for the continuous case is between two functions for example between a random function $f(x)$ and the eigenfunction $g_p(x)$ equal to:

$$g_p(x)\bullet f(x)\equiv\left(g_p(x),f(x)\right)=\int_{-\infty}^{\infty}g_p(x)^*f(x)dx\qquad\textbf{(17)}$$

But the above equation is known for us as the Fourier transform of

$$\left(g_p(x),f(x)\right)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{-i\frac{p}{\hbar}x}f(x)dx\equiv\tilde{f}(p)\qquad\textbf{(18)}$$

In analogy to equation**(9)**; every function $f(x)$ can be expressed as a continuous superposition of the set of eigenfunctions $g_p(x)$ if they satisfy certain conditions, the space one is working with must satisfy certain conditions itself; a very important notion; **completeness**; a space(metric space) M is complete if and only if every **Cauchy sequence** (which is a sequence x_n with distance between two elements;

$\left|x_n - x_m\right|$ converges as n and m become large) converges to a point in the space M. Intuitively this means that we have enough points in the space and not “missing” any, that we have enough limits to use the techniques of calculus. Examples of complete spaces are $\mathbb{R}$ and $\mathbb{C}$.We will stop here and continue with our work as it is not the subject of interest in this project.

A set of functions $\left\{g_p(x)\right\}$ must be complete in order to write every function as a super position of them. In the case of the momentum operator $g_p(x) = \frac{1}{\sqrt{2\pi}} e^{i\frac{p}{\hbar}x}$; they are complete and we have:

$$f(x) = \int_{-\infty}^{\infty} \left(g_p(x).f(x)\right) g_p(x) dp \tag{19}$$

Writing it explicitly:

$$f(x) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \tilde{f}(p) e^{i\frac{p}{\hbar}x} dp \tag{20}$$

What about the operator for position? Do we have a set of eigenfunctions and what are they? Well; $\hat{x}$ operating a function is just multiplication by the function “x” itself; so the eigenvalue equation is as following:

$$\hat{x} g_y(x) = x g_y(x) = y g_y(x) \tag{21}$$

In the above equation; we have “y” as the continuous eigenvalues of $\hat{x}$. Rearranging the above equation; we have:

$$\left(x - y\right) g_y(x) = 0 \tag{22}$$

In order to satisfy the above equation; the function $g_y(x)$ must be zero everywhere with one exception; it can be non-zero when $x = y$. The “function” that satisfies this condition is the well-known Dirac delta function among physicists [5], [6]. We have:

$$g_y(x) = \delta\left(x - y\right) \tag{23}$$

1.4 Hilbert space:

The Hilbert space is a generalization of the notion of vector space into functions, could be complex or real. Vectors in this space are abstract and could be written any basis of interest, not only in the position space. Hilbert space is a generalization of Euclidean space; the vector algebra and calculus are generalized from Euclidean 2 and three dimensions to any number of dimensions finite of infinite. It is an abstract vector space with some properties; more mathematically put; Hilbert space is complex (or real) inner product space which is complete metric space with respect to the distance induced by the inner product. In this project we use Dirac's notation as it is more practical for a physicist to work with.

The general theory of Hilbert space could be found in several mathematics literature books. A vector in Dirac's notation represented by a **Ket** vector $\left|V\right\rangle$ which is an abstract vector in Hilbert space; for every ket vector $\left|V\right\rangle$ there is **Bra** vector $\left\langle V\right|$ which the hermitian conjugate is of $\left|V\right\rangle$:

$$\left(\left|V\right\rangle\right)^{\dagger} = \left\langle V\right| \tag{24}$$

The hermitian conjugate of a superposition of two ket vectors each multiplied by scalars is:

$$\left(\alpha\left|V\right\rangle + \beta\left|W\right\rangle\right)^{\dagger} = \left\langle V\right|\alpha^{*} + \left\langle W\right|\beta^{*} \tag{25}$$

In the above equation; α^{*} and β^{*} are simply the complex conjugate of the scalars α and β .

If an operator $\hat{O}$ is acting on the ket vector $\left|V\right\rangle$ then the hermitian conjugate of the product is:

$$\left(\hat{O}\left|V\right\rangle\right)^{\dagger} = \left\langle V\right|\hat{O}^{\dagger} \tag{26}$$

If the operator $\hat{O}$ is hermitian; then it is equal to its hermitian conjugate:

$$\hat{O} = \hat{O}^{\dagger} \tag{27}$$

Finally the inner product in this space between two vectors $\left|V\right\rangle$ and $\left|W\right\rangle$ is multiplying the bra vector of the one by the ket vector of the other:

$$\left(\left|V\right\rangle, \left|W\right\rangle\right) = \left\langle V\right|\left|W\right\rangle \equiv \left\langle V\middle|W\right\rangle = \left(\left\langle W\middle|V\right\rangle\right)^{*} \tag{28}$$

In the above equation; we have the last equality because the product could be complex and we already know the when you change the order of multiplication in the inner product vectors; you get the complex conjugate. If $\left|V\right\rangle = \left|W\right\rangle$; then in similarity to usual vectors equation (28) becomes the length of the vector squared:

$$\left\langle V\middle|V\right\rangle = \left\|\left|V\right\rangle\right\|^{2} \tag{29}$$

Also if a vector $\left|\mathrm{C}\right\rangle$ that we get by operating some operator $\hat{\mathrm{P}}$ on a vector $\left|\mathrm{B}\right\rangle$; then the inner product between $\left|\mathrm{A}\right\rangle$ and $\left|\mathrm{C}\right\rangle$ is:

$$\left\langle \mathrm{A} \middle| \mathrm{C} \right\rangle = \left\langle \mathrm{A} \middle| \hat{\mathrm{P}} \middle| \mathrm{B} \right\rangle \tag{30}$$

We have the following equality:

$$\left\langle \mathrm{A} \middle| \hat{\mathrm{P}} \middle| \mathrm{B} \right\rangle = \left(\left\langle \mathrm{B} \middle| \hat{\mathrm{P}}^{\dagger} \middle| \mathrm{A} \right\rangle \right)^{\dagger} \tag{31}$$

The above equation is just the rule for the hermitian conjugate of product of several terms.

The eigenvalue equation in Hilbert space for an operator $\hat{\mathrm{A}}$ with a set of abstract eigenvectors $\left\{\left|\mathrm{A}\right\rangle\right\}$ and eigenvalues A which can be discrete but also can be continuous also is:

$$\hat{\mathrm{A}}\left|\mathrm{A}\right\rangle = \lambda\left|\mathrm{A}\right\rangle \tag{32}$$

It makes easier to see the operators, eigenvalues and eigenvectors of an eigenvalue equation because we can use the same letter more than once. The reason we can use the same letter is because there is no confusion that $\left|\mathrm{A}\right\rangle$ is a vector, not a number, $\hat{\mathrm{A}}$ is the operator and we call the "numbers" or the eigenvalues λ simply for A as well. For example the eigenvalue equation for the momentum operator $\hat{\mathrm{p}}$ in this notation is:

$$\hat{\mathrm{p}}\left|\mathrm{p}\right\rangle = \mathrm{p}\left|\mathrm{p}\right\rangle \tag{33}$$

But of course we can call the eigenvalues anything we want as long as we it is correct mathematically.

Finally if an operator $\hat{\mathrm{L}}$ is Hermitian ($\hat{\mathrm{L}}^{\dagger} = \hat{\mathrm{L}}$); then its eigenvalues are real; let us prove it: If we $\hat{\mathrm{L}}$ have the set of eigenvectors $\mathrm{L} = \left\{\left|\mathrm{L}_{\mathrm{n}}\right\rangle\right\}$ and eigenvalues L_{n}, we have:

$$\hat{\mathrm{L}}\left|\mathrm{L}_{\mathrm{n}}\right\rangle = \mathrm{L}_{\mathrm{n}}\left|\mathrm{L}_{\mathrm{n}}\right\rangle \tag{34}$$

Multiplying the above equation from left by bra eigenvector $\left\langle\mathrm{L}_{\mathrm{n}}\right|$ from the set L; we have:

$$\left\langle \mathrm{L}_{\mathrm{n}} \middle| \hat{\mathrm{L}} \middle| \mathrm{L}_{\mathrm{n}} \right\rangle = \mathrm{L}_{\mathrm{n}} \left\langle \mathrm{L}_{\mathrm{n}} \middle| \mathrm{L}_{\mathrm{n}} \right\rangle \tag{35}$$

Using equation**(31)**; we have:

$$\left\langle \mathrm{L}_{\mathrm{n}} \middle| \hat{\mathrm{L}} \middle| \mathrm{L}_{\mathrm{n}} \right\rangle = \left(\left\langle \mathrm{L}_{\mathrm{n}} \middle| \hat{\mathrm{L}}^{\dagger} \middle| \mathrm{L}_{\mathrm{n}} \right\rangle \right)^{\dagger} \tag{36}$$

But we know that $\hat{L}$ is hermitian; so we get:

$$\begin{aligned}&L_n\langle L_n|L_n\rangle=\langle L_n|\hat{L}|L_n\rangle=\left(\langle L_n|\hat{L}^{\dagger}|L_n\rangle\right)^{\dagger}\\&=\left(\langle L_n|\hat{L}|L_n\rangle\right)^{\dagger}=\left(L_n\langle L_n|L_n\rangle\right)^{\dagger}=L^{*}\langle L_n|L_n\rangle\end{aligned} \tag{37}$$

This means that the eigenvalues L_n are equal to their complex conjugate:

$$L_n=L_n^{*} \tag{38}$$

And this of course means that the eigenvalues L_n are real.

In similarity to equation**(12)**; we can find the projection of an abstract vector $|f\rangle$ in Hilbert space onto any desired basis; for example the eigenvalue equation for the position operator in Hilbert space is:

$$\hat{x}|x\rangle=y|x\rangle \tag{39}$$

So the vectors $|x\rangle$ are the eigenvectors of the position operator $\hat{x}$ and y are the eigenvalues of it. The projection of the abstract vector $|f\rangle$ onto an eigenvector for position in similarity with equation**(12)** is:

$$\langle x|f\rangle=f(x) \tag{40}$$

The function $f(x)$ is the projection of its abstract vector $|f\rangle$ in Hilbert space **[5]**, **[6]**. The projection of the eigenvector $|x\rangle$ itself on a particular eigenvector $|y\rangle$ in the same basis is the eigenvector function we found in equation **(23)**:

$$\langle y|x\rangle=g_y(x)=\delta(x-y) \tag{41}$$

The Schrödinger equation in abstract Hilbert space it is:

$$\hat{H}|\psi\rangle=E|\psi\rangle \tag{42}$$

In similarity with equation **(11)**; if a set of vectors $N=\{|n\rangle\}$ are an orthonormal basis; then we can write the abstract vector $|\psi\rangle$ as a superposition of the vectors:

$$|\psi\rangle=\sum_n|n\rangle\langle n|\psi\rangle \tag{43}$$

We can do similar thing for the Hamiltonian; then Schrödinger's equation in this basis becomes:

$$\hat{H}|\psi\rangle=\sum_n\hat{H}|n\rangle\langle n|\psi\rangle=\sum_n E|n\rangle\langle n|\psi\rangle \tag{44}$$

If we multiply the equation **(44)** by a vector $\langle m|$ that belongs to the same basis; we get:

$$\langle m|\hat{H}|\psi\rangle = \sum_n \langle m|\hat{H}|n\rangle\langle n|\psi\rangle = E\sum_n \langle m|n\rangle\langle n|\psi\rangle \tag{45}$$

The inner products $\langle m|n\rangle$ equal to kronecker delta δ_{mn} for an orthonormal basis N; then the product on the right hand of the above equations $\delta_{mn}\langle n|\psi\rangle = \langle m|\psi\rangle = \psi_m$. The symbol ψ_m is simply the projection of $|\psi\rangle$ onto $|m\rangle$ in the basis. Finally the projection of an operator $\hat{H}$ on vectors in a basis is the multiplication by basis vectors on both sides (operators are matrices in a basis, look at equation section (1.1), eigenvalue equation); we have $\langle m|\hat{H}|n\rangle = \hat{H}_{mn}$. The operator $\hat{H}_{mn}$ is the projection of $\hat{H}$ onto the vectors $|n\rangle$ and $|m\rangle$ in the basis N. The Schrödinger's equation then is:

$$\sum_n \hat{H}_{mn}\psi_n = E\psi_m \tag{46}$$

The above equation is a matrix equation:

$$\begin{pmatrix} H_{11} & H_{12} & . & . \\ H_{21} & . & & \\ . & & . & \\ . & & & . \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ . \\ . \end{pmatrix} = E\begin{pmatrix} \psi_1 \\ \psi_2 \\ . \\ . \end{pmatrix} \tag{47}$$

We have a very similar equation to **(46)** for the continuous case, only instead of a sum; we have an integral. For example the abstract vector $|\psi\rangle$ in position basis is:

$$|\psi\rangle = \int dy\,|y\rangle\langle y|\psi\rangle \tag{48}$$

Schrödinger's equation in this basis is:

$$\hat{H}|\psi\rangle = \int dy\hat{H}|y\rangle\langle y|\psi\rangle = E\int dy\,|y\rangle\langle y|\psi\rangle \tag{49}$$

Now we multiply by a particular vector $|x\rangle$ from the same basis; we get:

$$\int dy\,\langle x|\hat{H}|y\rangle\langle y|\psi\rangle = E\int dy\,\langle x|y\rangle\langle y|\psi\rangle \tag{50}$$

The right hand side of the above equation is equal to:

$$E\int dy\,\langle x|y\rangle\langle y|\psi\rangle = E\int dy\delta(y-x)\psi(y) = E\psi(x) \tag{51}$$

The left hand side of equation **(50)** is the well-known Hamiltonian operating on the function in position space:

$$\int dy\,\langle x|\hat{H}|y\rangle\langle y|\psi\rangle = \int dy\hat{H}(x,y)\psi(y) \tag{52}$$

In the above equation; The Hamiltonian $\hat{H}$ is:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{y}) \tag{53}$$

And with the commutation relation between $\hat{x}$ and $\hat{p}$ (look at section (1.5) below for commutation relations):

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = 1 \tag{54}$$

Using equations **(53)** and **(54)**; we have:

$$\langle x|\hat{H}|y\rangle = \hat{H}(x, y) = \left(-\frac{\hbar^2}{2m}\delta''(y-x) + V(y)\delta(y-x) \right) \tag{55}$$

And integration of the projection above gives:

$$\begin{aligned}
&\int dy \langle x|\hat{H}|y\rangle\langle y|\psi\rangle = \int dy\hat{H}(x, y)\psi(y) \\
&\int dy\left(-\frac{\hbar^2}{2m}\delta''(y-x) + V(y)\delta(y-x) \right)\psi(y) \\
&= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \right)\psi(x) = \hat{H}(x)\psi(x)
\end{aligned} \tag{56}$$

Finally the Schrödinger equation in position basis then is:

$$\hat{H}(x)\psi(x) = E\psi(x) \tag{57}$$

We can also project operators on a basis discrete or continuous; the projection of the Hamiltonian on the discrete basis $N = \{|n\rangle\}$ is:

$$\hat{H} = \sum_{n,m} |m\rangle\langle m|\hat{H}|n\rangle\langle n| = \sum_{n,m} \hat{H}_{mn}|m\rangle\langle n| \tag{58}$$

And the projection of the Hamiltonian operator on the continuous position space is:

$$\hat{H} = \int dxdy|x\rangle\langle x|\hat{H}|y\rangle\langle y| \tag{59}$$

Finally let us look at the transformation from one basis to another; let us for example take the transformation from the discrete basis N into the continuous position basis; each vector $|m\rangle \in N$ can be written in the position basis as:

$$|m\rangle = \int dx|y\rangle\langle m|y\rangle \tag{60}$$

We have the following identity:

$$\langle m|y\rangle = \varphi_m(x) \tag{61}$$

The function $\varphi_m(x)$ in position space is of course the projection of $|m\rangle$ onto the eigenvector $|y\rangle$ of position operator. We continue and with the use of equations **(60)** and **(61)** we find transformation of $\langle m|\hat{H}|n\rangle$ into the position space:

$$\begin{aligned}
\langle m|\hat{H}|n\rangle &= \langle m|\left(\int dxdy|x\rangle\langle x|\hat{H}|y\rangle\langle y|\right)|n\rangle \\
&= \int dxdy\langle m|x\rangle\langle x|\hat{H}|y\rangle\langle y|n\rangle \\
&= \int dxdy\varphi_m^*\hat{H}(x,y)\varphi_n(y) \\
&= \int \varphi_m^*(x)\left(\int \hat{H}(x,y)\varphi_n(y)dy\right)dx
\end{aligned} \tag{62}$$

Using equation **(56)** for the last equality of the above equation; we get:

$$\langle m|\hat{H}|n\rangle = \int \varphi_m^*\hat{H}(x)\varphi_n dx \tag{63}$$

And for the eigenvectors themselves:

$$\langle m|n\rangle = \int dx\langle m|x\rangle\langle x|n\rangle = \int dx\varphi_m^*(x)\varphi_n(x) = \delta_{mn} \tag{64}$$

We also have for a general statevector of a physical system:

$$\langle\psi|\psi\rangle = \sum_n \langle\psi|n\rangle\langle n|\psi\rangle = \sum_n \psi_n^*\psi_n = 1 \tag{65}$$

Or in continuous position space:

$$\int dx\langle\psi|x\rangle\langle x|\psi\rangle = \int dx\psi^*(x)\psi(x) = 1 \tag{66}$$

1.5 Commutators and Anticommutators:

The commutator is important in Quantum mechanics as we can determine whether two operators commute with each other and from that we can determine if they have common set of eigenvector or not. The commutator between two operators $\hat{A}$ and $\hat{B}$ written as $\left[\hat{A},\hat{B}\right]$ is defined as:

$$\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A} \tag{67}$$

Generally the commutators are not zero; $\left[\hat{A},\hat{B}\right]\neq 0$. If the commutator between the operators are zero; $\left[\hat{A},\hat{B}\right]=0$, we say the two operators **commute** with each other and they have common eigenvectors **[6]**.

Let us look at the case of non-degenerate eigenvectors; if the operator $\hat{A}$ has the eigenvectors $\left|n\right\rangle$ with the eigenvalues λ_n :

$$\hat{A}\left|n\right\rangle=\lambda_n\left|n\right\rangle \tag{68}$$

Using the commutator for two commuting operators we have:

$$\begin{aligned}&\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}=0\\&\Rightarrow \hat{A}\hat{B}=\hat{B}\hat{A}\end{aligned} \tag{69}$$

So if $\hat{A}$ is acting on a state $\hat{B}\left|n\right\rangle$; we get:

$$\hat{A}\left(\hat{B}\left|n\right\rangle\right)=\hat{A}\hat{B}\left|n\right\rangle=\hat{B}\hat{A}\left|n\right\rangle=\lambda_n\hat{B}\left|n\right\rangle \tag{70}$$

The above equation means that $\hat{B}\left|n\right\rangle$ must also be an eigenvector of $\hat{A}$; mathematically means:

$$\hat{B}\left|n\right\rangle=c_n\left|n\right\rangle \tag{71}$$

In the above equation; the coefficients c_n are scalars. In conclusion; the eigenvectors $\left|n\right\rangle$ are also eigenvectors of the operator $\hat{B}$ if it commutes with $\hat{A}$. This is a theorem about the above result; it also includes degenerate systems and can be proven that is holds the latter case too.

There is also something called the **Anticommutator** written as $\left\{\hat{A},\hat{B}\right\}$ defined as:

$$\left\{\hat{A},\hat{B}\right\}=\hat{A}\hat{B}+\hat{B}\hat{A} \tag{72}$$

Generally the anticommuation is non-zero $\left\{\hat{A},\hat{B}\right\}\neq 0$, but if they are equal to zero; $\left\{\hat{A},\hat{B}\right\}=0$ then we say that the operators **anticommute** each other. The commutation relation is important in physics for example it is used when working with particles with integer spin; Bosons. The anticommmutator is also used in physics for example it is used when working with particles that have half-integer spin; Fermions.

2. Physics

2.1 Quantum Mechanics:

Just as we have in Newtonian mechanics; the three laws of motion or the two postulates of the theory of special relativity; in quantum mechanics there are some postulates that the whole theory is based on, one either can write less number of postulates in a compact way or make a bigger list of postulates by separating some of them into two or more independent postulates to describe Quantum Mechanics, never the less there are set of important postulates that the theory is based on and have to be written [6]:

Postulate 1: For every measurable physical quantity; an observable A there is a linear hermitian operator belongs to it $\hat{A}$

Postulate 2: The state of a physical system is fully described by the complex vector $|\Psi\rangle$ in Hilbert space.

Postulate 3: The time evolution of the system is given by Schrödinger equation;

$$i\hbar\frac{\partial}{\partial t}\left|\Psi\right\rangle = \hat{H}\left|\Psi\right\rangle \quad \textbf{(73)}$$

$\hat{H}$ is the Hamiltonian of the system.

Postulate 4: The expectation value for an observable A is given by

$$\left\langle A\right\rangle = \left\langle \Psi\middle|\hat{A}\middle|\Psi\right\rangle \quad \textbf{(74)}$$

Postulate 5: The possible values of an observable A in a measurement are the eigenvalues A_n of it`s operator with the eigenstates $\left|\psi_n\right\rangle$ and satisfy the equation:

$$\hat{A}\left|\psi_n\right\rangle = A_n\left|\psi_n\right\rangle \quad \textbf{(75)}$$

2.2 Schrödinger equation:

In non-relativistic Quantum Mechanics; the time evolution of a system is given by Schrödinger equation;

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = \hat{H}\left|\Psi(t)\right\rangle \quad \textbf{(76)}$$

Here $\hat{H}$ is the Hamiltonian of the system.

The most important task in quantum mechanics is to find the right Hamiltonian $\hat{H}$. If we know Hamiltonian of the physical system and it is independent of time explicitly; we can solve the eigenvalue equation for the system at a fixed time t_0 (stationary), we can of course choose $t_0 = 0$; the eigenvalue equation is the Time-independent Schrödinger's equation and is given by **[7]**:

$$\hat{H}\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle \tag{77}$$

Where the eigenvalues E_n the possible energy values the system could have. We can choose $\left|\psi_n\right\rangle$ to be an orthonormal set of vectors in Hilbert space i.e. the inner product between two vectors is:

$$\left\langle\psi_n|\psi_m\right\rangle = \delta_{nm} \tag{78}$$

The symbol δ_{nm} in equation **(78)** is the kronecker delta; it is equal to 1 when m and n are equal to each other and 0 if they are different:

$$\delta_{nm} = \begin{cases} 1 if \ \ n = m \\ 0 if \ n \neq m \end{cases} \tag{79}$$

Of course for the non-degenerate case; the states are already orthogonal and we just make the norm equal to one. The stationary solutions of Schrödinger's equation are a complete set; We can write the general solution of the time-dependent Schrödinger equation of the physical system in time as a sum of the stationary solutions:

$$\left|\Psi(t)\right\rangle = \sum_n c_n \left|\psi_n\right\rangle \exp(-\mathrm{i}\ \mathrm{t}E_n / \hbar) \tag{80}$$

Here c_n are complex numbers and equal:

$$c_n = \left\langle\psi_n|\Psi(t)\right\rangle \exp(\mathrm{i}\ \mathrm{t}E_n / \hbar) \tag{81}$$

They are called probability amplitudes because their absolute value squared are interpreted as probabilities (Max Born`s interpretation):

$$\left|c_n\right|^2 = \left|\left\langle\varphi_n|\Psi(t)\right\rangle\right|^2 \tag{82}$$

The number $|c_n|^2$ is the probability to find the system in the eigenstate $\left|\psi_n\right\rangle$ at time t given that it was initially in the state $\Psi(t_0)$ at time t_0. The sum of these probabilities is equal to one:

$$\sum_n \left|c_n\right|^2 = 1 \tag{83}$$

2.3 One electron in a periodic potential:

In this section; we will look at the problem of one electron in a periodic potential, we start with one dimensional case, and then do for two or more dimensions. The one-electron in a periodic potential is very useful and applicable in condensed matter physics, we can apply it to a system of many particles given some approximations; in this one electron theory one looks at material where there are several non-interacting electrons moving in a static and periodic ion-lattice. The one-dimensional Hamiltonian for electron in a periodic potential is:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \tag{84}$$

Where the potential $V(x)$ satisfies the periodicity condition:

$$V(x+a) = V(x) \tag{85}$$

Here a is the period of the lattice, Look at Figure (3) below.

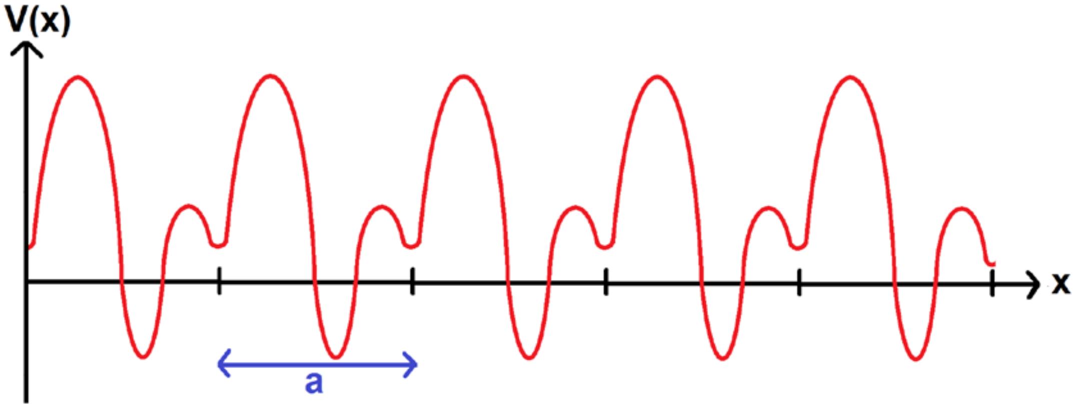


Figure (3); An example of a periodic potential with period a.

The fact that the potential is the same for each one dimensional cell of length a; gives the requirement that all physical properties of the system must be same for each cell; that is if F(x) is some physical property, then we have same properties each time we add the period to F(x); mathematically written:

$$F(x) = F(x+na) \tag{86}$$

Where n in the above equation is an integer.

Now let us be more specific; if we look at the time-independent Schrödinger equation for the periodic potential in equation **(85)**:

$$\hat{H}\psi(x) = E\psi(x) \tag{87}$$

Writing the time independent Schrödinger equation explicitly:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x) \tag{88}$$

The periodicity of the potential requires that the probability density must be the same for each cell; that is **[6]**:

$$\left|\psi(x)\right|^2=\left|\psi(x+a)\right|^2 \tag{89}$$

Equation **(89)** Implies that an eigenvector $\psi(x)$ must have the following form:

$$\psi(x+a)=e^{ika}\psi(x) \tag{90}$$

Or

$$\psi(x+na)=e^{inka}\psi(x) \tag{91}$$

We can derive equation **(91)** in a more formal way using translation operator and Fourier transform of the eigenvector:

We define the following translation operator $\hat{T}_a$ operating on an arbitrary function $G(x)$ and gives **[6]**:

$$\hat{T}_a G(x)=G(x+a) \tag{92}$$

The periodicity of the potential implies that the translation operator defined in equation **(92)** commutes with the Hamiltonian of the electron defined in equation **(84)**; we can easily prove this by direct calculation of the commutator

$$\left[\hat{T}_a,\hat{H}\right]\psi(x)=\left(\hat{T}_a\hat{H}-\hat{H}\hat{T}_a\right)\psi(x) \tag{93}$$

We write the Hamiltonian in terms of the kinetic part and the potential part:

$$\begin{aligned}\left[\hat{T}_a,\hat{H}\right]\psi(x)&=\left[\hat{T}_a,-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)\\&=\left[\hat{T}_a,-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi(x)+\left[\hat{T}_a,V(x)\right]\psi(x)\end{aligned} \tag{94}$$

Let us do each commutator in the last equality of equation **(94)** then sum them together; we start with the kinetic term:

$$\left[\hat{T}_a,-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi(x)=\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x+a)}{dx^2}\right)+\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(\psi(x+a)\right)=0 \tag{95}$$

Now we calculate the second commutator; the potential term:

$$\begin{aligned}&\left[\hat{T}_a, V(x)\right]\psi(x) = (\hat{T}_a V(x) - V(x)\hat{T}_a)\psi(x)\\&= \hat{T}_a(V(x)\psi(x)) - V(x)\hat{T}_a\psi(x)\\&= V(x+a)\psi(x+a) - V(x)\psi(x+a) = 0\end{aligned} \tag{96}$$

The last equality in equation **(96)** is because the potential is periodic as we so in equation **(85),** in conclusion the sum of the two terms in the last quality of equation **(94)** is zero i.e. $\hat{T}_a$ and $\hat{H}$:

$$\left[\hat{T}_a, -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi(x) + \left[\hat{T}_a, V(x)\right]\psi(x) = 0 \tag{97}$$

Since the translation operator commutes with the Hamiltonian; the two operators can have common or simultaneous eigenvectors (functions). We write the eigenvalue equation for the translation operator:

$$\hat{T}_a\psi(x) = t_a\psi(x) \tag{98}$$

We write the eigenvectors in terms of plane waves or simply the Fourier transform:

$$\psi(x) = \sum_{q=-\infty}^{\infty} C_q e^{iqx} \tag{99}$$

We put the expression from equation **(99)** into the eigenvalue equation **(98);** we get:

$$\begin{aligned}&\hat{T}_a\psi(x) = \hat{T}_a \sum_{q=-\infty}^{\infty} C_q e^{iqx} = \sum_{q=-\infty}^{\infty} C_q e^{iq(x+a)}\\&= \sum_{q=-\infty}^{\infty} C_q e^{iqa} e^{iqx} = t_a \sum_{q=-\infty}^{\infty} C_q e^{iqx}\end{aligned} \tag{100}$$

The last equality in equation **(100)** implies that e^{iqa} must be a constant; that is:

$$\begin{aligned}&e^{iqa} = const.\\&\Rightarrow qa = 2\pi n + const.\end{aligned} \tag{101}$$

Where n is an arbitrary integer; Equation **(101)** gives conditions on the values of the wave vector as following:

$$q = k + g \tag{102}$$

Where k is an arbitrary constant and g satisfies the following equation:

$$ga = 2\pi n \tag{103}$$

When we use the solutions for q above; then the eigenvalues of the translation operator must be:

$$t_{a,k} = e^{ika} \tag{104}$$

The eigenvectors are degenerate with respect to

$k + g$; We can write a general eigenvector for and eigenvalue $t_a = e^{ika}$ as a sum of eigenvectors over g:

$$\begin{aligned} \psi_k(x) &= \sum_{g=-\infty}^{\infty} c_{k+g} e^{i(k+g)x} \\ &= e^{ikx} \sum_{g=-\infty}^{\infty} c_{k+g} e^{igx} \equiv e^{ikx} u_k(x) \end{aligned} \tag{105}$$

Here k labels different eigenvalues and eigenvectors of the translation operator and we have defined the function $u_k(x)$ as:

$$u_k(x) = \sum_{g=-\infty}^{\infty} c_{k+g} e^{igx} \tag{106}$$

And it has the periodicity of the lattice.

Choosing k to be in the in one single cell in k-space is sufficient, because just as we had translation symmetry in real space; we have translation symmetry in k-space too, the single cell is called the Brillouin zone as we will see when we do the 3-dimensional case.

2.4 Electron in a periodic potential, 3D case:

WE extend the one dimensional case to 2-3 dimensions by using the same simple procedures we used for the one dimensional case; we simply start with the three dimensional Hamiltonian for an electron in a periodic potential:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \tag{107}$$

Here ∇^2 is the Laplace operator:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{108}$$

But of course we have similar for the two dimensional case, only with two variables instead of three.

We define the translation vector $\vec{R}$ as:

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \tag{109}$$

Here $\{n_1, n_2, n_3 \in \mathbb{Z}\}$; they are integers. The vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ are the basis vectors of the lattice; they are the vectors of the **primitive cell**; the primitive cell is the minimum volume (area in 2D) that construct the periodicity of the lattice, the minimum volume (area) that a particle crosses the lattice that is translation invariant.

The periodic potential then satisfies the condition:

$$V(\vec{r}+\vec{R}) = V(\vec{r}) \tag{110}$$

We define the translation operator $\hat{T}_{\vec{R}}$ on a function $G(\vec{r})$; in a similar way we did for the one dimensional case:

$$\hat{T}_{\vec{R}}G(\vec{r}) = G(\vec{r}+\vec{R}) \tag{111}$$

The translation operator $\hat{T}_{\vec{R}}$ commutes with the Hamiltonian operator from equation **(107)**:

$$\begin{aligned}[\hat{T}_{\vec{R}}, \hat{H}]\psi(\vec{r}) &= \left[\hat{T}_{\vec{R}}, -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) \\ &= \left(\left[\hat{T}_{\vec{R}}, -\frac{\hbar^2}{2m}\nabla^2\right] + \left[\hat{T}_{\vec{R}}, V(\vec{r})\right]\right)\psi(\vec{r})\end{aligned} \tag{112}$$

The first commutator in the last equality of equation **(112)** is simply the kinetic term and it is zero:

$$\begin{aligned}\left[\hat{T}_{\vec{R}}, -\frac{\hbar^2}{2m}\nabla^2\right]\psi(\vec{r}) &= \hat{T}_{\vec{R}}\left(-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})\right) - \left(-\frac{\hbar^2}{2m}\nabla^2\left(\hat{T}_{\vec{R}}\psi(\vec{r})\right)\right) \\ &= -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}+\vec{R}) + \frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}+\vec{R}) = 0\end{aligned} \tag{113}$$

The second commutator of equation **(112)** is also zero because of the periodicity of the potential:

$$\begin{aligned}\left[\hat{T}_{\vec{R}}, V(\vec{r})\right]\psi(\vec{r}) &= \hat{T}_{\vec{R}}(V(\vec{r})\psi(\vec{r})) - V(\vec{r})\left(\hat{T}_{\vec{R}}\psi(\vec{r})\right) \\ &= V(\vec{r}+\vec{R})\psi(\vec{r}+\vec{R}) - V(\vec{r})\psi(\vec{r}+\vec{R}) = 0\end{aligned} \tag{114}$$

The last equality is due to equation **(110)**.

Since the translation operator commutes with the Hamiltonian; there are common eigenstates for the two operators.

We write the eigenstate for the Hamiltonian from equation **(107)** in terms of plane waves or simply the Fourier transform just as we did in 1D:

$$\psi(\vec{r}) = \sum_{\vec{q}} c_{\vec{q}} e^{i\vec{q}\bullet\vec{r}} \tag{115}$$

So we have the following eigenvalue problem:

$$\hat{T}_{\vec{R}}\psi(\vec{r}) = t_{R}\psi(\vec{r}) \tag{116}$$

In terms of plane waves:

$$\begin{aligned} \hat{T}_{\vec{R}}\psi(\vec{r}) &= \hat{T}_{\vec{R}} \sum_{\vec{q}} c_{\vec{q}} e^{i\vec{q}\bullet\vec{r}} = \sum_{\vec{q}} c_{\vec{q}} e^{i\vec{q}\bullet(\vec{r}+\vec{R})} = \sum_{\vec{q}} c_{\vec{q}} e^{i\vec{q}\bullet\vec{r}} e^{i\vec{q}\bullet\vec{R}} \\ &= t_{R} \sum_{\vec{q}} c_{\vec{q}} e^{i\vec{q}\bullet\vec{r}} \end{aligned} \tag{117}$$

In order for the last equality of equation **(117)** to be true; we must have the following term be a constant:

$$e^{i\vec{q}\bullet\vec{R}} = Const. \tag{118}$$

That means:

$$\vec{q}\bullet\vec{R} = const. + 2\pi n \tag{119}$$

Where n is an integer; this means that we have several solutions because the last term of equation **(119)** does not contribute:

$$e^{i2\pi n} = 1 \tag{120}$$

The solutions of $\vec{q}$ are:

$$\vec{q} = \vec{k} + \vec{G} \tag{121}$$

Where $\vec{k}$ is an arbitrary vector and $\vec{G}$ is the **reciprocal lattice vector**; the reciprocal lattice is defined as **[9]**:

$$\left\{ \vec{G} \in Reciprocal - Space \mid e^{i\vec{G}\bullet\vec{R}} = 1 \right\} \tag{122}$$

Reciprocal space is simply the momentum-space or k-space to be exact of the real lattice i.e. the Fourier transform of the real space.

In conclusion; the solution of the eigenvalues $t_{R,k}$ is:

$$t_{R,k} = e^{i\vec{k}\bullet\vec{R}} \tag{123}$$

The eigenvalues $t_{R,k}$ are degenerate with respect to $\vec{k}+\vec{G}$, you can always add $\vec{G}\bullet\vec{R}$ to the solution of the eigenstate and still be an eigenstate of the eigenvalue $t_{R,k}$; so a general eigenvector of the eigenvalue $t_{R,k}$ is:

$$\psi_{\vec{k}}(\vec{r})=\sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i(\vec{k}+\vec{G})\bullet\vec{r}} = e^{i\vec{k}\bullet\vec{r}} \sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i\vec{G}\bullet\vec{r}} = e^{i\vec{k}\bullet\vec{r}} u_k(\vec{r}) \tag{124}$$

Where $u_k(\vec{r})$ is a periodic function with same period as the periodicity of the lattice, it is the 3D version of equation **(106)**, and is defined as:

$$u_k(\vec{r})=\sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i\vec{G}\bullet\vec{r}} \tag{125}$$

As we mentioned earlier in the previous section that it is sufficient to choose the vector $\vec{k}$ in the first **Brillouin Zone**; A Brillouin zone is the primitive cell of the reciprocal lattice in momentum-space, so just as we had a minimum cell in real space; there is a minimum cell in momentum space that is called a Brillouin zone.

Our conclusion for both the one and three dimensional case is simply **Bloch's theorem** which states; "the Eigenvectors $\psi_{\vec{k}}(\vec{r})$ of a periodic lattice are a product of the plane wave $e^{i\vec{k}\bullet\vec{r}}$ with a function $u_k(\vec{r})$ that satisfy the periodicity of the lattice".

2.5 Harmonic Oscillator:

The equation of quantum harmonic oscillator appears frequently in physics as an approximation to more complicated potentials or in equations involving charged particles in a magnetic field etc.; it is important to we go through it and using the simplest way of deriving the energy eigenvalues which is by using the ladder operators.

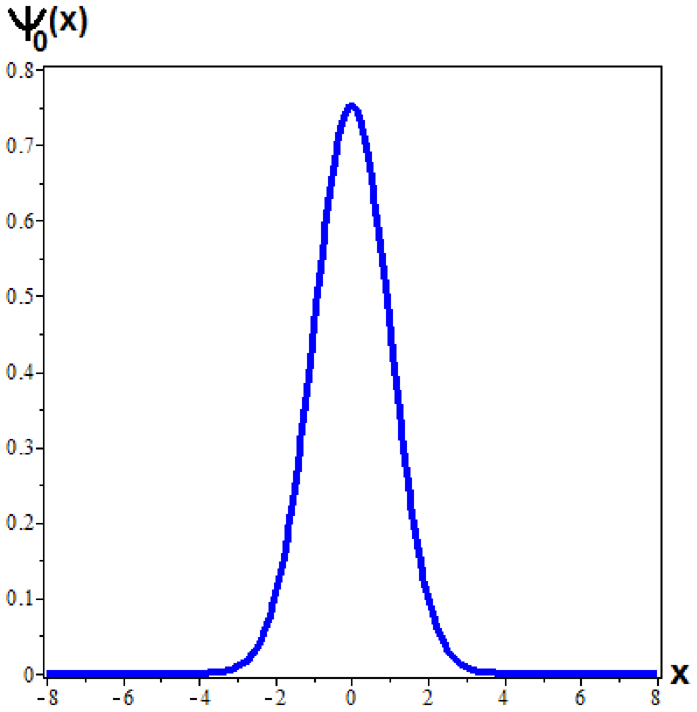


Figure (4): Ground state of the harmonic oscillator with $m\omega / \hbar = 1$

The Hamiltonian of the harmonic oscillator in quantum mechanics is the same as in classical mechanics, but one has to make the variables q, p into operators:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{q}^2 \qquad \textbf{(126)}$$

Where

$$\hat{q} = q \qquad \textbf{(127)}$$

And the momentum involves the derivative with respect to q; in more dimensions, it would involve partial derivative, but in 1D it is simply the total derivative with respect to q multiplied by a number:

$$\hat{p} = -i\hbar \frac{d}{dq} \qquad \textbf{(128)}$$

We can of course write the Hamiltonian in equation **(126)** more explicitly **[6]**, **[8]**:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2 q^2 \quad \textbf{(129)}$$

We rewrite the Hamiltonian in a way that is easier to see the energy eigenvalues:

$$\hat{H} = \hbar\omega(\frac{\hat{p}^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar}\hat{q}^2) \quad \textbf{(130)}$$

When the Hamiltonian $\hat{H}$ from equation **(130)** acts on one of its eigenvectors $\left|\psi_n\right\rangle$ it gives the eigenvalue E_n, we don't know what the eigenvectors and the eigenvalues of the Hamiltonian are, we just have defined them as eigenvectors $\left|\psi_n\right\rangle$ and eigenvalues E_n; or the equation:

$$\hat{H}\psi_n(q) = E_n\psi_n(q) \quad (131)$$

Or in abstract Hilbert space:

$$\hat{H}\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle \quad \textbf{(132)}$$

We will now look at which form does the Hamiltonian takes in abstract Hilbert space; We introduce new operators: The lowering operator

$$\begin{aligned} a(q) \equiv a &= \sqrt{\frac{m\omega}{2\hbar}}\hat{q} + i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p} \\ &= \sqrt{\frac{m\omega}{2\hbar}}q + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dq} \end{aligned} \quad \textbf{(133)}$$

And the raising operator

$$\begin{aligned} a^\dagger(q) \equiv a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\hat{q} - i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p} \\ &= \sqrt{\frac{m\omega}{2\hbar}}q - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dq} \end{aligned} \quad \textbf{(134)}$$

We will see later on why they are called so. Now we let us try express the Hamiltonian in in abstract Hilbert space in terms of a and $a^\dagger$ we start by looking at the operator $a^\dagger a$:

$$a^\dagger a = \frac{m\omega}{2\hbar}\hat{q}^2 + \frac{1}{2m\hbar\omega}\hat{p}^2 + \frac{i}{2\hbar}[\hat{q},\hat{p}] \quad \textbf{(135)}$$

Where the last term is the commutator:

$$\left[\hat{q},\hat{p}\right] = \hat{q}\hat{p} - \hat{p}\hat{q} = i\hbar \quad \textbf{(136)}$$

Where the last equality comes from the Heisenberg`s canonical commutation relation which implies Heisenberg`s uncertainty principle. This means:

$$a^{\dagger}a = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2} \tag{137}$$

Or the Hamiltonian is:

$$\hat{H} = \hbar\omega(a^{\dagger}a + \frac{1}{2}) \tag{138}$$

We do similar calculation for $aa^{\dagger}$ and find:

$$aa^{\dagger} = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \tag{139}$$

Then we can find the commutator:

$$\left[a, a^{\dagger}\right] = aa^{\dagger} - a^{\dagger}a = 1 \tag{140}$$

Of course we have the trivial commutation relations:

$$[a, a] = \left[a^{\dagger}, a^{\dagger}\right] = 0 \tag{141}$$

We could of course find the above commutation relation from the definitions in equations **(133)** and **(134)**. Now let us look at the norm $a\left|\psi_n\right\rangle$ using the inner product; first we have:

$$\left(a\left|\psi_n\right\rangle\right)^{\dagger} = \left\langle\psi_n\right|a^{\dagger} \tag{142}$$

Then it means the norm of $a\left|\varphi_n\right\rangle$ squared is to multiply it by its Hermitian conjugate:

$$\left\langle\psi_n\right|a^{\dagger}a\left|\psi_n\right\rangle \geq 0 \tag{143}$$

This expression must bigger than or equal to zero because it is the norm of a vector squared, the norm of any vector $\vec{r}$ is:

$$\left|\vec{r}\right| = (\vec{r}\cdot\vec{r})^{1/2} \tag{144}$$

We write the inner product in terms of the Hamiltonian, we get:

$$\begin{aligned}\left\langle\psi_n\right|a^{\dagger}a\left|\psi_n\right\rangle &= \left\langle\psi_n\right|\frac{1}{\hbar\omega}\hat{H} - \frac{1}{2}\left|\psi_n\right\rangle = \left\langle\psi_n\right|\frac{1}{\hbar\omega}E_n - \frac{1}{2}\left|\psi_n\right\rangle \\ &= \left\langle\psi_n|\psi_n\right\rangle\left(\frac{1}{\hbar\omega}E_n - \frac{1}{2}\right) = \left(\frac{1}{\hbar\omega}E_n - \frac{1}{2}\right) \geq 0\end{aligned} \tag{145}$$

Equation **(145)** gives the following inequality for the energy eigenvalues E_n:

$$E_n \geq \frac{1}{2}\hbar\omega \tag{146}$$

The lowest possible energy eigenvalue is $\frac{1}{2}\hbar\omega$.

Now let us calculate the commutation relations between the Hamiltonian and the operators raising and lowering:

$$\begin{aligned}
&\left[\hat{H},a\right]=\hbar\omega\left(a^{\dagger}a+\frac{1}{2}\right)a-\hbar\omega a\left(a^{\dagger}a+\frac{1}{2}\right)\\
&=\hbar\omega a^{\dagger}a+\frac{\hbar\omega}{2}a-\hbar\omega aa^{\dagger}a-\frac{\hbar\omega}{2}\\
&=\hbar\omega\left(a^{\dagger}aa-aa^{\dagger}a\right)=\hbar\omega\left(a^{\dagger}a-aa^{\dagger}\right)a\\
&=-\hbar\omega\left[a,a^{\dagger}\right]a=-\hbar\omega a
\end{aligned} \tag{147}$$

Similarly for $a^{\dagger}$:

$$\left[\hat{H},a^{\dagger}\right]=\hbar\omega a^{\dagger} \tag{148}$$

Now let us operate the Hamiltonian on the state $a\left|\psi_n\right\rangle$, the states of harmonic oscillators are also written just with index; $\left|n\right\rangle$ which is more convenient to write, but we stick with the first notation so reader can have better understanding that it is an eigenvector not a number and to resemble the eigenvector in real space $\psi_n(x)$:

$$\begin{aligned}
&\hat{H}\left(a\left|\psi_n\right\rangle\right)=\left(\hat{H}a+\left(-a\hat{H}+a\hat{H}\right)\right)\left|\psi_n\right\rangle\\
&=\left(\left(\hat{H}a-a\hat{H}\right)+a\hat{H}\right)\left|\psi_n\right\rangle\\
&=\left(\left[\hat{H},a\right]+a\hat{H}\right)\left|\psi_n\right\rangle\\
&=\left(-\hbar\omega a+aE_n\right)\left|\psi_n\right\rangle\\
&=\left(E_n-\hbar\omega\right)a\left|\psi_n\right\rangle
\end{aligned} \tag{149}$$

Where we have simply added and subtracted $a\hat{H}$ in equation **(149)** so it doesn't contribute anything but we get a more familiar term which is the commutator from equation **(147)**; $\left[\hat{H},a\right]=-\hbar\omega a$.

And similarly for $a^{\dagger}\left|\psi_n\right\rangle$:

$$\hat{H}\left(a^{\dagger}\left|\psi_n\right\rangle\right)=\left(E_n+\hbar\omega\right)a^{\dagger}\left|\psi_n\right\rangle \tag{150}$$

So when the operators $a^\dagger$ and a are acting on the eigenstate $|\psi_n\rangle$; we get new eigenstates with energy eigenvalues equal to the energy eigenvalue of the original state plus and minus a constant value $\hbar\omega$. That is why the operator a is called a lowering operator; it lowers the original state to a state with energy value $(E_n - \hbar\omega)$ and $a^\dagger$ raises the original state to a state with energy value $(E_n + \hbar\omega)$ hence: the raising operator. The combined name for both is ladder operators.

Now this means that if we act the raising and lowering operators on an eigenstate repeatedly; we can have energy values from $+\infty$ to $-\infty$ But the eigenvalues should satisfy the inequality $E_n \geq \frac{1}{2}\hbar\omega$ as we found out earlier, so there must be a **lowest** eigenstate $|\psi_0\rangle$ with minimum energy eigenvalue or the ground state energy; $E_0 = \frac{1}{2}\hbar\omega$ such that when we act the operator a we get zero:

$$a|\psi_0\rangle = 0 \tag{151}$$

This satisfies the minimum condition in inequality **(146)**:

$$\hat{H}|\psi_0\rangle = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|\psi_0\rangle = \frac{1}{2}\hbar\omega|\psi_0\rangle \tag{152}$$

Now if we act the raising operator on the ground state and using equation **(150)**; we can get the **second lowest** state or the first exited state:

$$a^\dagger|\psi_0\rangle = c_1|\psi_1\rangle \tag{153}$$

Where c_1 in equation **(153)** is a constant. If we repeat the operation again and again; we can get all the next states, a general state:

$$\left(a^\dagger\right)^n|\psi_0\rangle = c_n c_{n-1}\ldots\ldots c_1|\psi_n\rangle \tag{154}$$

Where $c_n, c_{n-1}, \ldots\ldots, c_0$ are constants; and:

$$a^\dagger|\psi_n\rangle = c_{n+1}|\psi_{n+1}\rangle \tag{155}$$

But we also can use equation **(149)** to write the states in terms of $a|\psi_n\rangle$:

$$a|\psi_n\rangle = c_n|\psi_{n-1}\rangle \tag{156}$$

In equation **(156)**; c_n is just a constant similarly to c_{n+1} but they are not the same. We have used the same set of constants $c_n, c_{n-1}, \ldots\ldots, c_0$ for both equations **(155)** and **(156)** because they are the same set of constants as we see later on in more detail.

Let us now find the energy eigenvalues of the eigenstates; if we act the Hamiltonian operator on a random state $\left|\psi_{n+1}\right\rangle$ then from the above results we have:

$$\hat{H}\left|\psi_{n+1}\right\rangle = E_{n+1}\left|\psi_{n+1}\right\rangle \tag{157}$$

Also if we operated on $a^{\dagger}\left|\psi_{n}\right\rangle$; we should get the same energy since $a^{\dagger}\left|\psi_{n}\right\rangle$ and $\left|\psi_{n+1}\right\rangle$ differ by only a constant:

$$\hat{H}\left(c_{n+1}\left|\psi_{n+1}\right\rangle\right) = c_{n+1}\hat{H}\left|\psi_{n+1}\right\rangle = c_{n+1}E_{n+1}\left|\psi_{n+1}\right\rangle = E_{n+1}\left(c_{n+1}\left|\psi_{n+1}\right\rangle\right) \tag{158}$$

But we know from equation **(155)** that $\left|\psi_{n+1}\right\rangle$ is just equal to $c_n a^{\dagger}\left|\psi_{n}\right\rangle$; so we can operate the Hamiltonian on $a^{\dagger}\left|\psi_{n}\right\rangle$ and using equation **(150)** to get:

$$\begin{aligned}&\hat{H}\left(c_{n+1}\left|\psi_{n+1}\right\rangle\right) = \hat{H}\left(a^{\dagger}\left|\psi_{n}\right\rangle\right)\\&=\left(E_n+\hbar\omega\right)a^{\dagger}\left|\psi_{n}\right\rangle\\&=\left(E_n+\hbar\omega\right)c_{n+1}\left|\psi_{n+1}\right\rangle\end{aligned} \tag{159}$$

Using equations **(157)** and **(159)**; we get a difference equation for the eigenvalues of the energy E_n:

$$E_{n+1} = \left(E_n+\hbar\omega\right) \tag{160}$$

Where $n\in\mathbb{N}$ equation **(160)** has the following solution for the eigenvalues:

$$E_n = E_0 + n\hbar\omega \tag{161}$$

The energy E_0 is a constant, which simply is the ground state energy; $E_0 = \frac{1}{2}\hbar\omega$. The energy eigenvalues are then:

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \tag{162}$$

The only thing left to do is finding the constants c_n; now let us look at the inner product between the eigenstates again:

$$\left\langle\psi_n\middle|\psi_m\right\rangle = \delta_{mn} \tag{163}$$

The symbol δ_{mn} is the kronecker delta defined in equation **(79)**. Now let us look at the following inner product:

$$\left\langle\psi_{n+1}\middle|c_{n+1}^{*}c_{n+1}\middle|\psi_{n+1}\right\rangle = \left|c_{n+1}\right|^2\left\langle\psi_{n+1}\middle|\psi_{n+1}\right\rangle = \left|c_{n+1}\right|^2 \tag{164}$$

But we can also write $\langle \psi_{n+1} | c_{n+1}^{*} c_{n+1} | \psi_{n+1} \rangle$ in terms of $\langle \psi_n | aa^{\dagger} | \psi_n \rangle$ and use equation **(139)** for $aa^{\dagger}$:

$$\begin{aligned}
&\langle \psi_{n+1} | c_{n+1}^{*} c_{n+1} | \psi_{n+1} \rangle = \langle \psi_n | aa^{\dagger} | \psi_n \rangle = \langle \psi_n | \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \right) | \psi_n \rangle \\
&= \langle \psi_n | \left(\frac{E_n}{\hbar\omega} + \frac{1}{2} \right) | \psi_n \rangle = \left(\frac{\frac{1}{2}\hbar\omega + n\hbar\omega}{\hbar\omega} + \frac{1}{2} \right) \langle \psi_n | \psi_n \rangle \\
&= (n+1) \langle \psi_n | \psi_n \rangle = n+1
\end{aligned} \tag{165}$$

Putting equations **(164)** and **(165)** equal to each other; we get the following equation:

$$|c_{n+1}|^2 = n+1 \tag{166}$$

Where θ in the above is an undetermined phase. We do similar calculations for a. We then have the following results:

$$a | \psi_n \rangle = c_n | \psi_{n-1} \rangle = \sqrt{n} e^{i\theta} | \psi_{n-1} \rangle \tag{167}$$

Similar calculations for $a^{\dagger}$ give:

$$a^{\dagger} | \psi_n \rangle = c_{n+1} | \psi_{n+1} \rangle = \sqrt{n+1} e^{i\theta} | \psi_{n+1} \rangle \tag{168}$$

And finally we can express all the eigenvectors in terms of the ground state using the raising operator:

$$| \psi_n \rangle = \frac{1}{\sqrt{n!}} \left(a^{\dagger} \right)^n | \psi_0 \rangle \tag{169}$$

The phase with angle θ is often ignored as it does not give any physical meaning, because the probabilities involve the absolute value of the eigenstates ; so the phase drops out.

Now lets us find the eigenstates of the harmonic oscillator in position space; we go back to the ladder operator in this space and we have:

$$a(q)\psi_n(q) = \left(\sqrt{\frac{m\omega}{2\hbar}} q + \sqrt{\frac{\hbar}{2m\omega}} \frac{\partial}{\partial q} \right) \psi_n(q) = c_n \psi_{n-1}(q) \tag{170}$$

This is exactly the same equation as equation **(167)** only in the more familiar position-space q; this means we have the following differential equation for the ground state $\psi_0(q)$ of the harmonic oscillator in position space:

$$a(q)\psi_0(q) = \left(\sqrt{\frac{m\omega}{2\hbar}} q + \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dq} \right) \psi_0(q) = 0 \tag{171}$$

Solving the above equation for the ground state; we get a Gaussian function (look at figure (4) above):

$$\psi_0(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega q^2}{2\hbar}} \tag{172}$$

Operating the ladder operator $a^\dagger(q)$ on the ground state $\psi_0(q)$ above and repeatedly; we get the all the exited states of the harmonic oscillator:

$$\psi_n(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{1}{2^n n!}} e^{-\frac{m\omega q^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} q\right) \tag{173}$$

2.6 Harmonic Oscillator in 2 and N-dimensional space:

The 2 and 3 or n-dimensional harmonic oscillators are similar to the one dimensional and in fact we use similar methods to obtain the energy eigenvalues of the time independent Hamiltonian; the Hamiltonian for the 2D Harmonic Oscillator is **[7]**:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{1}{2} m\omega^2 (x^2 + y^2) \tag{174}$$

Writing them in a explicit way

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2} m\omega^2 (x^2 + y^2) \tag{175}$$

And the eigenvalue equation is:

$$\hat{H}\psi(x,y) = E\psi(x,y) \tag{176}$$

We rewrite the Hamiltonian in terms of three brackets; each involving one variable:

$$\hat{H} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2\right) + \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2} m\omega^2 y^2\right) \tag{177}$$

Where:

$$\hat{H} = \sum_{n=1}^{2}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_n^2} + \frac{1}{2} m\omega^2 x_n^2\right) = \sum_{n=1}^{2} \hat{H}_n \tag{178}$$

We have written the variables in equation **(178)** in terms of $x_1 = x, x_2 = y$, of course for two dimensional, it is unnecessary to write it this way, but the purpose is that we can generalize it any number of dimensions just by summing these operators $\hat{H}_n$ which are operators where each one of them simply represents a bracket in equations **(177)** and **(178)**.

Each operator $\hat{H}_n$ is:

$$\hat{H}_n = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_n^2} + \frac{1}{2}m\omega^2 x_n^2 \tag{179}$$

And the Hamiltonian for the 2D case (equation **(175)** and equation **(177)**) becomes:

$$\hat{H} = \hat{H}_x + \hat{H}_y \tag{180}$$

The Hamiltonian in equation **(180)** is a sum of two independent operators; $\hat{H}_x$ depends only on x and $\hat{H}_y$ only depends on y. That means the eigenvalue equation **(176)** for the 2D Hamiltonian is separable and we can write the eigenfunction $\psi(x,y)$ as a product of two functions; one function $\psi_x(x)$ that only depends on x and another function $\psi_y(x)$:

$$\psi(x,y) = \psi_x(x)\psi_y(x) \tag{181}$$

And the eigenvalue equation **(176)** becomes:

$$\left(\hat{H}_x\psi_x(x)\right)\psi_y(x) + \psi_x(x)\left(\hat{H}_y\psi_y(x)\right) = \left(E_x + E_y\right)\psi_x(x)\psi_y(x) \tag{182}$$

The left hand side of equation **(182)** is because $\hat{H}_x$ only operates on $\psi_x(x)$, not on $\psi_y(x)$ and $\hat{H}_y$ only operates on $\psi_y(x)$, in the RHS of the equation; we simply wrote the energy E by <u>definition</u> as a sum of two constants; E_x and E_y which we see in a moment that it makes sense. Now let us divide both side of equation **(182)** by the eigenfunction $\psi(x,y) = \psi_x(x)\psi_y(x)$:

$$\frac{(\hat{H}_x\psi_x(x))\psi_y(x)}{\psi_x(x)\psi_y(x)} + \frac{\psi_x(x)(\hat{H}_y\psi_y(x))}{\psi_x(x)\psi_y(x)} = \frac{\left(E_x + E_y\right)\psi_x(x)\psi_y(x)}{\psi_x(x)\psi_y(x)} \tag{183}$$

Now we can cancel out $\psi_y(x)$ in the first term of the LHS of equation **(183)** because it is just a multiplication by a function, but not $\psi_x(x)$ because the operator $\hat{H}_x$ is acting on it. Similarly we cancel $\psi_x(x)$ in the second term and finally we can cancel the whole product $\psi_x(x)\psi_y(x)$ in the RHS of equation **(183)** because there is only a multiplication by a constant $E = E_x + E_y$, and we get:

$$\frac{\hat{H}_x\psi_x(x)}{\psi_x(x)} + \frac{\hat{H}_y\psi_y(x)}{\psi_y(x)} = E_x + E_y \tag{184}$$

In the left hand side of equation **(184)**; we have one term completely dependent on x and another completely dependent on y; that could happen only if each term of the LHS of equation **(184)** is a constant where by definition we called one of them E_x and E_y and we finally get two independent equations, one for x and one for y:

$$\frac{\hat{H}_x \psi_x(x)}{\psi_x(x)} = E_x \\ \Rightarrow \hat{H}_x \psi_x(x) = E_x \psi_x(x) \tag{185}$$

And a second equation for y:

$$\hat{H}_y \psi_y(x) = E_y \psi_y(x) \tag{186}$$

If we write equations **(185)** and **(186)** explicitly; we see that they are nothing but two independent harmonic oscillators:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi_x(x) = \left(\frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2 x^2\right)\psi_x(x) = E_x \psi_x(x) \tag{187}$$

And for y:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega^2 y^2\right)\psi_y(x) = \left(\frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2 y^2\right)\psi_y(x) = E_y \psi_y(x) \tag{188}$$

So solving each equation must have identical procedure as we did for one dimensional harmonic oscillator in the previous section, which is by ladder operators. We define the following ladder operators for x; the lowering operator:

$$a_n = \sqrt{\frac{m\omega}{2\hbar}}\hat{x}_n + i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p}_n = \sqrt{\frac{m\omega}{2\hbar}}x_n + \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x_n} \tag{189}$$

And the raising operator:

$$a_n^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x}_n - i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p}_n = \sqrt{\frac{m\omega}{2\hbar}}x_n - \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x_n} \tag{190}$$

In equation(190) above; $n = 1, 2$ or simply x and y, the ladder operators in equations **(189)** and **(190)** satisfy the commutation relations:

$$\left[a_n, a_m^\dagger\right] = \delta_{nm} \tag{191}$$

In equation **(191)**; $\mathrm{n,m} = 1, 2$ or simply x and y. Equation **(191)** is written for two independent oscillators N =2, however the equation is general for any number of independent oscillators, N could be very large number; that is N dimensional harmonic oscillator would be solved in identical procedures.

In conclusion; we solve equation **(176)** for the two dimensional harmonic oscillator by splitting it to two independent 1D harmonic oscillator equations **(185)** and **(186)**. Then solving each equation in identical procedure as in the 1D case we did with ladder operators satisfying equation **(191)**. That means that the general 1D eigenstates $\psi_x(x)$ and $\psi_y(x)$ have the following solutions:

$$\psi_{n_x}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{1}{2^{n_x} n_x!}} e^{-\frac{m\omega x^2}{2\hbar}} H_{n_x}\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \tag{192}$$

With the same form as the one dimensional case; energy E_x is equal to:

$$E_x = \hbar\omega\left(n_x + \frac{1}{2}\right) \tag{193}$$

And the same for y:

$$\psi_{n_y}(y) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{1}{2^{n_y} n_y!}} e^{-\frac{m\omega y^2}{2\hbar}} H_{n_y}\left(\sqrt{\frac{m\omega}{\hbar}} y\right) \tag{194}$$

With similar form for the energy E_y:

$$E_y = \hbar\omega\left(n_y + \frac{1}{2}\right) \tag{195}$$

Finally the general eigenstate $\psi(x, y)$ of the 2D case is a super position of all possible eigenstates:

$$\psi(x, y) = \sum_{n_x, n_y = 1}^{\infty} \psi_{n_x}(x)\psi_{n_y}(x) \tag{196}$$

And it`s energy E:

$$E = \hbar\omega\left(n_y + \frac{1}{2}\right) + \hbar\omega\left(n_x + \frac{1}{2}\right) \tag{197}$$

The indices n_x, n_y are the natural numbers; $n_x, n_y \in \mathbb{N}$. We can see from result above that the energies are degenerate in the two dimensional case and also higher dimensional cases of course **[6], [7]**.

The procedure for the 2D case helps us to see exactly what would the procedures for solving the harmonic oscillator for any number of dimensions; we simply start extending the equation **(178)** from the total number of dimensions n=2 to any number N dimensions; the energy of the N dimensional harmonic oscillator is:

$$E = \sum_{k=1}^{k=N} \hbar\omega\left(n_k + \frac{1}{2}\right) \tag{198}$$

The reason that we went thru the 2D and N dimensions case is because the methods used for harmonic oscillator like the ladder operators; is also used quite often in other physical problems, such as field quantization which involves infinite dimensional harmonic oscillators and also similarly used but exact the same rules for writing the tight binding model eigenfunctions in the second quantization form, the latter would be discussed in more detail later. The harmonic oscillator is kind of the starting point for applications in second quantization method.

2.7 Tight-binding Model:

The tight binding theory for solids is easy to imagine and have a simple intuitive picture of it. We can have a physical picture of the electronic interactions in real space. In the tight binding theory one assumes that the electrons are tightly bounded to the atoms they belong to and there are only weak interactions between electrons that belong to an atom and the rest of the atoms of the crystal.

The atoms are almost like individual atoms in empty space and only have small overlap between their wavefunctions. The system is described by a set of non-interacting wavefunctions that obey Fermi statistics.

We start with the single particle Schrödinger equation in the whole lattice:

$$\hat{H}\Psi(x) = E\Psi(x) \tag{199}$$

Then one assumes that the delocalized wavefunction $\Psi(x)$ in the above equation is approximately equal to a linear combination of the wavefunctions of isolated atoms each lying in one of the atomic sites of the lattice under study; in one dimension we have:

$$\psi(x) = \sum_{n}^{N} \alpha_n \varphi(x - x_n) \tag{200}$$

The positions of the atomic sites x_n (look at figure () below) are:

$$x_n = na \tag{201}$$

The positions of the atoms have the linear property (look at figure () below); that is for two vectors x_n and x_m in the lattice:

$$x_n \pm x_m = na \pm ma = (n \pm m)a = x_{n\pm m} \tag{202}$$

The atomic wavefunctions aren't necessarily orthonormal, but we can make them orthonormal. They overlap integrals between the atomic wavefunctions are often neglected. We assume here that they are orthonormal and we start with the following relation:

$$\int \varphi(x - x_n)^* \varphi(x - x_m)\,dx = \delta_{nm} \tag{203}$$

The wavefunction must be of the Bloch form as we have seen for periodic potentials in the section (2.3); that is it must satisfy:

$$\psi\left(x+x_m\right)=e^{ikx_m}\psi\left(x\right) \tag{204}$$

Let us use equation **(200)** to write the translated function $\psi\left(x+x_m\right)$ in space in terms of the atomic wavefunctions; we get:

$$\psi\left(x+x_m\right)=\sum_n^N \alpha_n\varphi\left(x-x_n+x_m\right)=\sum_n^N \alpha_n\varphi\left(x-\left(x_n-x_m\right)\right) \tag{205}$$

If we make the substitution $s=n-m \Rightarrow n=s+m$ and use the linear property from equation **(202)**; we get the following:

$$\psi\left(x+x_m\right)=\sum_s^N \alpha_{s+m}\varphi\left(x-x_s\right) \tag{206}$$

Putting the expression above into equation **(204)**; then we get:

$$\begin{aligned}\psi\left(x+x_m\right)&=\sum_s^N \alpha_{s+m}\varphi\left(x-x_s\right)\\ &=e^{ikx_m}\psi\left(x\right)=e^{ikx_m}\sum_s^N \alpha_s\varphi\left(x-x_s\right)=\sum_s^N e^{ikx_m}\alpha_s\varphi\left(x-x_s\right)\end{aligned} \tag{207}$$

From equation we can find the recurrence relation:

$$\alpha_{s+m}=e^{ikx_m}\alpha_s \tag{208}$$

The solution for the recurrence relation above is given by:

$$\alpha_m=e^{ikx_m}\alpha_0 \tag{209}$$

In order to find α_0; we use the probability requirement that the inner product of the delocalized wavefunction over the whole space is equal to one:

$$\begin{aligned}1&=\int\psi\left(x\right)^*\psi\left(x\right)dx=\sum_{n,m=1}^N\int\alpha_n^*\alpha_m\varphi\left(x-x_n\right)^*\varphi\left(x-x_m\right)dx\\ &=\left|\alpha_0\right|^2\sum_{n,m=1}^N e^{ikx_m-ikx_n}\delta_{nm}=\left|\alpha_0\right|^2\sum_{n,m=1}^N 1=\left|\alpha_0\right|^2 N\end{aligned} \tag{210}$$

The solution for the coefficient α_0 then is:

$$\alpha_0=\frac{1}{\sqrt{N}} \tag{211}$$

We can of course multiply the coefficient by a phase in equation **(211)**, but it does not give any physical meaning since it drops out when we take the absolute value of α_0.

Finally we have the delocalized function for single electrons in the whole lattice written as a linear combination of the atomic wavefunctions **[10]**:

$$\psi(x) = \frac{1}{\sqrt{N}} \sum_{n}^{N} e^{ikx_n} \varphi(x - x_n) \tag{212}$$

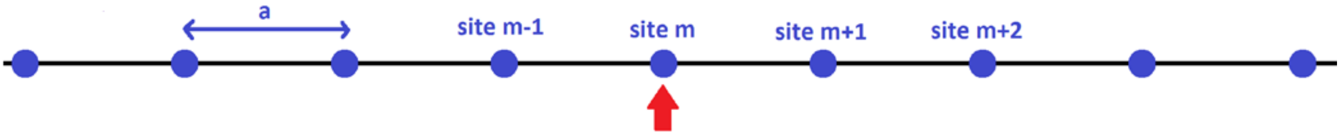


Figure (5): straight line of infinite atoms with distance a.

The energy spectrum can be found by simply take the mean value of the Hamiltonian operator:

$$E = \int \psi(x)^* \hat{H} \psi(x) dx = \frac{1}{N} \sum_{n,m}^{N} \int e^{ik(x_n - x_m)} \varphi^*(x - x_m) \hat{H} \varphi(x - x_n) dx \tag{213}$$

The overlap integrals (interactions between atomic of the lattice) can be written as coefficients (hopping energies) ε_{mn} :

$$\varepsilon_{mn} = \int \varphi^*(x - x_m) \hat{H} \varphi(x - x_n) dx \tag{214}$$

In the absence of a magnetic field; we can have the interaction coefficients ε_{mn} to be real; which simply comes from the fact that the potentials in the Hamiltonian operator above $\hat{H}$ are real. The hopping energies ε_{mn} are dependent on the distance between the wave functions of the atomic sites in the integrand of the above equation:

$$\varepsilon_{mn} = \varepsilon(x_n - x_m) = \varepsilon_{n-m} \tag{215}$$

We last equality of the above equation comes from **(202)**. Then the solutions of the energy spectrum **(213)** are:

$$E = \int \psi(x)^* \hat{H} \psi(x) dx = \frac{1}{N} \sum_{n,m}^{N} \varepsilon_{n-m} e^{ik(x_n - x_m)} \tag{216}$$

We write $\delta = n - m \Rightarrow n = \delta + m$; we get:

$$E = \frac{1}{N} \sum_{\delta,m}^{N} \varepsilon_\delta e^{ik\delta} = \sum_{\delta}^{N} \varepsilon_\delta e^{ik\delta} \tag{217}$$

We have summed δ over the whole one dimensional lattice in the above equation. For nearest neighbor; $\delta = \pm a$ where a the physical distance (in real space) between nearest neighboring atoms and $\varepsilon_+ = \varepsilon_- \equiv \varepsilon$; then we have [11]:

$$E = E_0 + \varepsilon\left(e^{ika} + e^{-ika}\right) = E_0 + 2\varepsilon\cos\left(ka\right) \tag{218}$$

Where in the above equation; E_0 is the onsite energy for the lattice, it is not very interesting; all we have to do is include it in the energy E.

2.8 Tight binding Model 2D and 3D:

The 2D and 3D case are similar to the 1D case. We work with 3D case here, but the 2D case is identical to it, only we have two primitive vectors instead of three. We start with writing the general vector for the lattice under study:

$$\vec{R}_{\vec{n}} = n_1\vec{e}_1 + n_2\vec{e}_2 + n_3\vec{e}_3 \tag{219}$$

In the above equation; we have $n_1, n_2, n_3 \in \mathbb{Z}$. The vectors $\vec{e}_1, \vec{e}_2$ and $\vec{e}_3$ are the primitive lattice vectors; the vector $\vec{R}_{\vec{n}}$ has the linear property:

$$\begin{aligned}\vec{R}_{\vec{n}} \pm \vec{R}_{\vec{m}} &= \left(n_1\vec{e}_1 + n_2\vec{e}_2 + n_3\vec{e}_3\right) \pm \left(m_1\vec{e}_1 + m_2\vec{e}_2 + m_3\vec{e}_3\right)\\ &= \left(n_1 \pm m_1\right)\vec{e}_1 + \left(n_2 \pm m_2\right)\vec{e}_2 + \left(n_3 \pm m_3\right)\vec{e}_3\\ &= \vec{R}_{\vec{n}\pm\vec{m}}\end{aligned} \tag{220}$$

We start with the Schrödinger equation

$$\hat{H}\psi\left(\vec{r}\right) = E\psi\left(\vec{r}\right) \tag{221}$$

We again start with assuming that the statevector $\psi\left(\vec{r}\right)$ can be approximated to the superposition of the statevectors of atoms in the whole lattice if they were isolated from each other [10], [12]:

$$\psi\left(\vec{r}\right) = \frac{1}{\sqrt{N}}\sum_{\vec{n}}^{N} e^{i\vec{k}\bullet\vec{R}_{\vec{n}}}\varphi\left(\vec{r} - \vec{R}_{\vec{n}}\right) \tag{222}$$

Then we take the expectation value of the Hamiltonian $\hat{H}$ and get:

$$\begin{aligned}E &= \int \psi^*\left(\vec{r}\right)\hat{H}\psi\left(\vec{r}\right)d^3r = \frac{1}{N}\sum_{\vec{n},\vec{m}}^{N} e^{i\vec{k}\bullet\left(\vec{R}_{\vec{n}} - \vec{R}_{\vec{m}}\right)}\int \varphi^*\left(\vec{r} - \vec{R}_{\vec{m}}\right)\hat{H}\varphi\left(\vec{r} - \vec{R}_{\vec{n}}\right)d^3r\\ &= \frac{1}{N}\sum_{\vec{n},\vec{m}}^{N} e^{i\vec{k}\bullet\left(\vec{R}_{\vec{n}} - \vec{R}_{\vec{m}}\right)}\varepsilon_{\vec{m}\vec{n}}\end{aligned} \tag{223}$$

Equation **(215)** holds for the 3D case; that is $\varepsilon_{\vec{m}\vec{n}} = \varepsilon_{\vec{n}-\vec{m}}$ so if we make the substitution: $\vec{n} - \vec{m} = \vec{s}$ and we also get $\vec{n} = \vec{s} + \vec{m}$; the above equation becomes:

$$E = \frac{1}{N}\sum_{\vec{s},\vec{m}}^{N} e^{i\vec{k}\bullet\vec{R}_{\vec{s}}}\varepsilon_{\vec{s}} = \sum_{\vec{s}}^{N} e^{i\vec{k}\bullet\vec{R}_{\vec{s}}}\varepsilon_{\vec{s}} \tag{224}$$

In the above equation we summed over $\vec{m}$ which simply gives a factor N. The above sum includes all the interactions between the atoms of the whole lattice. The hopping energies $\varepsilon_{\vec{s}}$ becomes weaker and weaker the further the atoms are from each other, so often only the nearest neighboring terms are included when using the tight binding approximation and we e take next nearest correction if needed otherwise drop most of the rest of the terms. In the case of nearest neighboring approximation; we have only one interaction coefficient:

$$E = \varepsilon_0 \sum_{\vec{\delta}} e^{i\vec{k}\bullet\vec{R}_{\vec{\delta}}} \tag{225}$$

In the above equation; ε_0 is the hopping energy between nearest neighboring atoms in the lattice under study and the sum over $\vec{\delta}$ are the nearest neighboring vectors. Let us look at an example; for the square lattice, the primitive vectors are $\vec{a}_1 = (1,0)$ and $\vec{a}_2 = (0,1)$ and vector for the atomic sites are (look at Figure (6) below):

$$\vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2 \tag{226}$$

The nearest neighboring vectors $\vec{R}_{\vec{\delta}}$ are:

$$\vec{R}_{1,0} = (1,0)a,\ \vec{R}_{0,1} = (0,1)a,\ \vec{R}_{-1,0} = (-1,0)a,\ \vec{R}_{0,-1} = (0,-1)a \tag{227}$$

The letter a in the equation above stands for the real atomic distance which translates from an atom to the next one. The energy band for the square lattice considering only nearest neighboring atoms then is (with $\vec{k} = (k_x, k_y)$ **[11]**:

$$\begin{aligned} E &= \varepsilon_0 \sum_{\vec{\delta}} e^{i\vec{k}\bullet\vec{R}_{\vec{\delta}}} = E_0 + \varepsilon_0\left(e^{ik_xa} + e^{-ik_xa}\right) + \varepsilon_0\left(e^{ik_ya} + e^{-ik_ya}\right) \\ &= E_0 + 2\varepsilon_0 \cos(k_xa) + 2\varepsilon_0 \cos(k_ya) \end{aligned} \tag{228}$$

We can again absorb the constant on site term E_0 into the energy E and is not very interesting. In later calculations for any dimensions; we don't write the onsite term anymore and assume that we have absorbed it into the energy E at least when we are working systems without external fields.

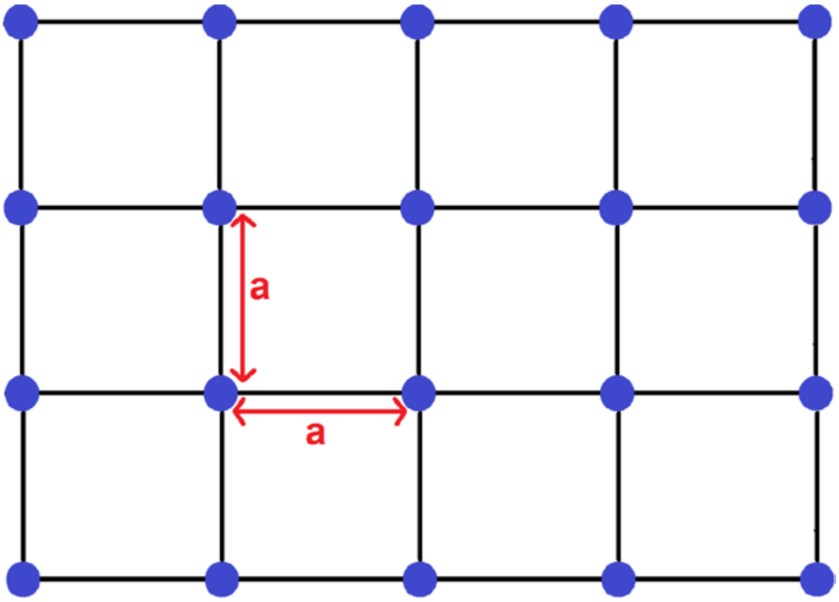


Figure (6): shows the square lattice with nearest neighboring atoms at distance a *from each other*

If considered the next nearest neighboring interactions too; we simply have to include more terms to the energy spectrum in addition to the nearest neighboring terms:

$$\mathrm{E}=\varepsilon_0\sum_{\vec{\delta}}\mathrm{e}^{\mathrm{i}\vec{\mathrm{k}}\bullet\vec{\mathrm{R}}_{\vec{\delta}}}+\varepsilon\sum_{\vec{\Delta}}\mathrm{e}^{\mathrm{i}\vec{\mathrm{k}}\bullet\vec{\mathrm{R}}_{\vec{\Delta}}} \qquad \textbf{(229)}$$

The first term on the right hand side of the above equation is just the sum from equation **(228)** , the second term is the sum over next nearest neighboring vectors labeled $\vec{\mathrm{R}}_{\vec{\Delta}}$ multiplied by the interaction coefficient ε between next nearest neighboring atoms. The next nearest neighboring vectors $\vec{\mathrm{R}}_{\vec{\Delta}}$ are (look at figure (7) below):

$$\vec{\mathrm{R}}_{1,1}=(1,1)\mathrm{a},\ \ \vec{\mathrm{R}}_{-1,1}=(-1,1)\mathrm{a},\ \ \vec{\mathrm{R}}_{1,-1}=(1,-1)\mathrm{a},\ \ \vec{\mathrm{R}}_{-1,-1}=(-1,-1)\mathrm{a} \qquad \textbf{(230)}$$

Inserting those vectors into equation **(229)**; we get the energy band for a square lattice with next nearest neighboring terms included:

$$E(\vec{k})=2\varepsilon_0\left(\cos\left(k_xa\right)+\cos\left(k_ya\right)\right)+4\varepsilon\cos\left(k_xa\right)\cos\left(k_ya\right) \qquad \textbf{(231)}$$

We can of course include more terms involving interactions between neighboring atoms of greater distances, but often only the nearest neighboring and the next nearest neighboring atoms are included when we looking at the overlap between atomic wavefunctions in a given lattice.

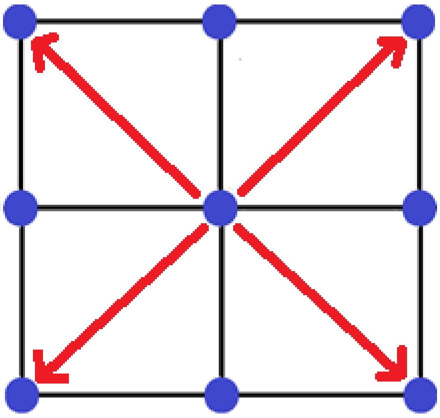


Figure (7): shows the four next nearest neighbor vectors representing the four next nearest atomic sites; the red arrows in the picture are the four next nearest neighboring vectors.

We look at the values of the energy when k is close to the corner; $\vec{k}=\vec{K}_1+\vec{q}$ with $\vec{q}=\left(q_x,q_y\right)$ being a small deviation from the corner point $\vec{K}_1$; that is:

$$\vec{k}=\vec{K}_1+\vec{q}=\left(\frac{\pi}{a}+q_x,\frac{\pi}{a}q_x\right) \tag{232}$$

We have

$$E=E_0+2\varepsilon_0\cos\left(\left(\frac{\pi}{a}+q_x\right)a\right)+2\varepsilon_0\cos\left(\left(\frac{\pi}{a}+q_y\right)a\right) \tag{233}$$

We use the formula for the cosine of the sum of two angles:

$$\cos\left(\left(\frac{\pi}{a}+q_j\right)a\right)=\cos\left(\pi+q_ja\right)=\cos\left(\pi\right)\cos\left(q_ja\right)-\sin\left(\pi\right)\sin\left(q_ja\right)=-\cos\left(q_ja\right) \tag{234}$$

In the above equation; we have $q_j=q_x,q_y$. We then expand the energy and keep only up lowest order in $\vec{q}$:

$$\cos\left(q_ja\right)\approx1-\left(q_ja\right)^2 \tag{235}$$

Using the above equation; the energy near corner point from equation **(233)** then is **[10]**:

$$\begin{aligned}E&\approx E_0-2\varepsilon_0\left(1-\frac{1}{2}q_x^2a^2\right)-2\varepsilon_0\left(1-\frac{1}{2}q_y^2a^2\right)\\&=E_0-4\varepsilon_0+\varepsilon_0a^2\left(q_x^2+q_y^2\right)\end{aligned} \tag{236}$$

The energy band is parabolic (quadratic in q_x and q_y) near the corners for the square lattice. The interesting property of graphene is that it is linear near the corners of the Brillouin zone as we see later, not only that but more, we also get an effective Hamiltonian that is like the Dirac equation in two dimensions, more details will come when we work with graphene.

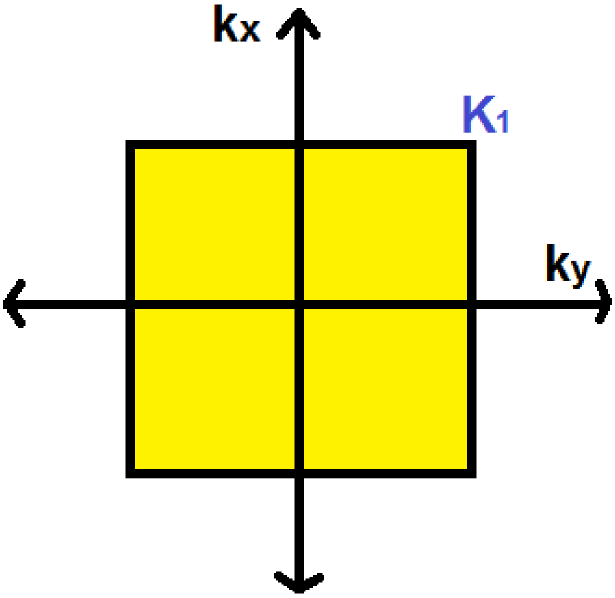


Figure (8): The first Brillouin zone for the square lattice

2.9 Second Quantization:

In the second quantized form on simply writes the quantum numbers of the physical system; we worked previously a little with the ladder operators when we studied the harmonic oscillator; the quantum numbers were simply the states of different energy levels. In the second quantization the ladder operators are important and we make use of them. In the context of many body systems the ladder operators are called creation and annihilation operators as we see why a little later. The creation and annihilation operators are essential in quantizing fields, it is fundamental in the theory of many-body-systems that every operator can be written in terms of the annihilation and creation operators.

Particles with integer spins; **Bosons** and particles with half integer spins; **Fermions** obey different kind of rules. If a physical system is occupied by a number M of particles in each state for example; we have [13]:

$$\left|\ldots\ldots, M_{m-1}, M_m, M_{m+1}, \ldots\ldots\right\rangle \qquad \textbf{(237)}$$

The number operator $\hat{M}_m$ or the occupation number is defined as:

$$\hat{M}_m \left|\ldots\ldots, M_{m-1}, M_m, M_{m+1}, \ldots\ldots\right\rangle = M_m \left|\ldots\ldots, M_{m-1}, M_m, M_{m+1}, \ldots\ldots\right\rangle \qquad \textbf{(238)}$$

In the above equation M_m is simply the number of particles occupying the state m. That means if we sum the number of particles in each state we get the total number M of course:

$$\sum_m M_m = M \qquad \textbf{(239)}$$

A collection of bosons can occupy the same state in the same time while no two fermions can be in one same quantum state; so for a state with fermions can have one particle or zero or no particles occupy it:

$$\begin{gathered} \mathrm{M_m} \in \{0,1\} \text{ for fermions} \\ \text{and} \\ \mathrm{M_m} \in \{0,1,2,......\} \text{ for bosons} \end{gathered} \qquad \textbf{(240)}$$

Bosons:

The operator $\mathrm{a_m}$ in this context called **annihilation** operator because it annihilate a particle in the given state m. The operator $\mathrm{a_m^\dagger}$ is called creation operator because of course it creates a particle in the given state m:

$$\mathrm{a_m^\dagger} \left|......., \mathrm{M_{m-1}}, \mathrm{M_m}, \mathrm{M_{m+1}}, ...\right\rangle = \left|......., \mathrm{M_{m-1}}, \mathrm{M_m}+1, \mathrm{M_{m+1}}, ...\right\rangle \qquad \textbf{(241)}$$

And for the annihilation operator we have:

$$\mathrm{a_m} \left|......., \mathrm{M_{m-1}}, \mathrm{M_m}, \mathrm{M_{m+1}}, ...\right\rangle = \left|......., \mathrm{M_{m-1}}, \mathrm{M_m}-1, \mathrm{M_{m+1}}, ...\right\rangle \qquad \textbf{(242)}$$

When the annihilation operator operates on the ground state; it simply gives zero just as we had for the harmonic oscillator:

$$\mathrm{a_m}\left|0\right\rangle = 0 \qquad \textbf{(243)}$$

Bosons obey the commutations relations just like we had for the harmonic oscillator in section ():

$$\left[a_n, a_m^\dagger\right] = a_n a_m^\dagger - a_m^\dagger a_n = \delta_{nm} \qquad \textbf{(244)}$$

Creation (annihilation) operators commute with other creations (annihilations) operators: we have:

$$\left[a_n^\dagger, a_m^\dagger\right] = \left[a_n, a_m\right] = 0 \qquad \textbf{(245)}$$

The above equation means symmetry under permutation a property of bosons; if two successive operators $a_n^\dagger a_m^\dagger$ are acting on the ground state $\left|0\right\rangle$:

$$a_n^\dagger a_m^\dagger \left|0\right\rangle \qquad \textbf{(246)}$$

Using equation **(245)**; we prove the symmetry under permutation of n and m(could be two different particles with integer spin):

$$a_n^\dagger a_m^\dagger \left|0\right\rangle = \left(\left[a_n^\dagger, a_m^\dagger\right] + a_m^\dagger a_n^\dagger\right)\left|0\right\rangle = a_m^\dagger a_n^\dagger \left|0\right\rangle \qquad \textbf{(247)}$$

Finally the number operator we defined in equation **(238)** could be written in terms of the creation and annihilation operator:

$$\hat{\mathrm{M}}_{\mathrm{m}} = \mathrm{a}_{\mathrm{m}}^{\dagger}\mathrm{a}_{\mathrm{m}} \tag{248}$$

Fermions:

For each quantum state; the occupancy can only be zero **[13]**, no two identical fermions can occupy the same quantum state. An example of a general state for a collection of fermions would look like:

$$\left|1,0,1,1,0,0,0,1,0,0,0,1,1,0,1,0,1,1,1,1,0,0,0,1,............\right\rangle \tag{249}$$

If we start with a ground state of a system; then when a creation operator $\mathrm{c}_{\mathrm{m}}^{\dagger}$ for fermions operating on the ground state would fill the m'th state with one fermion (an electron etc.)

$$\mathrm{c}_{\mathrm{m}}^{\dagger}\left|0,.................,\underset{(\mathrm{m})}{0},............0\right\rangle = \left|0,.................,\underset{(\mathrm{m})}{1},............0\right\rangle \tag{250}$$

And the operator c_{m} annihilates a particle in the m'th state:

$$\mathrm{c}_{\mathrm{m}}\left|0,.................,\underset{(\mathrm{m})}{1},............0\right\rangle = \left|0,.................,\underset{(\mathrm{m})}{0},............0\right\rangle \tag{251}$$

The anticommutation relations are:

$$\left\{c_n, c_m^{\dagger}\right\} = c_n c_m^{\dagger} + c_m^{\dagger} c_n = \delta_{nm} \tag{252}$$

In similar way for commutation relations; the annihilation operator c_n acting on the ground state in the anticommuting case also gives zero:

$$c_n\left|0\right\rangle = 0 \tag{253}$$

And of course for the relation between creation operators and annihilation operators by themselves:

$$\left\{c_n^{\dagger}, c_m^{\dagger}\right\} = \left\{c_n, c_m\right\} = 0 \tag{254}$$

The anticommutation relations are important; they are connected to fermions in that they implement the Pauli Exclusion Principle; that is they are **antisymmetric** under permutation of n and m, which could represent different particles, it is very simple to check; if look at the following the operator $a_n^{\dagger}a_m^{\dagger}$ acting on the ground state, we have:

$$c_n^{\dagger}c_m^{\dagger}\left|0\right\rangle \tag{255}$$

Then if we use the anticommutator from equation **(254)**; we minus the permutation of m and n i.e. they are antisymmetric:

$$c_n^\dagger c_m^\dagger \left|\psi_0\right\rangle = -c_m^\dagger c_n^\dagger \left|\psi_0\right\rangle \tag{256}$$

We can check that in the fermions you can't have more than one fermion in a given state; we operate the some given state by the same creation operator twice and use the result from the equation above to get **[8]**:

$$\begin{aligned} & c_n^\dagger c_n^\dagger \left|\psi\right\rangle = -c_n^\dagger c_n^\dagger \left|\psi\right\rangle \\ & \Rightarrow \left|\psi\right\rangle = -\left|\psi\right\rangle \\ & \Rightarrow \left|\psi\right\rangle = 0 \end{aligned} \tag{257}$$

The above result is what we expected that there cannot be more than one particle in a given state. Finally the number operator $\hat{M}_m$ for fermions is defines similarly to the bosons, only now we have either zero or one:

$$\hat{M}_m = c_m^\dagger c_m \tag{258}$$

2.10 Tight binding in the second quantized form:

If the states of each individual atoms in a lattice are filled shells and there is only one state that is half filled for each atomic site in a lattice (an unoccupied state can have two electrons because of their spins and if there is already an electron occupying the state of interest, then it is half filled); then there is place only for one electron on each atomic state. In the tight binding we are interested in the half filled shells or the state with an unoccupied electron, because this state can interact with neighboring atoms and bond covalently with them. If we start with one dimension and define the vector $\left|n\right\rangle$ as an abstract version of the atomic state in Hilbert space; that is:

$$\left\langle x \middle| n\right\rangle = \varphi\left(x - x_n\right) \tag{259}$$

In the above equation; we have $\varphi\left(x - x_n\right)$ as the atomic state of a single isolated atom in one dimension just as we defined it in the previous section. If we start with a ground state; that is no electron occupying the available atomic states; then by operating the creation operator $c_n^\dagger$ on the ground state; we get an electron in the nth atomic site or simply the state $\left|n\right\rangle$ (that is the state that describes an electron in the m'th atomic site):

$$\left|n\right\rangle = c_n^\dagger \left|0\right\rangle \tag{260}$$

The annihilation operator c_n acted on the ground state gives zero in the usual way:

$$c_n \left|0\right\rangle = 0 \tag{261}$$

The delocalized state $|\mathrm{k}\rangle$ for a single electron in the lattice just as we did in the previous section is a linear combination of the atomic states

$$|\mathrm{k}\rangle=\frac{1}{\sqrt{\mathrm{N}}}\sum_{\mathrm{n}}\mathrm{e}^{\mathrm{ikx_n}}|\mathrm{n}\rangle \tag{262}$$

The vector $|\mathrm{k}\rangle$ is the abstract version of the delocalized vector we had in equation **(212)** for the single electron in a one dimensional lattice:

$$\langle \mathrm{x}|\mathrm{k}\rangle=\psi_{\mathrm{k}}(\mathrm{x}) \tag{263}$$

We have written $\psi_{\mathrm{k}}(\mathrm{x})$ Instead of the way we wrote it in the previous section $\psi(\mathrm{x})$, but the k simply specifies the k-dependence as we know that the most general solution of Schrödinger equation is the sum (or integral in the continuous case) of all solutions with different k. Now when we use the creation operator; we can write the delocalized state as:

$$|k\rangle=\frac{1}{\sqrt{N}}\sum_{n}e^{ikx_n}c_n^{\dagger}|0\rangle \tag{264}$$

We know from equation **(58)** that we can write a Hamiltonian with respect to a given basis. If we use the states of the atoms in the lattice under study as the basis and use the creation operator from equation **(260)**; we get:

$$\hat{H}=\sum_{n.m}^{N}|m\rangle\langle m|\hat{H}|n\rangle\langle n|=\hat{H}=\sum_{n.m}^{N}\varepsilon_{mn}c_m^{\dagger}|0\rangle\langle 0|c_n \tag{265}$$

In the above equation we used the identity from equation **(63)** and equation **(214)** for the atomic sites to write:

$$\varepsilon_{mn}=\langle m|\hat{H}|n\rangle \tag{266}$$

When we take the expectation value of the Hamiltonian $\langle k|\hat{H}|k\rangle$; the result would be exactly the same if wrote the Hamiltonian only in terms of the creation and annihilation operators:

$$\hat{H}=\sum_{n.m}^{N}\varepsilon_{nm}c_n^{\dagger}c_m \tag{267}$$

And as we will see it is right; it gives exactly the same result as we got in equation **(217)** for the one dimension. Let us start with Schrödinger equation the second quantized form:

$$\hat{H}|k\rangle=\frac{1}{\sqrt{N}}\left(\sum_{n.m}^{N}\varepsilon_{nm}c_n^{\dagger}c_m\right)\sum_{s}^{N}e^{ikx_s}c_s^{\dagger}|0\rangle \tag{268}$$

Now we make use of the anticommutation relations from equation **(252)** and **(254)** for the creation and annihilation operators to continue the calculations:

$$
\begin{aligned}
E\left|k\right\rangle &= \hat{H}\left|k\right\rangle = \frac{1}{\sqrt{N}}\sum_{s}^{N}\sum_{n.m}^{N} e^{ikx_s}\varepsilon_{nm}c_n^{\dagger}c_m c_s^{\dagger}\left|0\right\rangle \\
&= \frac{1}{\sqrt{N}}\sum_{s}^{N}\sum_{n.m}^{N} e^{ikx_s}\varepsilon_{nm}c_n^{\dagger}\left(\delta_{sm} - c_s^{\dagger}c_m\right)\left|0\right\rangle \\
&= \frac{1}{\sqrt{N}}\sum_{n.m}^{N} e^{ikx_m}\varepsilon_{nm}c_n^{\dagger}\left|0\right\rangle
\end{aligned}
\tag{269}
$$

Now if we multiply the above equation by the ket of the general vector of the system $\left\langle k\right|$; we get the expectation value of the Hamiltonian operator i.e. the energies because $\left|k\right\rangle$ is the eigenvector of the Hamiltonian; we get:

$$
\begin{aligned}
E\left\langle k\middle|k\right\rangle &= E = \left\langle k\right|\hat{H}\left|k\right\rangle = \left(\frac{1}{\sqrt{N}}\sum_{l}^{N} e^{-ikx_l}\left\langle 0\right|c_l\right)\frac{1}{\sqrt{N}}\sum_{n.m}^{N} e^{ikx_m}\varepsilon_{nm}c_n^{\dagger}\left|0\right\rangle \\
&= \frac{1}{N}\sum_{l}^{N}\sum_{n.m}^{N} e^{ikx_m - ikx_l}\varepsilon_{nm}\left\langle 0\right|c_l c_n^{\dagger}\left|0\right\rangle = \frac{1}{N}\sum_{l}^{N}\sum_{n.m}^{N} e^{ikx_m - ikx_l}\varepsilon_{nm}\delta_{nl} \\
&= \frac{1}{N}\sum_{n.m}^{N} e^{ikx_m - ikx_n}\varepsilon_{nm}
\end{aligned}
\tag{270}
$$

We again have the hopping energies ε_{mn} only depend on the distance between the two atoms as we had in equation **(215)**; $\varepsilon_{mn} = \varepsilon_{n-m}$ so we make the similar substitution: $\delta = n - m \Rightarrow n = \delta + m$ and we get the exact same answer as we had in equation **(217)**:

$$
E = \frac{1}{N}\sum_{n.m}^{N} e^{ikx_m - ikx_n}\varepsilon_{nm} = \frac{1}{N}\sum_{\delta,m}^{N}\varepsilon_{\delta}e^{ikx_{\delta}} = \sum_{\delta}^{N}\varepsilon_{\delta}e^{ikx_{\delta}}
\tag{271}
$$

The three dimensional version is exactly the same; the only difference is that the indices are over three dimensions (three indices for n and m in the above equation) and all the hopping vectors to the atomic sites of the lattice under study are also three-dimensional vectors.

When working with tight binding; often one starts with only nearest neighboring terms in the Hamiltonian; in that case almost all of the terms in equation **(267)** will be neglected; the only two sets of operators kept: the hops to the nearest neighboring atoms in the lattice and the terms that are hopping back to nearest neighboring atoms(i.e. the hermitian conjugate of the nearest neighboring hops); so the Hamiltonian in the nearest neighboring case(in 3D) is :

$$
\hat{H} = \varepsilon_0 \sum_{\vec{n}}^{N}\sum_{\vec{\delta}}\left(c_{\vec{n}}^{\dagger}c_{\vec{n}+\vec{\delta}} + c_{\vec{n}+\vec{\delta}}^{\dagger}c_{\vec{n}}\right)
\tag{272}
$$

In the above equation; the indices $\vec{\delta}$ are only the indices of the nearest neighboring atoms. Notice that we ignored the onsite energy E_0 we had in equation **(218)** from the equation above which as previously discussed could be absorbed into the energy, but of course that is only when are looking at the system without any external fields applied to it.

If we included the spin $\sigma = \left(\uparrow, \downarrow\right)$ of the electrons; then the Hamiltonian from equation **(272)** would be **[15]**:

$$\hat{H} = \varepsilon_0 \sum_{\vec{n},\sigma}^{N} \sum_{\vec{\delta}} \left(c_{\vec{n},\sigma}^{\dagger} c_{\vec{n}+\vec{\delta},\sigma} + c_{\vec{n}+\vec{\delta},\sigma}^{\dagger} c_{\vec{n},\sigma} \right) \tag{273}$$

In this case the anticommutation relations between the annihilation operators $c_{\vec{n},\sigma}$ and the creation operators $c_{\vec{m},\tau}^{\dagger}$ are:

$$\left\{ c_{\vec{n},\sigma}, c_{\vec{m},\tau}^{\dagger} \right\} = \delta_{\vec{n}\vec{m}} \delta_{\sigma\tau} \tag{274}$$

We now drop the spin indices; we include them when we are interested in the full system, but first we are interested in the atomic states without the spin.

2.11 Lattices containing different sublattices:

The final thing we have to study is when there are different sublattices: suppose there are two types of atoms in straight one line of atoms in a one dimensional lattice (see figure (9) below): in this case we have two types of creation and annihilation operators for example $a_{\vec{n}} \left(a_{\vec{n}}^{\dagger} \right)$ and $b_{\vec{m}} \left(b_{\vec{m}}^{\dagger} \right)$. In this case the general Hamiltonian for the whole lattice would be:

$$\hat{\mathrm{H}} = \sum_{\mathrm{n,m}}^{\mathrm{N}} \varepsilon_{\mathrm{nm}} \left(\mathrm{a}_{\mathrm{n}}^{\dagger} \mathrm{b}_{\mathrm{m}} + \mathrm{b}_{\mathrm{m}}^{\dagger} \mathrm{a}_{\mathrm{n}} \right) + \sum_{\mathrm{n,m}}^{\mathrm{N}} \tilde{\varepsilon}_{\mathrm{nm}} \left(\mathrm{a}_{\mathrm{n}}^{\dagger} \mathrm{a}_{\mathrm{m}} + \mathrm{b}_{\mathrm{n}}^{\dagger} \mathrm{b}_{\mathrm{m}} \right) \tag{275}$$

The creation and annihilations operators $a_{\vec{n}} \left(a_{\vec{n}}^{\dagger} \right)$ and $b_{\vec{m}} \left(b_{\vec{m}}^{\dagger} \right)$ follow the anticommuation relations we had in equation **(252)**. The operator $a_{\vec{n}} \left(a_{\vec{n}}^{\dagger} \right)$ creates (annihilates) an electron in the sublattice B(blue colored balls in figure (9) below) and $b_{\vec{m}} \left(b_{\vec{m}}^{\dagger} \right)$ creates(annihilates) an electron in the aublattice R(red colored balls in figure(9)). The first sum of the Hamiltonian involves hops between atoms of different sublattices(Band R) with hopping energies $\varepsilon_{\vec{n}\vec{m}}$ and the second sum involves hops between atoms of same sublattices (B and B, R and R) with hopping energies $\tilde{\varepsilon}_{\vec{n}\vec{m}}$.

Figure (9): shows one dimensional lattice with two different sublattices labeled B(blue) and R(red).

The Schrödinger equation in this case is similar to the one type of atoms in the previous section; however the general eigenstate $\left|k\right\rangle$ is also similar but not exact form:

$$\hat{H}\left|k\right\rangle = E\left|k\right\rangle \tag{276}$$

In the above equation; the eigenstate $\left|k\right\rangle$ is:

$$\left|k\right\rangle = B\left|B_k\right\rangle + R\left|R_k\right\rangle \tag{277}$$

In the above equation B and R are just complex scalars, $\left|B_k\right\rangle$ is the general vector for the B-sublattice and could be written as a linear combination of all atomic eigenstates of the B-sublattice:

$$\left|B_k\right\rangle = \frac{1}{\sqrt{N}}\sum_{\alpha}^{N} e^{ikB_\alpha}\left|\alpha, k\right\rangle \tag{278}$$

And similarly for the general vector $\left|R_k\right\rangle$ which is for the R-sublattice is a linear combination of all atomic eigenstates of the R-sublattice:

$$\left|R_k\right\rangle = \frac{1}{\sqrt{N}}\sum_{\beta}^{N} e^{ikR_\beta}\left|\beta, k\right\rangle \tag{279}$$

In equations (278) and (279) above; B_α and R_β represent the positions of the atoms in B and R-sublattices:

$$B_\alpha = 2a\alpha \tag{280}$$

And

$$R_\beta = B_\beta + a = a\left(2\beta + 1\right) \tag{281}$$

In two equations above; $\alpha, \beta \in \mathbb{Z}$ and a is the real distance between two neighboring atoms. The vectors $\left|\alpha, k\right\rangle$ and $\left|\beta, k\right\rangle$ are the eigenstates of single individual atoms of the sublattices B and R and just as we had in the previous section; the eigenstates of the atoms could be normalized:

$$\left\langle \alpha, k \middle| \tilde{\alpha}, k \right\rangle = \delta_{\alpha\tilde{\alpha}} \tag{282}$$

And for the sublattice R:

$$\left\langle \beta, k \middle| \tilde{\beta}, k \right\rangle = \delta_{\beta\tilde{\beta}} \tag{283}$$

And last for the inner product between eigenvectors of different sublattices; we have:

$$\left\langle \alpha, k \middle| \beta, k \right\rangle = 0 \tag{284}$$

The three equations above and the equations **(278)** and **(279)** make the general vectors $\left|\mathrm{B_k}\right\rangle$ and $\left|\mathrm{R_k}\right\rangle$ normalized too:

$$\left\langle \mathrm{B_k} \middle| \mathrm{B_k} \right\rangle = \left\langle \mathrm{R_k} \middle| \mathrm{R_k} \right\rangle = 1 \tag{285}$$

And inner product between general vectors of different sublattices:

$$\left\langle \mathrm{B_k} \middle| \mathrm{R_k} \right\rangle = 0 \tag{286}$$

Getting back to Schrödinger equation **(276)**; solving it in this case is similar to the case of one type of atoms lattices only here we get two coupled equations; one for B and one for R. We get the two coupled equations by multiplying Schrödinger equation by the ket vector of the general vectors of each sublattice; the first one is by multiplication with $\left\langle \mathrm{B_k} \right|$:

$$\begin{aligned} &\left\langle \mathrm{B_k} \middle| \hat{\mathrm{H}} \middle| \mathrm{k} \right\rangle = \left\langle \mathrm{B_k} \middle| \hat{\mathrm{H}} \middle| \mathrm{B_k} \right\rangle \mathrm{B} + \left\langle \mathrm{B_k} \middle| \hat{\mathrm{H}} \middle| \mathrm{R_k} \right\rangle \mathrm{R} \\ &= \mathrm{E}\left(\left\langle \mathrm{B_k} \middle| \mathrm{B_k} \right\rangle \mathrm{B} + \left\langle \mathrm{B_k} \middle| \mathrm{R_k} \right\rangle \mathrm{R} \right) = \mathrm{EB} \end{aligned} \tag{287}$$

Similarly we get the second coupled equation by multiplication with $\left\langle \mathrm{R_k} \right|$ and we get:

$$\left\langle \mathrm{R_k} \middle| \hat{\mathrm{H}} \middle| \mathrm{B_k} \right\rangle \mathrm{B} + \left\langle \mathrm{R_k} \middle| \hat{\mathrm{H}} \middle| \mathrm{R_k} \right\rangle \mathrm{R} = \mathrm{ER} \tag{288}$$

We can write equations **(287)** and **(288)** as a 2x2 matrix equation:

$$\begin{pmatrix} \left\langle B_k \middle| \hat{H} \middle| B_k \right\rangle & \left\langle B_k \middle| \hat{H} \middle| R_k \right\rangle \\ \left\langle R_k \middle| \hat{H} \middle| B_k \right\rangle & \left\langle R_k \middle| \hat{H} \middle| R_k \right\rangle \end{pmatrix} \begin{pmatrix} B \\ R \end{pmatrix} = E \begin{pmatrix} B \\ R \end{pmatrix} \tag{289}$$

The elements of the above equation are computed exactly the same way it was done for a lattice with one type atoms (the diagonal terms of the above equation):

$$\left\langle B_k \middle| \hat{H} \middle| B_k \right\rangle = \left\langle R_k \middle| \hat{H} \middle| R_k \right\rangle = \sum_{\Delta}^{N} \tilde{\varepsilon}_{\Delta} e^{ikx_{\Delta}} \tag{290}$$

The symbol Δ above runs over all the distances between atoms of the same sublattice. The off-diagonal terms of equation **(289)** are:

$$\left\langle B_k \middle| \hat{H} \middle| R_k \right\rangle = \sum_{\delta}^{N} \varepsilon_{\delta} e^{ikx_{\delta}} \tag{291}$$

The last term $\left\langle R_k \middle| \hat{H} \middle| B_k \right\rangle$ (by hermiticity of the physical operator i.e. the Hamiltonian $\hat{H}$) is simply the complex conjugate of the above expression. The δ in the above equation is the index of all the distances between atoms of different sublattices. Finally for the 3D case; simply make δ and Δ each become the three indices one for each dimension. Also x_{Δ} and x_{δ} simply become three dimensional vectors.

Let us apply the above result to the 1D case when we only consider the nearest neighboring hops between atoms of the lattice. The off-diagonal terms of equation (289) will only have two terms $x_{\pm 1} = \pm a$ and we get a simply expression:

$$\langle B_k | \widehat{H} | R_k \rangle = \varepsilon_0 \left(e^{ika} + e^{-ika} \right) = 2\varepsilon_0 \cos(ka) \tag{292}$$

The diagonal terms of equation **(289)** are zero when we only consider nearest neighboring hops between atoms. The complete coupled equation in k-space then is:

$$\begin{pmatrix} 0 & 2\varepsilon_0 \cos(ka) \\ 2\varepsilon_0 \cos(ka) & 0 \end{pmatrix} \begin{pmatrix} B \\ R \end{pmatrix} = E \begin{pmatrix} B \\ R \end{pmatrix} \tag{293}$$

The eigenvalue equation above has the solutions for the energy:

$$E = \pm 2\varepsilon_0 \cos(ka) \tag{294}$$

The graphene lattice is a two dimensional lattice with two different types of sublattices; so it is a little similar to the above equation and as we have seen that we get a matrix equation.

In the case of graphene; we have a two component (coupled) matrix equation with off-diagonal terms being linear near the corners of the Brillouin zone and the energy is linear in the momentum i.e. they follow a differential equation that is like The Dirac equation (see section (2.12) below) in 2D only with different constants (e.g. c is not speed of light in graphene). We study graphene in detail later on in this project.

2.12 Dirac Equation:

Dirac equation is:

$$\mathrm{i}\hbar\gamma^{\mu}\partial_{\mu}\psi - \mathrm{mc}\psi = 0 \tag{295}$$

Where γ^{μ} are four4×4 matrices; $\mu = 0,1,2,3$ that we can write in terms of pauli-matrices, the identity matrix and the zero matrix **[6]**:

$$\gamma^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \gamma^1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}, \gamma^2 = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}, \gamma^3 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \tag{296}$$

Or in a more compact and elegant way:

$$\gamma^0 = \begin{pmatrix} \mathrm{I} & 0 \\ 0 & -\mathrm{I} \end{pmatrix} \quad \gamma^1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix} \quad \gamma^2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix} \quad \gamma^3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix} \tag{297}$$

That is we simply write them in terms of 2×2 Pauli matrices and the identity matrix:

$$\mathrm{I}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\quad 0=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix},\ \sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0 & -i\\ \mathrm{i} & 0\end{pmatrix},\ \sigma_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \qquad \textbf{(298)}$$

Dirac's equation describes relativistic particles with half integer spin (Fermions). It is the equivalent of the Schrödinger equation when we include relativistic effects, but only describes fermions as the case gets more complicated when we include special relativity, there are other equations that describe bosons such as the Klein Gordon equation which also includes solutions to the Dirac equation, but that is not the subject of interest in this project, so we stop there.

Later when we work with graphene; we would be interested in Dirac's equation in two dimensions. So we need to study the two dimensional version of Dirac's equation; we know from Einstein's theory of special relativity that the energy squared can be written as:

$$E^2 = p^2c^2 + m^2c^4 \qquad (299)$$

The approach that Dirac took which he did for the 3+1 dimensional space-time is keeping the equation linear in time derivative so if we try the same for the two dimensional case; we must have:

$$\begin{aligned} E &= \vec{\alpha}\bullet\vec{p}c + \beta m \\ &= \alpha_x p_x c + \alpha_y p_y c + \beta mc^2 \end{aligned} \qquad (300)$$

Now in order for the above equation to be valid; the square of the energy E must satisfy the relativistic equation for the energy:

$$\begin{aligned} E^2 &= \left(\alpha_x p_x c + \alpha_y p_y c + \beta mc^2\right)^2 \\ &= \alpha_x^2 p_x^2 c^2 + \alpha_y^2 p_y^2 c^2 + \beta^2 m^2 c^4 \\ &+ p_x p_y c^2\left(\alpha_x\alpha_y + \alpha_y\alpha_x\right) + p_x mc^3\left(\alpha_x\beta + \beta\alpha_x\right) + p_y mc^3\left(\alpha_y\beta + \beta\alpha_y\right) \end{aligned} \qquad (301)$$

So in order for equations **(300)** and **(301)** to be valid; the last three terms in the parenthesis of the above equation must be zero, that is:

$$\left(\alpha_x\alpha_y + \alpha_y\alpha_x\right) = \left(\alpha_x\beta + \beta\alpha_x\right) = \left(\alpha_y\beta + \beta\alpha_y\right) = 0 \qquad (302)$$

These symbols α_x, α_y and β must be matrices in order to fulfill equation **(301)**. If we make the following ansatz for a matrix A_-:

$$\mathrm{A}_- = \begin{pmatrix} \mathrm{mc}^2 & \mathrm{c}\left(\mathrm{p_x} - \mathrm{ip_y}\right) \\ \mathrm{c}\left(\mathrm{p_x} + \mathrm{ip_y}\right) & -\mathrm{mc}^2 \end{pmatrix} \qquad (303)$$

Then the squared of the above matrix is:

$$\begin{aligned} A_-^2 &= \begin{pmatrix} c^2\left(p_x^2+p_y^2\right)+m^2c^4 & 0 \\ 0 & c^2\left(p_x^2+p_y^2\right)+m^2c^4 \end{pmatrix} \\ &= \left(p_x^2c^2+p_y^2c^2+m^2c^4\right)I = E^2 I \end{aligned} \tag{304}$$

The above equation means that the matrix A_- fulfills the requirements of the relativistic energy. That means we can have the following solutions for the matrices α_x, α_y and β :

$$\alpha_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \alpha_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{305}$$

And the time-independent Dirac equation in 2D can be written as:

$$\begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} p_x c + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} p_x c + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 \tag{306}$$

The time-dependent Dirac equation becomes:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} i\hbar \frac{\partial \psi}{\partial t} = -i\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\partial \psi}{\partial x} - i\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{\partial \psi}{\partial y} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 \tag{307}$$

One can express the 2D Dirac's equation in different ways by simple matrix transformation. We also have the matrix A_+ which does satisfy the conditions for relativistic energy:

$$A_+ = \begin{pmatrix} mc^2 & p_x + ip_y \\ p_x - ip_y & -mc^2 \end{pmatrix} \tag{308}$$

It is actually a theorem in relativistic quantum mechanics that we also have A_+ which has to do with chirality, the matrices A_- and A_+ describe particles with opposite chirality related to their spins and the direction of momentum. As for graphene; there are pseudo spins related simply to two inequivalent Dirac points as we shall in the next part of this project.

Part ll: Electronic Structure of Graphene, Single Layer, Bilayer and Fewlayers Graphene

3. Monolayer Graphene

3.1 Introduction to Graphene

Graphene is a two dimensional allotrope of carbon. It has a hexagonal shaped lattice; each carbon atom has four valence electrons. Three of those four form tight bonds (the strong σ bonds) with neighboring atoms in the graphene plane and this band will have filled shells because the Pauli principle (look at figure (10) below. They form a trigonal structure on the plane (the sp^2 hybridization between ones orbital and two p orbitals) **[14]**,**[15]**. The strong σ bond between Carbon atoms is the reason for robustness of graphene. The three tight bounded electrons don't play part in the conductivity.

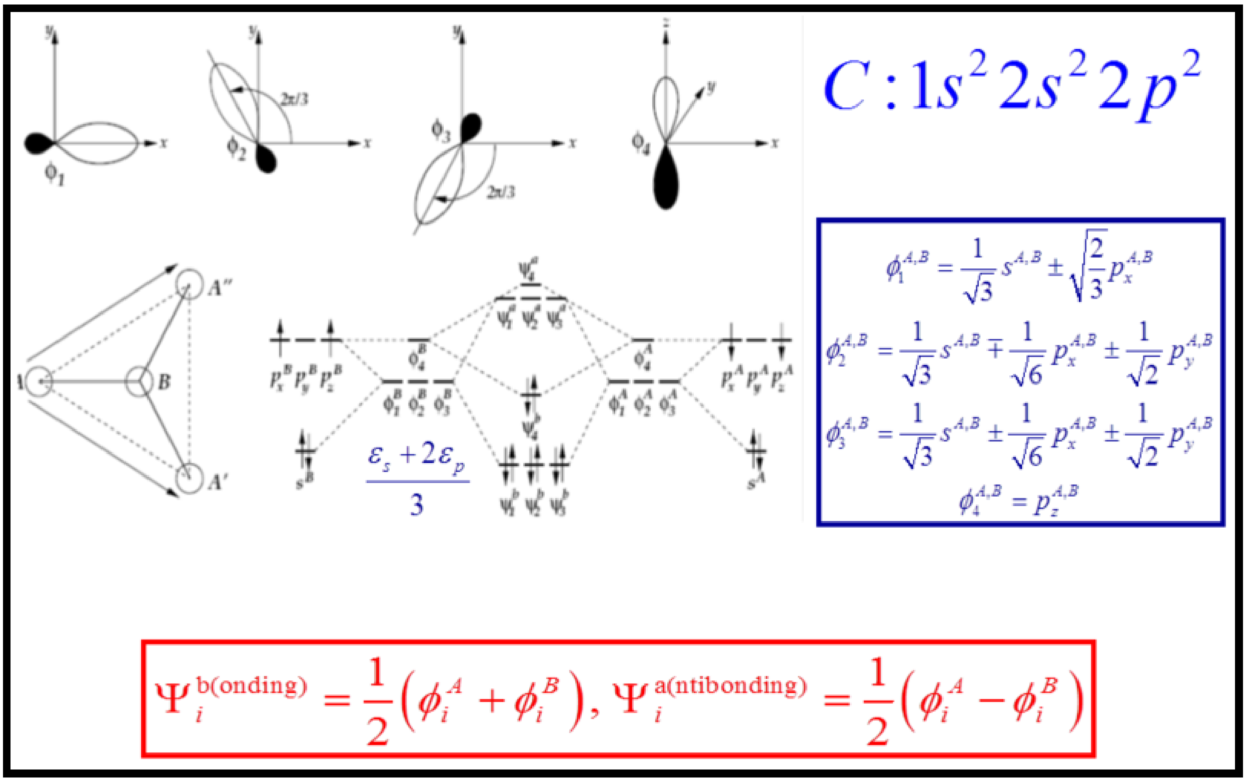


Figure (10): shows the chemistry of graphene, the sp^2 *hybridization the* sp^2 *hybridization between the one s orbital and the two p orbitals and covalent bonds* **[14]**.

The fourth electron is considered to be in the $2p_z$ state perpendicular to the planar structure; it bonds covalently with neighboring Carbon atoms. The fourth electron forms a π bond with neighboring carbon atoms. Since there is only electron in each $2p_z$ orbital; then they make half-filled bands, so only the fourth electron will play part in the conductivity. We therefore can treat graphene as having one conduction electron in the $2p_z$ state **[16]**.

In the rest of the project we will only be interested in the $2p_z$ state of individual atoms and study the overlap between the state wavefunctions between carbon atoms of the whole graphene lattice in the tight binding approximation.

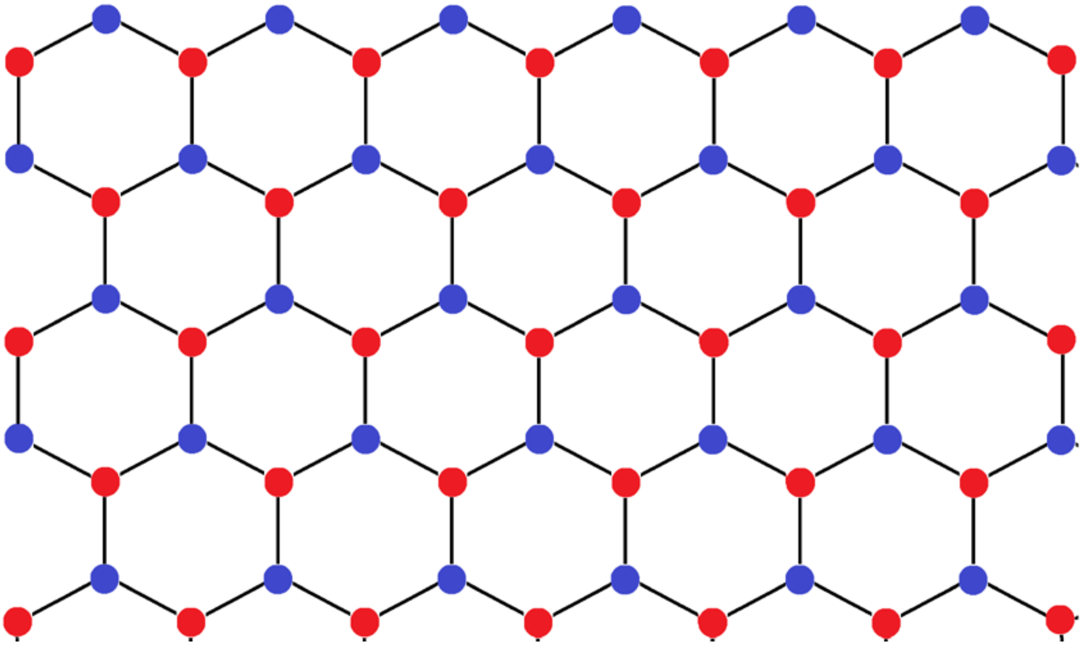


Figure (11): Graphene lattice (hexagonal shape)

In most articles; they are have chosen the letters A and B for labeling of the two sublattices of graphene lattice; in this project the two sublattices are labeled B for blue and R for red, almost all of the Figures have the color blue and red to distinguish the two sublattices.

Let us now write all the vectors of atomic sites in a graphene lattice explicitly in terms of primitive vectors; $\vec{e}_1$ and $\vec{e}_2$ (look at Figure (12) below) defined as:

$$\vec{e}_1 = \left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right)\mathrm{a} \quad , \quad \vec{e}_1 = \left(-\frac{\sqrt{3}}{2}, \frac{3}{2}\right)a \qquad (309)$$

We have to start somewhere, so we choose the origin at the blue site; the position vectors $\vec{B}_{\vec{n}}$ are positions of all atomic sites for sublattice B, since graphene is two dimensional; $\vec{n}$ is only indices n_1 and n_2; where $n_1, n_2 \in \mathbb{Z}$. The vectors $\vec{B}_{\vec{n}}$ for the blue sublattice can be written as:

$$\vec{B}_{\vec{n}} \equiv \vec{B}_{n_1,n_2} = n_1\vec{e}_1 + n_2\vec{e}_2 \qquad \mathbf{(310)}$$

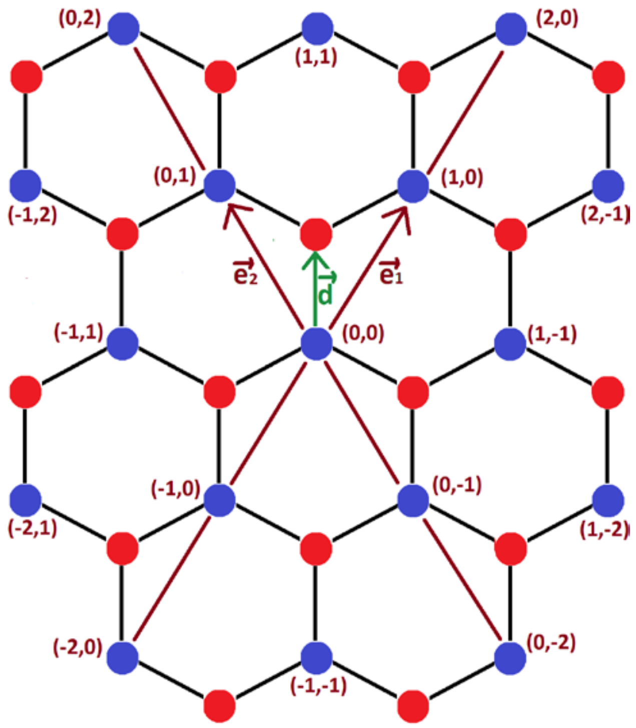


Figure (12) show a discrete coordinate system representing atomic sites in a graphene lattice with origin lies on an atom from the blue sublattice B.

The R-sublattice vectors differ from the B-sublattice vectors by a translation $\vec{d} = a\left(0,1\right)$ otherwise similar (look at figure (12) above), and the vectors for R-Sublattice; $\vec{R}_{\vec{m}}$ is then:

$$\vec{R}_{\vec{m}} \equiv \vec{R}_{m_1,m_2} = m_1\vec{e}_1 + m_2\vec{e}_2 + \vec{d} = \vec{B}_{m_1,m_2} + \vec{d} \qquad \textbf{(311)}$$

Where in the above equation; $m_1, m_2 \in \mathbb{Z}$. We can construct a general Hamiltonian for graphene considering all neighboring atoms similar to the Hamiltonian from equation **(275)** but with vector sign over the indices m and n as we are working with two-dimensional substance here:

$$\begin{aligned} \hat{H}_{gen} &= \sum_{\vec{n},\vec{m}}^{N} \varepsilon_{\vec{n}\vec{m}} \left(a^{\dagger}_{\vec{n}} b_{\vec{m}} + b^{\dagger}_{\vec{m}} a_{\vec{n}} \right) + \sum_{\vec{n},\vec{m}}^{N} \tilde{\varepsilon}_{\vec{n}\vec{m}} \left(a^{\dagger}_{\vec{n}} a_{\vec{m}} + b^{\dagger}_{\vec{n}} b_{\vec{m}} \right) \\ &= \hat{H}_{gen,0} + \hat{H}_{gen,1} \end{aligned} \qquad \textbf{(312)}$$

The first term $\hat{H}_{gen,0}$ in the last equality of the above equation **(312)** represents for all hops to neighboring of different sublattices (B to R and R to B) with hopping energies $\varepsilon_{\vec{m},\vec{n}}$:

$$\hat{H}_{gen,0} = \sum_{\vec{m},\vec{n}} \varepsilon_{\vec{m},\vec{n}} \left(a^{\dagger}_{\vec{m}} b_{\vec{n}} + b^{\dagger}_{\vec{n}} a_{\vec{m}} \right) \qquad \textbf{(313)}$$

The second term $\hat{H}_{gen,1}$ of the last equality of equation **(312)** represents all the hops to neighboring atoms of same sublattice (B to B and R to R) with hopping energies $\tilde{\varepsilon}_{\vec{m},\vec{n}}$:

$$\hat{H}_{gen,1} = \sum_{\vec{m},\vec{n}} \tilde{\varepsilon}_{\vec{m},\vec{n}} \left(a_{\vec{m}}^{\dagger} a_{\vec{n}} + b_{\vec{m}}^{\dagger} b_{\vec{n}} \right) \tag{314}$$

The operator $a_{\vec{n}}^{\dagger}(a_{\vec{n}})$ Creates (annihilates) an electron on atomic site $\vec{B}_{\vec{n}}$ and on B-sublattice (blue) and $b_{\vec{m}}^{\dagger}(b_{\vec{m}})$ creates (annihilates) an electron on atomic site $\vec{R}_{\vec{m}}$ and on R-sublattice(red), (look at figure()) below.

The Anticommutations relations from equations **(252)** and **(254)**) hold for the each ladder operator $a_{\vec{n}}$ and $b_{\vec{m}}$:

$$\left\{ \mathrm{a}_{\vec{n}}, \mathrm{a}_{\vec{m}}^{\dagger} \right\} = \delta_{\vec{n}\vec{m}} \tag{315}$$

And the same for the R-sublattice:

$$\left\{ \mathrm{b}_{\vec{n}}, \mathrm{b}_{\vec{m}}^{\dagger} \right\} = \delta_{\vec{n}\vec{m}} \tag{316}$$

And last the operators for the B-sublattice; $\mathrm{a}_{\vec{n}}, \mathrm{a}_{\vec{n}}^{\dagger}$ anticommute with the operators of the R-sublattice $\mathrm{b}_{\vec{m}}, \mathrm{b}_{\vec{m}}^{\dagger}$ anticommute with each other:

$$\left\{ a_{\vec{n}}, b_{\vec{m}} \right\} = \left\{ a_{\vec{n}}, b_{\vec{m}}^{\dagger} \right\} = \left\{ a_{\vec{n}}^{\dagger}, b_{\vec{m}} \right\} = \left\{ a_{\vec{n}}^{\dagger}, b_{\vec{m}} \right\} = 0 \tag{317}$$

The delocalized statevector of the whole system is a superposition of two statevectors, one vector for each sublattice:

$$\left| \psi_{\vec{k}} \right\rangle = B \left| B_{\vec{k}} \right\rangle + R \left| R_{\vec{k}} \right\rangle \tag{318}$$

The coefficients B and R in the above equation are just complex numbers. The statevectors $\left| B_k \right\rangle$ and $\left| R_k \right\rangle$ are a superposition of all atomic states for each atomic site in their sublattices B(blue) or R(red) respectively which combined makes up the whole lattice atoms in one graphene layer and taking into account the translations symmetry i.e. the Bloch form of the statevectors $\left| B_k \right\rangle$ and $\left| R_k \right\rangle$; we have:

$$\left| B_{\vec{k}} \right\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{u}=1}^{N} e^{i\vec{k}\bullet\vec{B}_{\vec{u}}} \left| \vec{u}, B \right\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{u}=1}^{N} e^{i\vec{k}\bullet\vec{B}_{\vec{u}}} a_{\vec{u}}^{\dagger} \left| 0 \right\rangle \tag{319}$$

And the eigenvector $\left|R_{\vec{k}}\right\rangle$ is:

$$\left|R_{\vec{k}}\right\rangle = \frac{1}{\sqrt{N}}\sum_{\vec{v}=1}^{N} e^{i\vec{k}\bullet\vec{R}_{\vec{v}}}\left|\vec{v},R\right\rangle = \frac{1}{\sqrt{N}}\sum_{\vec{v}=1}^{N} e^{i\vec{k}\bullet\vec{R}_{\vec{v}}} b_{\vec{v}}^{\dagger}\left|0\right\rangle \qquad \textbf{(320)}$$

Where in the two equations above; we have used the creation operator to rewrite the statevectors of individual atoms belonging to the atomic sites of graphene lattice in terms of the creation operators and the ground state of the atomic states (or simply the state with an unoccupied electron just as we had in equation **(260)** from section (2.10):

$$\left|\vec{u},B\right\rangle = a_{\vec{u}}^{\dagger}\left|0\right\rangle \qquad (321)$$

And

$$\left|\vec{v},R\right\rangle = b_{\vec{v}}^{\dagger}\left|0\right\rangle \qquad (322)$$

They are the eigenvectors of the atoms in each sublattice in Hilbert space:

$$\left\langle x\middle|\vec{u},B\right\rangle = \varphi_{B}\left(\vec{r}-\vec{r}_{\vec{u}}\right) \qquad (323)$$

And

$$\left\langle x\middle|\vec{v},R\right\rangle = \varphi_{R}\left(\vec{r}-\vec{r}_{\vec{v}}\right) \qquad (324)$$

Where $\left|0\right\rangle$ is the ground state of the whole system; we also have the following conditions:

$$a_{\vec{n}}\left|0\right\rangle = b_{\vec{m}}\left|0\right\rangle = 0 \qquad \textbf{(325)}$$

We can always choose the atomic statevector to be normalized (we neglect overlap terms); for the B-sublattice we have:

$$\left\langle \vec{\mathrm{w}},\mathrm{B}\middle|\vec{\mathrm{u}},\mathrm{B}\right\rangle = \left\langle 0\middle|\mathrm{a}_{\vec{\mathrm{w}}}\mathrm{a}_{\vec{\mathrm{u}}}^{\dagger}\middle|0\right\rangle = \delta_{\vec{\mathrm{u}}\vec{\mathrm{v}}} \qquad \textbf{(326)}$$

And for the R-sublattice we have similar equation:

$$\left\langle \vec{\mathrm{w}},\mathrm{R}\middle|\vec{\mathrm{u}},\mathrm{R}\right\rangle = \left\langle 0\middle|\mathrm{b}_{\vec{\mathrm{w}}}\mathrm{b}_{\vec{\mathrm{v}}}^{\dagger}\middle|0\right\rangle = \delta_{\vec{\mathrm{w}}\vec{\mathrm{v}}} \qquad \textbf{(327)}$$

Last we have the inner product between the two sulattice atomic statevectors are equal to zero:

$$\left\langle \vec{\mathrm{w}},\mathrm{B}\middle|\vec{\mathrm{u}},\mathrm{R}\right\rangle = \left\langle 0\middle|\mathrm{a}_{\vec{\mathrm{w}}}\mathrm{b}_{\vec{\mathrm{u}}}^{\dagger}\middle|0\right\rangle = \left\langle \vec{\mathrm{u}},\mathrm{R}\middle|\vec{\mathrm{w}},\mathrm{B}\right\rangle = \left\langle 0\middle|\mathrm{b}_{\vec{\mathrm{u}}}\mathrm{a}_{\vec{\mathrm{w}}}^{\dagger}\middle|0\right\rangle = 0 \qquad \textbf{(328)}$$

We can also make the delocalized states $\left|B_{\vec{k}}\right\rangle$ and $\left|R_{\vec{k}}\right\rangle$ orthonormal when the atomic states are orthonormal, so the normalization of the atomic states is the more difficult task; the delocalized ones are easy normalize.

We make the delocalized statevectors for each sublattice $\left|B_{\vec{k}}\right\rangle$ and $\left|R_{\vec{k}}\right\rangle$ orthonormal by simply multiplying by the inverse square root of the total number of atomic sites $\frac{1}{\sqrt{N}}$; such that we have the following relations too:

$$\begin{aligned}\left\langle B_{\vec{k}} \middle| B_{\vec{k}}\right\rangle &= \frac{1}{N}\sum_{\vec{u},\vec{w}=1}^{N} e^{i\vec{k}\bullet\left(\vec{B}_{\vec{u}}-\vec{B}_{\vec{w}}\right)}\left\langle \vec{w},B \middle| \vec{u},B\right\rangle \\ &= \frac{1}{N}\sum_{\vec{u},\vec{w}=1}^{N} e^{i\vec{k}\bullet\left(\vec{B}_{\vec{u}}-\vec{B}_{\vec{w}}\right)}\delta_{\vec{u}\vec{w}} \\ &= \frac{1}{N}\sum_{\vec{u}=1}^{N}1=1\end{aligned} \tag{329}$$

Similarly for the eigenvector $\left|R_{\vec{k}}\right\rangle$ for the R-sublattice:

$$\left\langle R_{\vec{k}} \middle| R_{\vec{k}}\right\rangle = 1 \tag{330}$$

Last we have the inner product between general vectors of different sublatties equal to zero:

$$\left\langle B_k \middle| R_k\right\rangle = \left\langle R_k \middle| B_k\right\rangle = 0 \tag{331}$$

3.2 Tight-binding Hamiltonian 1.nearest neighbors

We start by considering only nearest neighboring atoms; that is to say that the statevectors of farther atoms distance than nearest ones have very small overlap with each other; which means $\tilde{\varepsilon}_{\vec{m},\vec{n}}$ is zero in equation **(314)** and $\varepsilon_{\vec{m},\vec{n}}$ are only non-zero for the nearest neighbor atoms which they have the same value $\varepsilon_0 \approx 2.8eV$ **[15]**; the Hamiltonian of the system then is:

$$\hat{H}_0 = -\varepsilon_0 \sum_{\vec{n},m} a_{\vec{n}}^{\dagger} b_{\vec{n}+\vec{\delta}_m} + b_{\vec{n}+\vec{\delta}_m}^{\dagger} a_{\vec{n}} \tag{332}$$

The indices $\vec{\delta}_m$ in the above equation are indices of the nearest neighboring vectors. Now using equations **(332)** and **(318)**; Schrödinger equation becomes:

$$\hat{H}_0\left|\psi_k\right\rangle = \hat{H}_0\left(B\left|B_k\right\rangle + R\left|R_k\right\rangle\right) = E\left(B\left|B_k\right\rangle + R\left|R_k\right\rangle\right) \tag{333}$$

We get two coupled equations, one for each statevector and we have to solve an eigenvalue equation to find the energy dispersion relation for graphene. We multiply the above equation from the left side by the bra vector $\langle B_k |$; we get:

$$\begin{aligned} \langle B_k | \hat{H}_0 | \psi_k \rangle &= \langle B_k | \hat{H}_0 | B_k \rangle B + \langle B_k | \hat{H}_0 | R_k \rangle R \\ &= E \langle B_k | B_k \rangle B + E \langle R_k | R_k \rangle R \end{aligned} \tag{334}$$

Using the orthonormality relations from equations **(329)** and **(331)**; the above equation becomes:

$$\langle B_k | \hat{H}_0 | B_k \rangle B + \langle B_k | \hat{H}_0 | R_k \rangle R = E(k) B \tag{335}$$

We now multiply Schrödinger equation **(333)** by the second statevector $\langle R_k |$; we get a similar equation to equation **(335)** above; only for the R-sublattice:

$$\langle R_k | \hat{H}_0 | B_k \rangle B + \langle R_k | \hat{H}_0 | R_k \rangle R = E(k) R \tag{336}$$

Equations **(335)** and **(336)** are coupled equations as expected and they are written in k-space, we write both equations in one matrix equation just as we did in equation **(289)** i.e. Schrödinger equation for the whole system:

$$\begin{pmatrix} \langle B_k | \hat{H}_0 | B_k \rangle & \langle B_k | \hat{H}_0 | R_k \rangle \\ \langle R_k | \hat{H}_0 | B_k \rangle & \langle R_k | \hat{H}_0 | R_k \rangle \end{pmatrix} \begin{pmatrix} B \\ R \end{pmatrix} = E \begin{pmatrix} B \\ R \end{pmatrix} \tag{337}$$

Now if we use the Hamiltonian $\hat{H}_0$ from equation **(332)** and the expressions for $| R_k \rangle$ and $| B_k \rangle$ from equations **(319)** and **(320)**; it is very easy to compute the matrix elements of the matrix in the above equation; we start by operating $\hat{H}_0$ on the statevectors $| R_k \rangle$ and $| B_k \rangle$; for $| R_k \rangle$ we have:

$$\langle B_k | \hat{H}_0 | R_k \rangle = -\varepsilon_0 \sum_{m=1}^{3} e^{i\vec{k} \bullet \vec{\delta}_m} = -\varepsilon_0 \left(e^{-i\vec{k} \bullet \vec{\delta}_1} + e^{-i\vec{k} \bullet \vec{\delta}_2} + e^{-i\vec{k} \bullet \vec{\delta}_3} \right) = -\varepsilon_0 g(\vec{k}) \tag{338}$$

Where we have defined the function $g(\vec{k})$ as:

$$g(\vec{k}) = \sum_{m=1}^{3} e^{i\vec{k} \bullet \vec{\delta}_m} = e^{i\vec{k} \bullet \vec{\delta}_1} + e^{i\vec{k} \bullet \vec{\delta}_2} + e^{i\vec{k} \bullet \vec{\delta}_3} \tag{339}$$

The values nearest neighbor $\vec{\delta}_m$ vectors are:

$$\vec{\delta}_1 = (0,1)\mathrm{a}\,,\ \vec{\delta}_2 = \left(\frac{\sqrt{3}}{2}, -\frac{1}{2} \right) \mathrm{a} \text{ and } \vec{\delta}_3 = \left(-\frac{\sqrt{3}}{2}, -\frac{1}{2} \right) a \tag{340}$$

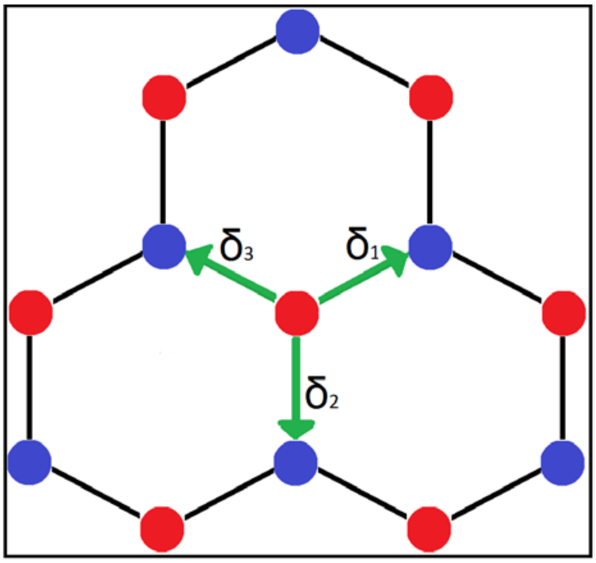


Figure (13) a: red site jumps

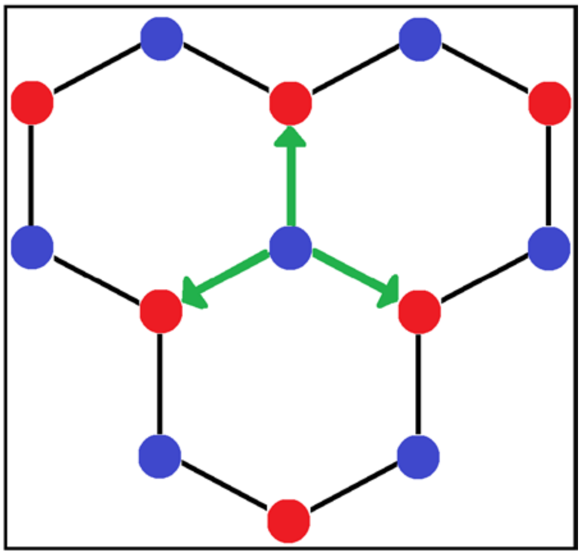


Figure (13) b: blue site jumps

We calculate $g(\vec{k})$ explicitly putting the values of $\vec{\delta}_1, \vec{\delta}_2$ and $\vec{\delta}_3$, we have $\vec{k} = \left(k_x, k_y\right)$ is simply the random momentum vector in momentum (more accurate Fourier k-vector in k-space, but related to momentum); then $g(\vec{k})$ is:

$$g(\vec{k}) = 2\cos\left(\frac{\sqrt{3}}{2}k_x a\right)e^{ik_y a/2} + e^{-ik_y a} \qquad \textbf{(341)}$$

We calculate the matrix elements from equation **(337)**:

$$\begin{aligned} \langle B_k | \hat{H}_0 | B_k \rangle &= \langle B_k | \varepsilon_0 g(\vec{k}) | R_k \rangle \\ &= -\varepsilon_0 g(\vec{k}) \langle B_k | R_k \rangle = 0 \end{aligned} \qquad (342)$$

We also get zero for $\langle R_k | \hat{H}_0 | R_k \rangle = 0$ in the same way; the last term is:

$$\langle R_k | \hat{H}_0 | B_k \rangle = -\varepsilon_0 g(\vec{k})^* \qquad (343)$$

Now finally we can write the Schrödinger equation **(337)** in k-space explicitly:

$$\hat{H}_0(\vec{k})\begin{pmatrix} B \\ R \end{pmatrix} = \begin{pmatrix} 0 & -\varepsilon_0 g(\vec{k}) \\ -\varepsilon_0 g(\vec{k})^* & 0 \end{pmatrix}\begin{pmatrix} B \\ R \end{pmatrix} = E\begin{pmatrix} B \\ R \end{pmatrix} \qquad \textbf{(344)}$$

Let us move the right hand side of equation **(344)** to the left hand side; we get:

$$\left(\hat{H}_0(k) - EI\right)\begin{pmatrix} B \\ R \end{pmatrix} = \begin{pmatrix} -E & -\varepsilon_0 g(\vec{k}) \\ -\varepsilon_0 g(\vec{k})^* & -E \end{pmatrix}\begin{pmatrix} B \\ R \end{pmatrix} = 0 \qquad \textbf{(345)}$$

It is very easy to solve the above eigenvalue equation, by simply putting the determinant of $\hat{H}_0(k)-E(k)I$ equal to zero:

$$\det\left(\hat{H}_0(\vec{k})-EI\right)=0 \tag{346}$$

Equation **(346)** gives:

$$\left(E\right)^2-\varepsilon_0^2 g(\vec{k})g(\vec{k})^*=0 \tag{347}$$

And finally the energy dispersion relation (look at figure (16) below):

$$E(\vec{k})=\pm\varepsilon_0\left|g(\vec{k})\right| \tag{348}$$

The absolute value of $\left|g(\vec{k})\right|$ is equal to:

$$\left|g(\vec{k})\right|=\left(g(\vec{k})g(\vec{k})^*\right)^{1/2}=\left(1+4\cos^2\left(\frac{\sqrt{3}}{2}k_x a\right)+4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{3}{2}k_y a\right)\right)^{1/2} \tag{349}$$

So the dispersion relation for one layer graphene considering only nearest neighbor approximations is:

$$E(\vec{k})=\pm\varepsilon_0\left(1+4\cos^2\left(\frac{\sqrt{3}}{2}k_x a\right)+4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{3}{2}k_y a\right)\right)^{1/2} \tag{350}$$

Now let us find the eigenvectors of equation by inserting the result from equation **(348)** for the energy into equation **(345)**; we get:

$$\begin{pmatrix}-E & \varepsilon_0 g(\vec{k})\\ \varepsilon_0 g(\vec{k})^* & -E\end{pmatrix}\begin{pmatrix}B\\ R\end{pmatrix}=\begin{pmatrix}\mp\varepsilon_0\left|g(\vec{k})\right| & \varepsilon_0 g(\vec{k})\\ \varepsilon_0 g(\vec{k})^* & \mp\varepsilon_0\left|g(\vec{k})\right|\end{pmatrix}\begin{pmatrix}B\\ R\end{pmatrix}=0 \tag{351}$$

Then the state vectors are equal to:

$$\begin{pmatrix}B\\ R\end{pmatrix}=\begin{pmatrix}1\\ \pm\dfrac{g(\vec{k})^*}{\left|g(\vec{k})\right|}\end{pmatrix} \tag{352}$$

Now if we consider the next nearest neighbor approximations hopping energy in addition to the nearest one; then the Hamiltonian becomes:

$$\hat{H}=-\varepsilon_0\sum_{\vec{n},m}\left(a_{\vec{n}}^{\dagger}b_{\vec{n}+\vec{\delta}_m}+b_{\vec{n}+\vec{\delta}_m}^{\dagger}a_{\vec{n}}\right)-\varepsilon\sum_{\vec{n},s}^{N}\left(a_{\vec{n}}^{\dagger}a_{\vec{n}+\vec{\Delta}_s}+a_{\vec{n}+\vec{\Delta}_s}^{\dagger}a_{\vec{n}}\right)-\varepsilon\sum_{\vec{n},s}^{N}\left(b_{\vec{n}}^{\dagger}b_{\vec{n}+\vec{\Delta}_s}+b_{\vec{n}+\vec{\Delta}_s}^{\dagger}b_{\vec{n}}\right) \tag{353}$$

Where we have added the next neighbor $\hat{H}_1$ term to $\hat{H}_0$ from equation **(332)**:

$$\hat{H}_1 = -\varepsilon \sum_{\vec{n},s}^{N} \left(a_{\vec{n}}^{\dagger} a_{\vec{n}+\vec{\Delta}_s} + a_{\vec{n}+\vec{\Delta}_s}^{\dagger} a_{\vec{n}} \right) - \varepsilon \sum_{\vec{n},s}^{N} \left(b_{\vec{n}}^{\dagger} b_{\vec{n}+\vec{\Delta}_s} + b_{\vec{n}+\vec{\Delta}_s}^{\dagger} b_{\vec{n}} \right) \qquad \textbf{(354)}$$

Where ε is the next nearest neighbor hopping energy between the same sublattices B-B (R-R). There are six points for each sublattice (look at Figure (14) below):

$$\Delta_1 = \left(\frac{\sqrt{3}}{2}, \frac{3}{2} \right) a, \quad \Delta_2 = \left(\sqrt{3}, 0 \right) a, \quad \Delta_3 = \left(\frac{\sqrt{3}}{2}, -\frac{3}{2} \right) a \qquad \textbf{(355)}$$

The other three next nearest neighbor vectors are simply the minus of these three vectors above.

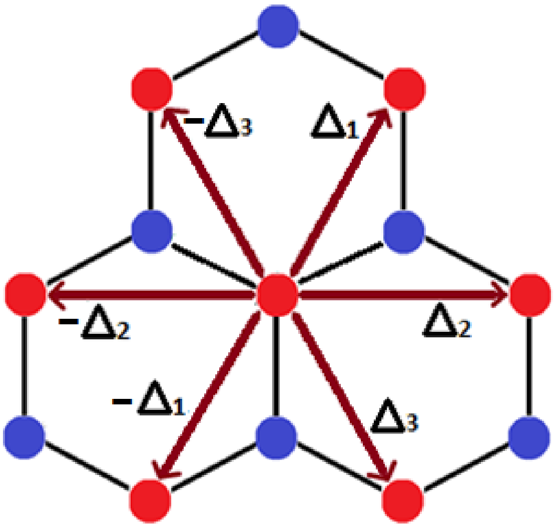


Figure (14) a: blue site jumps

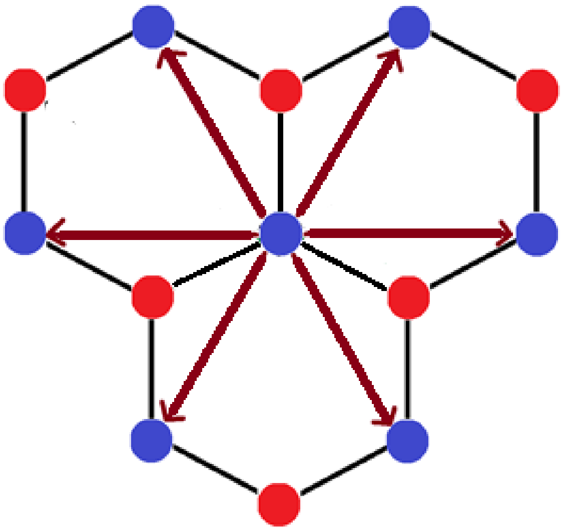


Figure (14) b: red site jumps

The Schrödinger equation from **(337)** preserves its form when added the next-nearest neighbor approximation term; the only difference is that now the Hamiltonian $\hat{H}$ is a sum of the two terms; $\hat{H}_0$ and $\hat{H}_1$:

$$\begin{pmatrix} \langle B_k | \hat{H} | B_k \rangle & \langle B_k | \hat{H} | R_k \rangle \\ \langle R_k | \hat{H} | B_k \rangle & \langle R_k | \hat{H} | R_k \rangle \end{pmatrix} \begin{pmatrix} B \\ R \end{pmatrix} = E \begin{pmatrix} B \\ R \end{pmatrix} \qquad (356)$$

Using the expression from equation **(320)** for the general statevector of R-sublattice $|R_k\rangle$ and the values of the six next nearest neighbor vectors; we get:

$$\langle R_k | \hat{H} | R_k \rangle = -\varepsilon \sum_{s=1}^{6} e^{i\vec{k}\cdot\vec{\Delta}_s} = -\varepsilon f(\vec{k}) \qquad \textbf{(357)}$$

Where $f(\vec{k})$ in the above equation is:

$$f(\vec{k}) \equiv \sum_{s=1}^{6} e^{i\vec{k}\cdot\vec{\Delta}_s} \tag{358}$$

If we operate $\hat{H}$ on the B-sublattice statevector; we get exactly the same result as above:

$$\left\langle B_k \middle| \hat{H} \middle| B_k \right\rangle = -\varepsilon f(\vec{k}) \tag{359}$$

Putting the values of $\vec{\Delta}_s$ from equation **(355)** for next nearest neighbor vectors to calculate $f(\vec{k})$ explicitly; we get:

$$f(\vec{k}) = 4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{3}{2}k_y a\right) + 2\cos\left(\sqrt{3}k_x a\right) \tag{360}$$

We know all the terms in the Hamiltonian **(356)**:

$$\hat{H}(\vec{k})\begin{pmatrix} B \\ R \end{pmatrix} = \left(\begin{pmatrix} -\varepsilon f(\vec{k}) & -\varepsilon_0 g(\vec{k}) \\ -\varepsilon_0 g(\vec{k})^* & -\varepsilon f(\vec{k}) \end{pmatrix}\right)\begin{pmatrix} B \\ R \end{pmatrix} = E\begin{pmatrix} B \\ R \end{pmatrix} \tag{361}$$

Finding the dispersion relation means that we again have to solve the eigenvalue equation

$$\det\left(\hat{H}(\vec{k}) - EI\right) = 0 \tag{362}$$

This gives the equation:

$$\left(\varepsilon f(\vec{k}) - E\right)^2 - \varepsilon_0^2 g(\vec{k}) g(\vec{k})^* = 0 \tag{363}$$

Solving for E The equation above gives the dispersion relation:

$$E(\vec{k}) = -\varepsilon f(\vec{k}) \pm \varepsilon_0 \left|g(\vec{k})\right| \tag{364}$$

Writing the above equation explicitly using the expressions for $\left|g(\vec{k})\right|$ and $f(\vec{k})$ from equations **(349)** and **(360)**; we have the dispersion relation:

$$\begin{aligned} E(\vec{k}) &= -2\varepsilon\cos\left(\sqrt{3}k_x a\right) - 4\varepsilon\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{3}{2}k_y a\right) \\ &\pm \varepsilon_0\left(1 + 4\cos^2\left(\frac{\sqrt{3}}{2}k_x a\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{3}{2}k_y a\right)\right)^{1/2} \end{aligned} \tag{365}$$

We can use the following identity:

$$4\cos^2\left(\frac{\sqrt{3}}{2}k_x a\right)=4\left(\frac{\cos\left(\sqrt{3}k_x a\right)+1}{2}\right) \tag{366}$$

And write the solution for the energy in terms of $f(\vec{k})$:

$$E(\vec{k})=-\varepsilon f(\vec{k})\pm\varepsilon_0\left(3+f(\vec{k})\right)^{1/2} \tag{367}$$

The answer looks nicer in the above form **[15]**.

3.3 Solutions near Dirac points:

Let us go back to the Hamiltonian $\hat{H}_0(k)$ from the matrix equation **(344)** for the nearest neighbor approximation for graphene; we had:

$$\hat{H}_0(k)=\begin{pmatrix} 0 & \varepsilon_0 g(k) \\ \varepsilon_0 g(k)^* & 0 \end{pmatrix} \tag{368}$$

We want study the effective Hamiltonian for graphene near Fermi energy; he hexagonal Brillion zone of graphene has six corners of which only two are inequivalent, the rest can be expressed in terms Dirac points; $\vec{K}_+$ and $\vec{K}_-$ (they are equivalent points to those two):

$$\vec{K}_+=\frac{2\pi}{3\sqrt{3}a}\left(1,-\sqrt{3}\right) \text{ and } \vec{K}_-=\frac{2\pi}{3\sqrt{3}a}\left(-1,-\sqrt{3}\right) \tag{369}$$

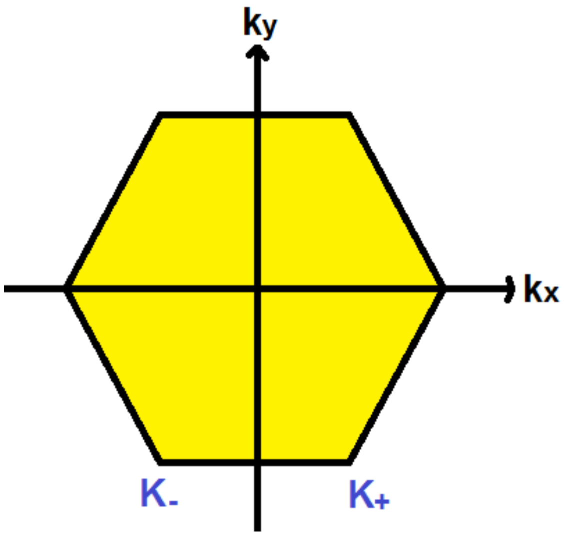


Figure (15): shows the first Brillion zone for graphene lattice in reciprocal space and two inequivalent Dirac points; $\vec{K}_+$ *and* $\vec{K}_-$ *.*

We start with $\vec{K}_+$ and look at $\vec{k}$ in the following circle in $\vec{k}-space$:

$$\vec{k} \approx \vec{K}_+ + \vec{q} \tag{370}$$

Where in the above equation; $\vec{q}$ is a small deviation from the Dirac point $\vec{K}_+$. Let us use the expression for $\vec{k}$ from the above equation into the function $g(k)$ from equation **(339)**:

$$g(\vec{K}_+ + \vec{q}) = \sum_{m=1}^{3} e^{i\left(\vec{K}_+ + \vec{q}\right)\bullet\vec{\delta}_m} = \sum_{j=1}^{3} e^{i\vec{K}_+\bullet\vec{\delta}_m} e^{i\vec{q}\bullet\vec{\delta}_m} \tag{371}$$

Now since $\vec{q}$ is a small number; we can expand $e^{i\vec{q}\bullet\vec{\delta}_m}$ and only the first order term in $\vec{q}$ (the linear term) would be dominating, the other ones become very small; we get:

$$e^{i\vec{q}\bullet\vec{\delta}_m} = 1 + \vec{q}\bullet\vec{\delta}_m + O\left(\vec{q}^2\right) \approx 1 + \vec{q}\bullet\vec{\delta}_m \tag{372}$$

Putting the above expression into equation **(371)**; we get:

$$\begin{aligned} g(\vec{K}_+ + \vec{q}) &= \sum_{m=1}^{3} e^{i\vec{K}_+\bullet\vec{\delta}_m} e^{i\vec{q}\bullet\vec{\delta}_m} = \sum_{m=1}^{3} e^{i\vec{K}_+\bullet\vec{\delta}_m} \left(1 + i\vec{q}\bullet\vec{\delta}_m\right) \\ &= \underbrace{\sum_{m=1}^{3} e^{i\vec{K}_+\bullet\vec{\delta}_m}}_{=0} + i\sum_{j=1}^{3} e^{i\vec{K}_+\bullet\vec{\delta}_m} \vec{q}\bullet\vec{\delta}_m \end{aligned} \tag{373}$$

The first term in the in the last equality of the above equation is zero because it is simply the function $g(k)$ and it is exactly zero at Dirac points; so we have:

$$\begin{aligned} g(\vec{K}_+ + \vec{q}) &= i\sum_{m=1}^{3} e^{i\vec{K}_+\bullet\vec{\delta}_m} \vec{q}\bullet\vec{\delta}_m \\ &= ie^{i\vec{K}_+\bullet\vec{\delta}_1} \vec{q}\bullet\vec{\delta}_1 + ie^{i\vec{K}_+\bullet\vec{\delta}_2} \vec{q}\bullet\vec{\delta}_2 + ie^{i\vec{K}_+\bullet\vec{\delta}_3} \vec{q}\bullet\vec{\delta}_3 \end{aligned} \tag{374}$$

We put the values of $\vec{\delta}_m$ from equation **(340)** into the above equation and after a little algebra; we get the final result which is linear in $\vec{q}$ **[14]**, **[17]**:

$$g(\vec{K}_+ + \vec{q}) \approx -\frac{3a}{2}\left(\frac{1}{2} + i\frac{\sqrt{3}}{2}\right)\left(q_x + iq_y\right) = \frac{3a}{2} e^{i\frac{2\pi}{3}} \left(q_x - iq_y\right) \tag{375}$$

Now we can write the effective Hamiltonian for graphene near Dirac point; $\vec{K}_+$:

$$\hat{H}_0(\vec{K}_+ + \vec{q}) = \begin{pmatrix} 0 & \varepsilon_0 g(\vec{K}_+ + \vec{q}) \\ \varepsilon_0 g(\vec{K}_+ + \vec{q})^* & 0 \end{pmatrix} \approx -\frac{3a\varepsilon_0}{2} \begin{pmatrix} 0 & e^{i\frac{2\pi}{3}} q_- \\ e^{-i\frac{2\pi}{3}} q_+ & 0 \end{pmatrix} \tag{376}$$

In the above equation; we have $q_- \equiv q_x - iq_y$ and $q_+ \equiv q_x + iq_y$.The phases $e^{\pm i\frac{2\pi}{3}}$ are not important; they cancel out when we solve the energy eigenvalue equation; so we can ignore them. We can do exactly similar calculations for the second Dirac point $\vec{K}_-$; (ignoring the phases); we get:

$$\hat{H}_0(\vec{k})_{\vec{k}=\vec{K}_-+\vec{q}} \approx -\frac{3a\varepsilon_0}{2}\begin{pmatrix} 0 & q_+ \\ q_- & 0 \end{pmatrix} \qquad \textbf{(377)}$$

The energy $E(k)$ is proportional to $\left(g(\vec{k})g(\vec{k})^*\right)^{1/2}$ as we have seen in equation **(348)**; the product becomes a product of two linear terms now, using the above equation we see that the energy is proportional to:

$$E(\vec{q}) \sim \left(\left(-e^{-i\frac{2\pi}{3}}\left(q_x - iq_y\right)\right)\left(-e^{i\frac{2\pi}{3}}\left(q_x + iq_y\right)\right)\right)^{1/2} = \frac{3a}{2}\sqrt{q_x^2 + q_y^2} = \frac{3a}{2}|\vec{q}| \qquad \textbf{(378)}$$

The energy is independent of the factor $-e^{-i\frac{2\pi}{3}}$, it doesn't have any physical effect; we might as well drop it and write the Hamiltonian in the linear form in momentum which is the interesting property of quasiparticles in graphene; $\hat{H}_0(\vec{q})_+ \equiv \hat{H}_0(\vec{k})_{\vec{k}=\vec{K}_++\vec{q}}$ as:

$$\hat{H}_0(\vec{q})_+ = \varepsilon_0\frac{3a}{2}\begin{pmatrix} 0 & \left(q_x - iq_y\right) \\ \left(q_x + iq_y\right) & 0 \end{pmatrix} = \hbar v_F\begin{pmatrix} 0 & \left(p_x - ip_y\right) \\ \left(p_x + ip_y\right) & 0 \end{pmatrix} \qquad \textbf{(379)}$$

The Hamiltonian around the second Dirac point is similar to above, only helicity is reversed:

$$\hat{H}_0(\vec{q})_- = \hbar v_F\begin{pmatrix} 0 & \left(p_x + ip_y\right) \\ \left(p_x - ip_y\right) & 0 \end{pmatrix} \qquad \textbf{(380)}$$

Where in the above equation v_F is the Fermi velocity and equal to:

$$v_f = \frac{3\varepsilon_0 a}{2\hbar} \approx 10^6\,\frac{m}{s} = c/300 \qquad \textbf{(381)}$$

The letter c in the above equation is of course the speed of light. We could have also seen that $E(k)$ is proportional to $|\vec{q}|$ near Dirac's point directly from equations**(350)** by expanding it around Dirac's points **[15]:**

$$E(\vec{K}_+ + \vec{q}) = \pm\varepsilon_0\left|g(\vec{K}_+ + \vec{q})\right| \approx \pm\varepsilon_0\frac{3a}{2}|\vec{q}| + O\left(|\vec{q}|^2\right) \qquad \textbf{(382)}$$

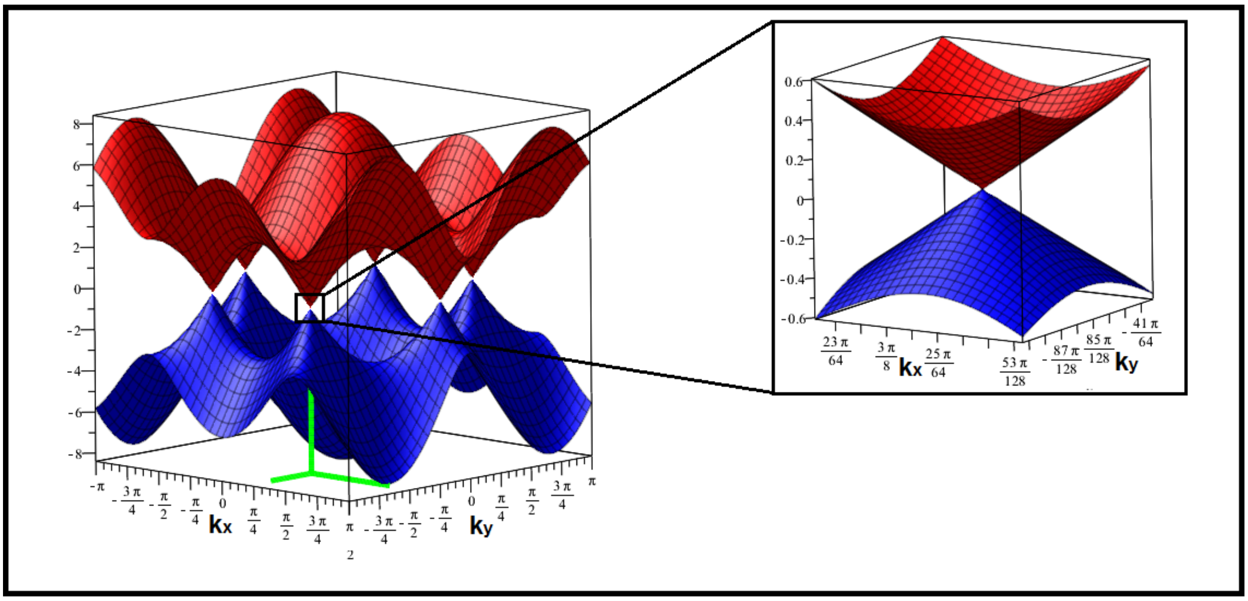


Figure (16): Left; shows the energy band of graphene in the tight binding model nearest neighboring approximation, Right; shows the behavior near Dirac's point $\vec{K}_+$ *shown in large.*

Now let us look at Schrödinger equation near Dirac's point $\vec{K}_+$; we have:

$$\hat{H}_0(\vec{q})_+ \begin{pmatrix} B \\ R \end{pmatrix} = \hbar v_F \begin{pmatrix} 0 & (q_x - iq_y) \\ (q_x + iq_y) & 0 \end{pmatrix} \begin{pmatrix} B \\ R \end{pmatrix} = E(\vec{q}) \begin{pmatrix} B \\ R \end{pmatrix} \tag{383}$$

We can rewrite the above equation in terms of Pauli matrices; the Hamiltonian $\hat{H}_0(\vec{q})_+$ can be written as:

$$\begin{aligned} \hbar v_F \begin{pmatrix} 0 & (q_x - iq_y) \\ (q_x + iq_y) & 0 \end{pmatrix} &= \hbar v_F \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} q_x + \hbar v_F \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} q_y \\ &= \hbar v_F \sigma_x q_x + \hbar v_F \sigma_y q_y = \hbar v_F (\sigma_x, \sigma_y) \bullet (\hat{q}_x, \hat{q}_y) = \hbar v_F \hat{\sigma} \bullet \vec{q} \end{aligned} \tag{384}$$

Let us solve the eigenvalues for equation **(383)**; we get:

$$E(\vec{q})^2 - \left(\frac{3a\varepsilon_0}{2} \right)^2 |\vec{q}|^2 = 0 \tag{385}$$

Then the dispersion relation is:

$$E(\vec{q}) = \pm \frac{3a\varepsilon_0}{2} |\vec{q}| = \pm \hbar v_F |\vec{q}| \tag{386}$$

If we included the next nearest neighboring term in our calculations up to first order; we find that it only contributes with a constant:

$$E(\vec{q}) = 3\varepsilon \pm \hbar v_F |\vec{q}| \qquad \textbf{(387)}$$

So the first order in the next nearest neighboring term is not interesting, it just shifts the energy by a constant 3ε. If one includes in the calculations the second order in $\vec{q}$; then the dispersion relation would be direction dependent, but the second order term has an effect for higher momentums.

As you can see from equations **(379)** and **(386)** that both the energy $E(\vec{q})$ and the Hamiltonian $\hat{H}_0(\vec{q})_+$ themselves are linear in $\vec{q}$ near Dirac points; which is a unique property of graphene lattice.

Equation **(383)** is like Dirac equation in momentum space for particles with mass equal to zero (ultrarelativistic particles, but of course with Fermi velocity not the speed of light) and with spin equal to half. The Solutions near Dirac points $\vec{K}_-$ and $\vec{K}_+$ look like "antiparticles", which of course they are not. The form of the Hamiltonian for graphene near Dirac points raises the question; do we get similar phenomenon for the lattice to what we get for the spin ½ particles Dirac equation? This has to be determined experimentally. The Klein paradox has been experimentally observed for graphene.

3.4 General symmetry of graphene around Dirac's points:

Let us investigate the zeros of the function $g(\vec{k})$:

$$g(\vec{k})^* g(\vec{k}) = 1 + 4\cos^2\left(\frac{\sqrt{3}}{2}k_x a\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{3}{2}k_y a\right) = 0 \qquad (388)$$

The above equation is second degree polynomial in cosines; we make a substitution to look simpler:

$$A = \cos\left(\frac{\sqrt{3}}{2}k_x a\right),\ b = \cos\left(\frac{3}{2}k_y a\right), \quad -1 \le A \le 1, \quad -1 \le b \le 1 \qquad (389)$$

Then equation **(388)** becomes:

$$1 + 4bA + 4A^2 = 0 \qquad (390)$$

We get the solutions for A:

$$\mathrm{A} = -\frac{\mathrm{b}}{2} \pm \frac{1}{2}\sqrt{\mathrm{b}^2 - 1} \qquad (391)$$

The solutions of b have the condition for cosine:

$$\mathrm{b} = \pm 1 \Rightarrow \mathrm{A} = \mp \frac{1}{2} \tag{392}$$

We finally have the solutions, we either have:

$$\begin{aligned} & b = -1 \Rightarrow K_y = \pm \frac{2}{3}(\pi + 2\pi N) \\ & \Rightarrow A = +\frac{1}{2} \Rightarrow K_x = \pm \frac{2}{\sqrt{3}}\left(\frac{\pi}{3} + 2\pi N\right), \;\; K_x = \pm \frac{2}{\sqrt{3}}\left(\frac{5\pi}{3} + 2\pi N\right) \end{aligned} \tag{393}$$

Or for the plus solution; we have:

$$\begin{aligned} & b = +\frac{1}{2} \Rightarrow K_y = \pm \frac{2}{3}(0 + 2\pi N) \\ & \Rightarrow A = -\frac{1}{2} \Rightarrow K_x = \pm \frac{2}{\sqrt{3}}\left(\frac{2\pi}{3} + 2\pi N\right), \;\; K_x = \pm \frac{2}{\sqrt{3}}\left(\frac{4\pi}{3} + 2\pi N\right) \end{aligned} \tag{394}$$

Which among the solutions; we have the two inequivalent Dirac points from equation**(369)**. If one takes consideration the whole lattice vectors and not just nearest neighbor ones; one can wonder whether other terms can dominating when the nearest neighbor function $g(k)$ is zero. If there are points where the functions of the whole lattice is zero; it has to be one of Dirac's points because that is only where the nearest neighbor is zero term is zero.

When we looked at the next-nearest neighbor approximation in the previous section; we only had the terms of equation **(313)** that correspond to nearest neighbor vectors; $\vec{R}_{0,0}, \vec{R}_{-1,0}, \vec{R}_{0,-1}$ with hopping energies:

$$\tilde{\varepsilon}_{0,0} = \tilde{\varepsilon}_{0,-1} = \tilde{\varepsilon}_{-1,0} \equiv \varepsilon_0 \tag{395}$$

And also only the first term of equation **(314)** with hopping energies:

$$\tilde{\varepsilon}_{1,0} = \tilde{\varepsilon}_{0,1} = \tilde{\varepsilon}_{-1,0} = \tilde{\varepsilon}_{0,-1} = \tilde{\varepsilon}_{1,-1} = \tilde{\varepsilon}_{-1,1} \equiv \varepsilon \tag{396}$$

The Schrödinger equation for the general Hamiltonian is:

$$\hat{H}_{gen}\left|\psi_k\right\rangle = E\left|\psi_k\right\rangle \tag{397}$$

Writing it in terms of statevectors of each sublattice:

$$\hat{H}_{gen}\left|\psi_k\right\rangle = \hat{H}_{gen}\left|B_k\right\rangle + \hat{H}_{gen}\left|R_k\right\rangle = E\left|B_k\right\rangle + E\left|R_k\right\rangle \tag{398}$$

The above equation for the general Hamiltonian is similar to what we considered for the next nearest neighbor approximation, only we have to add contributions from all neighboring atoms.

Let us write equation **(398)** as two coupled equations for each statevector $\left|B_k\right\rangle$ and $\left|R_k\right\rangle$ of the above equation separately; do so by the usual way of multiplication by $\left\langle B_k\right|$:

$$\begin{aligned}&\left\langle B_k\right|\hat{H}_{gen}\left|\psi_k\right\rangle=\left\langle B_k\right|\hat{H}_{gen}\left|B_k\right\rangle B+\left\langle B_k\right|\hat{H}_{gen}\left|R_k\right\rangle R\\&=E\left\langle B_k\middle|B_k\right\rangle B+\left\langle B_k\middle|R_k\right\rangle R\end{aligned}\qquad\textbf{(399)}$$

And we get the second one by multiplying Schrödinger equations by $\left\langle R_k\right|$:

$$\begin{aligned}&\left\langle R_k\right|\hat{H}_{gen}\left|\psi_k\right\rangle=\left\langle R_k\right|\hat{H}_{gen}\left|B_k\right\rangle B+\left\langle R_k\right|\hat{H}_{gen}\left|R_k\right\rangle R\\&=E\left\langle R_k\middle|B_k\right\rangle B+\left\langle R_k\middle|R_k\right\rangle R\end{aligned}\qquad(400)$$

We can calculate each term in equations **(399)** and **(400)** in the usual way we do for tight binding; we start with the off diagonal terms:

$$\left\langle B_k\right|\hat{H}_{gen}\left|R_k\right\rangle=\sum_{m,n}\varepsilon_{m,n}e^{i\vec{k}\bullet\vec{R}_{m,n}}\equiv G(\vec{k})\qquad\textbf{(401)}$$

And the other one is simply the complex conjugate of the above expression as it should be in order for the matrix to be hermitian:

$$\left\langle R_k\right|\hat{H}_{gen}\left|B_k\right\rangle=G^*(\vec{k})\qquad(402)$$

The last two diagonal terms, which must be real and they are:

$$\left\langle B_k\right|\hat{H}_{gen}\left|B_k\right\rangle=\left\langle R_k\right|\hat{H}_{gen}\left|R_k\right\rangle=\sum_{m,n}\tilde{\varepsilon}_{m,n}e^{i\vec{k}\bullet\vec{B}_{m,n}}\equiv F(\vec{k})\qquad(403)$$

The function $F(\vec{k})$ in the above equation represents all the hops between atoms of the same sublattice blue to blue. In the next nearest neighbor approximation; $F(\vec{k})$ is reduced to $\varepsilon f(\vec{k})$ as we already have seen. And the function $G(\vec{k})$ represents all hops of atoms different from different sublattices blue to red. In the next nearest neighbor approximation; $G(\vec{k})$ is reduced to $\varepsilon_0 g(\vec{k})$ which also is already known. We have two equations in k-space:

$$F(\vec{k})B+G(\vec{k})R=EB\qquad\textbf{(404)}$$

And

$$G(\vec{k})^*B+F(\vec{k})R=ER\qquad\textbf{(405)}$$

Writing them in matrix form:

$$\begin{pmatrix}F(\vec{k}) & G(\vec{k})\\ G(\vec{k})^* & F(\vec{k})\end{pmatrix}\begin{pmatrix}B\\R\end{pmatrix}=E(\vec{k})\begin{pmatrix}B\\R\end{pmatrix}\qquad\textbf{(406)}$$

Then it is easier to see that all we need is to solve for the eigenvalue equation for the energy of the whole lattice:

$$\begin{pmatrix} F(\vec{k})-E(\vec{k}) & G(\vec{k}) \\ G(\vec{k})^* & F(\vec{k})-E(\vec{k}) \end{pmatrix}\begin{pmatrix} B \\ R \end{pmatrix}=0 \tag{407}$$

Putting the determinant of the above equation equal to zero in the usual way; we get the following equation:

$$\left(F(\vec{k})-E(\vec{k})\right)^2-G(\vec{k})G(\vec{k})^*=0 \tag{408}$$

The dispersion relation for the general case in the tight binding approximation for a graphene lattice is then:

$$E(\vec{k})=F(\vec{k})\pm\left|G(\vec{k})\right| \tag{409}$$

In order to study the whole lattice near Dirac points; we expand the general functions for the entire lattice around Dirac points $\vec{k}=\vec{K}_+ +\vec{q}$ where $\vec{q}$ is small, just as we did for the nearest neighbor approximation and only keep the terms up to first order and study the behavior in that area. We start with diagonal term:

$$F(\vec{K}_+ +\vec{q})=\sum_{m,n}\tilde{\varepsilon}_{m,n}e^{i(\vec{K}_+ +\vec{q})\bullet\vec{B}_{m,n}}=\sum_{m,n}\tilde{\varepsilon}_{m,n}e^{i\vec{K}_+\bullet\vec{B}_{m,n}}e^{i\vec{q}\bullet\vec{B}_{m,n}} \tag{410}$$

Keeping only the first order term in $\vec{q}$ of the above equation; we get:

$$\begin{aligned} F(\vec{K}_+ +\vec{q}) &\approx \sum_{m,n}\tilde{\varepsilon}_{m,n}e^{i\vec{K}_+\bullet\vec{B}_{m,n}}\left(1+i\vec{q}\bullet\vec{B}_{m,n}\right) \\ &=\sum_{m,n}\tilde{\varepsilon}_{m,n}e^{i\vec{K}_+\bullet\vec{B}_{m,n}}+i\sum_{m,n}\tilde{\varepsilon}_{m,n}\vec{q}\bullet\vec{B}_{m,n}e^{i\vec{K}_+\bullet\vec{B}_{m,n}} \\ &\equiv f_{1mn}+f_{2mn} \end{aligned} \tag{411}$$

And for the off diagonal term:

$$G(\vec{K}_+ +\vec{q})=\sum_{m,n}\varepsilon_{m,n}e^{i(\vec{K}_+ +\vec{q})\bullet\vec{R}_{m,n}}=\sum_{m,n}\varepsilon_{m,n}e^{i\vec{K}_+\bullet\vec{R}_{m,n}}e^{i\vec{q}\bullet\vec{R}_{m,n}} \tag{412}$$

$$\begin{aligned} G(\vec{K}_+ +\vec{q}) &\approx \sum_{m,n}\varepsilon_{m,n}e^{i\vec{K}_+\bullet\vec{R}_{m,n}}\left(1+i\vec{q}\bullet\vec{R}_{m,n}\right) \\ &=\sum_{m,n}\varepsilon_{m,n}e^{i\vec{K}_+\bullet\vec{R}_{m,n}}+i\sum_{m,n}\varepsilon_{m,n}\vec{q}\bullet\vec{R}_{m,n}e^{i\vec{K}_+\bullet\vec{R}_{m,n}} \\ &\equiv g_{1mn}+g_{2mn} \end{aligned} \tag{413}$$

In order for the effective to be linear, that is Dirac-like equation; the diagonal function $F(\vec{k})$ must go to zero in the linear term (the term proportional to $\vec{q}$; f_{2mn}) and only have up to a real constant in f_{1mn}, which is not very interesting; it simply means we can absorb it into the energy. The diagonal term on the other hand should be non-zero for the linear term g_{2mn} if it is going to be a Dirac-like equation behavior. The other term g_{1mn} is zero as we see below as it is exactly at Dirac's point.

The next procedure is to study the rotational symmetries of the lattice, and also the translation symmetry. The interaction coefficients $\varepsilon_{m,n}$ only depend on the distance between the atoms, a rotated vector where lies on another point of the same lattice with the same distance have the same interaction coefficient $\varepsilon_{m,n}$.

This means not all of the coefficients $\varepsilon_{m,n}$ are unique and we can add terms where they have the same coefficients. This way it would be easier to see if the whole sum in the general functions of graphene lattice cancel out to zero in first order: For the diagonal terms which represent hop from one atomic sit to another in the same sublattice; we look at six rotations each with 60 degrees with next one:

$$\begin{aligned}&\mathrm{Rot}(60^0)\vec{\mathrm{B}}_{\mathrm{mn}} \equiv \vec{\mathrm{B}}^{60}_{\mathrm{mn}} = \mathrm{mRot}(60^0)\vec{\mathrm{e}}_1 + \mathrm{nRot}(60^0)\vec{\mathrm{e}}_2\\ &= \mathrm{m}\left(\vec{\mathrm{e}}_2\right) + \mathrm{n}\left(\vec{\mathrm{e}}_2 - \vec{\mathrm{e}}_1\right)\\ &= -\mathrm{n}\vec{\mathrm{e}}_1 + \left(\mathrm{m}+\mathrm{n}\right)\vec{\mathrm{e}}_2\end{aligned} \tag{414}$$

Rotating the vector $\vec{\mathrm{B}}_{\mathrm{mn}}$ by 120:

$$\vec{\mathrm{B}}^{120}_{\mathrm{mn}} = -\left(\mathrm{m}+\mathrm{n}\right)\vec{\mathrm{e}}_1 + \mathrm{m}\vec{\mathrm{e}}_2 \tag{415}$$

Rotating by 180 degrees:

$$\vec{\mathrm{B}}^{180}_{\mathrm{mn}} = -\mathrm{m}\vec{\mathrm{e}}_1 - \mathrm{n}\vec{\mathrm{e}}_2 \tag{416}$$

Rotating by 240 degrees

$$\vec{\mathrm{B}}^{240}_{\mathrm{mn}} = \mathrm{n}\vec{\mathrm{e}}_1 - \left(\mathrm{m}+\mathrm{n}\right)\mathrm{n}\vec{\mathrm{e}}_2 \tag{417}$$

And the last rotation is 300 degrees:

$$\vec{\mathrm{B}}^{300}_{\mathrm{mn}} = \left(\mathrm{m}+\mathrm{n}\right)\vec{\mathrm{e}}_1 - \mathrm{m}\vec{\mathrm{e}}_2 \tag{418}$$

We add those six terms and we can see that the sum for f_{1mn} in equation **(411)** into a sum where each term is a sum of six rotations and they are all just real constants:

$$\begin{aligned}&\tilde{\varepsilon}_{mn}\left(e^{i\vec{k}\bullet\vec{B}_{m,n}} + e^{i\vec{K}_+\bullet\vec{B}^{60}_{mn}} + e^{i\vec{K}_+\bullet\vec{B}^{120}_{mn}} + e^{i\vec{K}_+\bullet\vec{B}^{180}_{mn}} + e^{i\vec{K}_+\bullet\vec{B}^{240}_{mn}} + e^{i\vec{K}_+\bullet\vec{B}^{300}_{mn}}\right)\\ &= 6\tilde{\varepsilon}_{m,n}\cos\frac{2\pi}{3}\left(n-m\right)\end{aligned} \tag{419}$$

The result we got in equation **(419)** for any integers n and m is a real number independent of q as we expected. Now let us sum each six terms of the same distance of the second term f_{2mn} of equation **(411)**; we get:

$$\begin{aligned}
&i\tilde{\varepsilon}_{m,n}\begin{pmatrix}\vec{q}\bullet\vec{B}_{mn}e^{i\vec{k}\bullet\vec{B}_{m,n}}+\vec{q}\bullet\vec{B}_{mn}^{60}e^{i\vec{K}_{+}\bullet\vec{B}_{mn}^{60}}+\vec{q}\bullet\vec{B}_{mn}^{120}e^{i\vec{K}_{+}\bullet\vec{B}_{mn}^{120}}+\vec{q}\bullet\vec{B}_{mn}^{180}e^{i\vec{K}_{+}\bullet\vec{B}_{mn}^{180}}\\ +\vec{q}\bullet\vec{B}_{mn}^{240}e^{i\vec{K}_{+}\bullet\vec{B}_{mn}^{240}}+\vec{q}\bullet\vec{B}_{mn}^{300}e^{i\vec{K}_{+}\bullet\vec{B}_{mn}^{300}}\end{pmatrix}\\
&=i2\tilde{\varepsilon}_{m,n}\sin\frac{2\pi}{3}(n-m)\begin{pmatrix}\left(\frac{\sqrt{3}}{2}(m-n)q_x+\frac{3}{2}(m+n)q_y\right)+\left(\frac{\sqrt{3}}{2}(m+2n)q_x-\frac{3}{2}mq_y\right)\\ +\left(-\frac{\sqrt{3}}{2}(2m+n)q_x-\frac{3}{2}nq_y\right)\end{pmatrix}\\
&=0
\end{aligned}\tag{420}$$

So the linear term in of the diagonal term **(411)** of the general functions of graphene lattice is zero just as it supposes to be. We get the interesting well known graphene behavior near Dirac points. Now let us work on the off diagonal term from equation **(413)**; for the off diagonal terms we need three rotated terms each with 120 degrees with the next one:

$$\begin{aligned}
&\vec{\mathrm{R}}_{\mathrm{mn}}^{120}\equiv\mathrm{Rot}(120^{0})\vec{\mathrm{R}}_{\mathrm{mn}}=\mathrm{mRot}(120^{0})\vec{\mathrm{e}}_{1}+\mathrm{nRot}(120^{0})\vec{\mathrm{e}}_{2}+\mathrm{Rot}(120^{0})\vec{\mathrm{d}}\\
&=-(\mathrm{m}+\mathrm{n}+1)\vec{\mathrm{e}}_{1}+\mathrm{m}\vec{\mathrm{e}}_{2}+\vec{\mathrm{d}}
\end{aligned}\tag{421}$$

$$\vec{\mathrm{R}}_{\mathrm{mn}}^{240}=\mathrm{n}\vec{\mathrm{e}}_{1}-(\mathrm{m}+\mathrm{n}+1)\vec{\mathrm{e}}_{2}+\vec{\mathrm{d}}\tag{422}$$

The first term g_{1mn} of equation **(413)** is exactly at Dirac point; so when we add each three rotated term of the sum so we should get zero:

$$\begin{aligned}
&\varepsilon_{mn}\left(e^{i\vec{K}_{+}\bullet\vec{R}_{mn}}+e^{i\vec{K}_{+}\bullet\vec{R}_{mn}^{120}}+e^{i\vec{K}_{+}\bullet\vec{R}_{mn}^{240}}\right)\\
&=\varepsilon_{mn}\left(e^{i\frac{2\pi}{3}(n-m-1)}+e^{i\frac{2\pi}{3}(n-m)}+e^{i\frac{2\pi}{3}(n-m+1)}\right)\\
&=\varepsilon_{mn}e^{i\frac{2\pi}{3}(n-m)}\left(e^{-i\frac{2\pi}{3}}+1+e^{i\frac{2\pi}{3}}\right)\\
&=0
\end{aligned}\tag{423}$$

The last term that we have to look at the sum of each three rotated terms of the same distance of the term g_{2mn} equation **(413)** that is linear in $\vec{q}$:

$$i\varepsilon_{mn}\left(\vec{q}\bullet\vec{R}_{mn}e^{i\vec{K}_{+}\bullet\vec{R}_{mn}}+\vec{q}\bullet\vec{R}_{mn}^{120}e^{i\vec{K}_{+}\bullet\vec{R}_{mn}^{120}}+\vec{q}\bullet\vec{R}_{mn}^{240}e^{i\vec{K}_{+}\bullet\vec{R}_{mn}^{240}}\right)\tag{424}$$

The sum is a little long, but elementary algebraic calculation; we have three long terms:

$$ia\varepsilon_{mn}\begin{pmatrix} \left(\frac{\sqrt{3}}{2}(m-n)q_x+\left(\frac{3}{2}(m+n)+1\right)q_y\right)e^{i\frac{2\pi}{3}(n-m-1)} \\ +\left(-\frac{\sqrt{3}}{2}(2m+n+1)q_x-\left(\frac{3}{2}(n+1)-1\right)q_y\right)e^{i\frac{2\pi}{3}(n-m)} \\ +\left(\frac{\sqrt{3}}{2}(m+2n+1)q_x-\left(\frac{3}{2}(m+1)-1\right)q_y\right)e^{i\frac{2\pi}{3}(n-m+1)} \end{pmatrix} \qquad \textbf{(425)}$$

Summing these three terms in the above equation; we get:

$$-\frac{3a\varepsilon_{mn}}{2}e^{i\frac{2\pi}{3}(n-m)}\left(-\frac{1}{2}(3n+1)+i\frac{\sqrt{3}}{2}(2m+n+1)\right)\left(q_x-iq_y\right) \qquad \textbf{(426)}$$

The sum is non-zero and linear in momentum; that means that we have a general symmetry of the hexagonal shaped lattice of graphene which behave like ultrarelativistic fermions.

4 Bilayer:

4.1 Bilayer Lattice

Once we have done the work for the monolayer; it is easy to generalize the ideas to two layers or any number of layers. The Hamiltonian matrix is larger than for the monolayer; however the elements in the bilayer and N-layer have similarities and some of the same symmetries as the monolayer. Graphene layers in nature don’t lie directly above each other, only half of the atoms of each layer lie directly above each other; the other half don’t, instead they lie in the empty space in the center of the hexagonal cells of the second layer **[17]**:

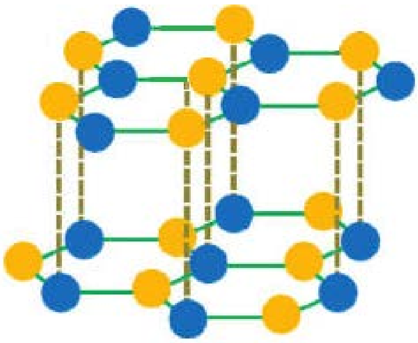


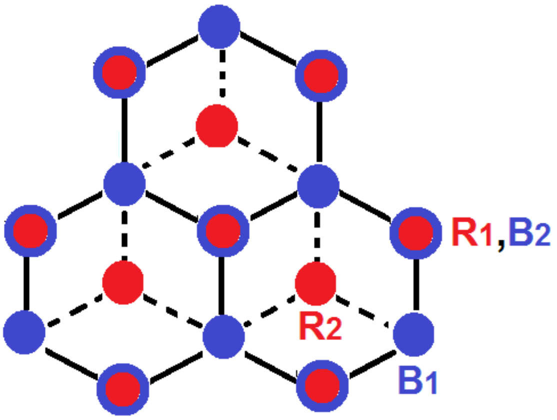
Figure (17): shows Bilayer Graphene for the transformed matrix; the blue colored balls are the B-sublattice atoms and the yellow colored balls are the R-sublattice atoms, we see that the atoms of the R-sublattice of the top layer lie directly above the atoms of the B-sublattice of the bottom layer.The rest of the atoms of the two layers are not directly above each other ***[21]****.*

If we label the sublattices of the first layer by B1 and R1-sublattices, and the second layer by B2 and R2-sublattices; then one choice of labeling is that R1-sublattice lies directly above B2-sublattice; that is the Carbon atoms of the sublattice R1 (red sublattice of layer 1) lie above the Carbon atoms B2(blue sublattice of layer 2), while the Carbon atoms of the B1-sublattice in the first layer(top layer) lie in the empty center of the hexagonal cell of the bottom layer and finally the similarly for R2; it lies in the empty center of the hexagonal cell of the top layer.

The strongest interaction between the two layers comes from the atoms that are directly above each other. The Hamiltonian for the Bilayer graphene is:

$$\begin{aligned}\hat{H}_{Bilayer} &= -\varepsilon_0 \sum_{l=1}^{2} \sum_{\langle \vec{m},\vec{n}\rangle} \left(a^\dagger_{l,\vec{m}} b_{l,\vec{n}} + H.c.\right) - \gamma_1 \sum_{\vec{m}} \left(a^\dagger_{1,\vec{m}} a_{2,\vec{m}} + H.c.\right) \\ &-\gamma_3 \sum_{\vec{m}} \left(b^\dagger_{1,\vec{m}} b_{2,\vec{m}} + H.c.\right) - \gamma_4 \sum_{\vec{m}} \left(+a^\dagger_{1,\vec{m}} b_{2,\vec{m}} + b^\dagger_{1,\vec{m}} a_{2,\vec{m}} + H.c.\right)\end{aligned} \qquad \textbf{(427)}$$

The experimental value of $\gamma_1 = 0,4eV$ **[15]**, which represents the hopping parameter for those atoms in different layers that are directly above each other (B1 to B2 in Figure (18) below), the experimental value of $\gamma_3 = 0,3eV$ which is the hopping parameter of R1 to R2 and finally the value of $\gamma_4 = 0,04eV$ is the hoping parameter of the hops B1 to R2 and R1 to B2.



Figure(18): shows bilayer, the R1-sublattice of the first(top) layer is directly above the B2-sublattice of the second (bottom) layer, however the R2-sublattice of the bottom layer is in center of the hexagonal cell of the top layer i.e. R2 and B1 are are in empty hexagonal cells of the opposite layer.

The state vector $\left|\psi_{\vec{k}}\right\rangle$ for the bilayer case has four components; two vectors $\left|B_1\right\rangle$ (statevector for the B-sublattice) and $\left|R_1\right\rangle$ (statevector for the R-sublattice) for the first layer and two vectors $\left|B_2\right\rangle$ and $\left|R_2\right\rangle$ for the second layer; so the state vector could be written as:

$$\left|\psi_{\vec{k}}\right\rangle = B_1\left|B_1\right\rangle + R_1\left|R_1\right\rangle + B_2\left|B_2\right\rangle + R_2\left|R_2\right\rangle \qquad \textbf{(428)}$$

The coefficients B_1, R_1, B_2, R_2 in equation **(428)** are complex numbers.

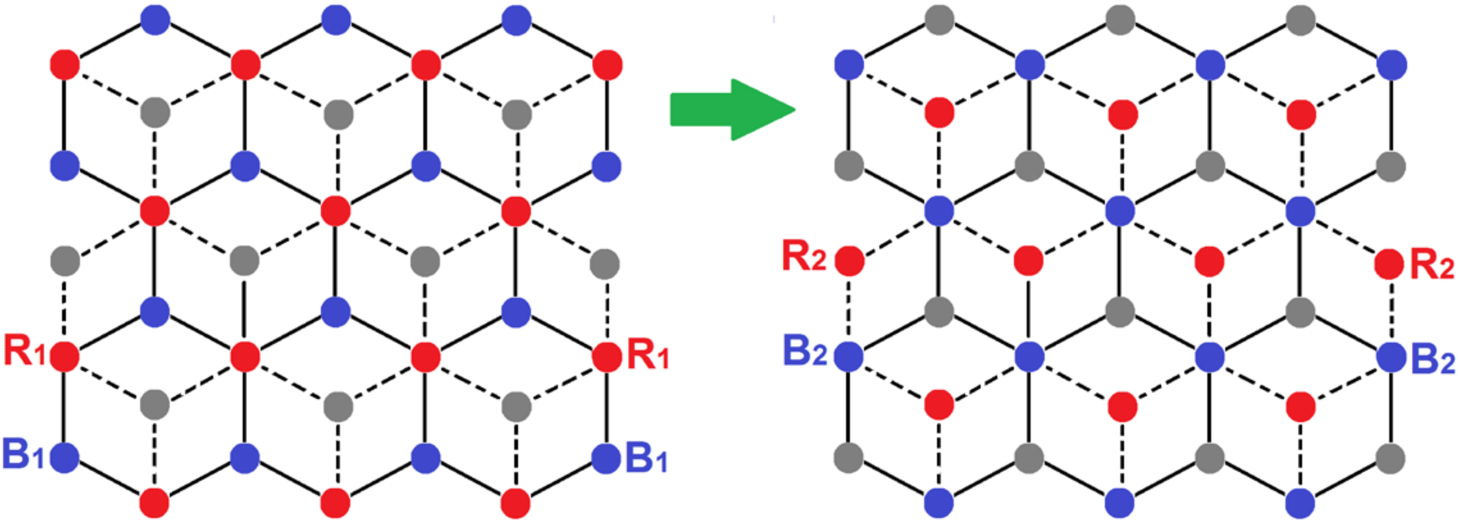


Figure (19) a *Figure (19) b*

*Figure (19 : a): in the left shows the top layer in color; the bottom layer in gray, b) on the right shows the bottom layer in color and the top layer in gray*Then we write the vector $\left|\psi_{\vec{k}}\right\rangle$ in k-space which is simply the coefficients from equation **(428)** taking account all four sublattices of the bilayer graphene; we have:

$$\psi_{\vec{k},n} = \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} \tag{429}$$

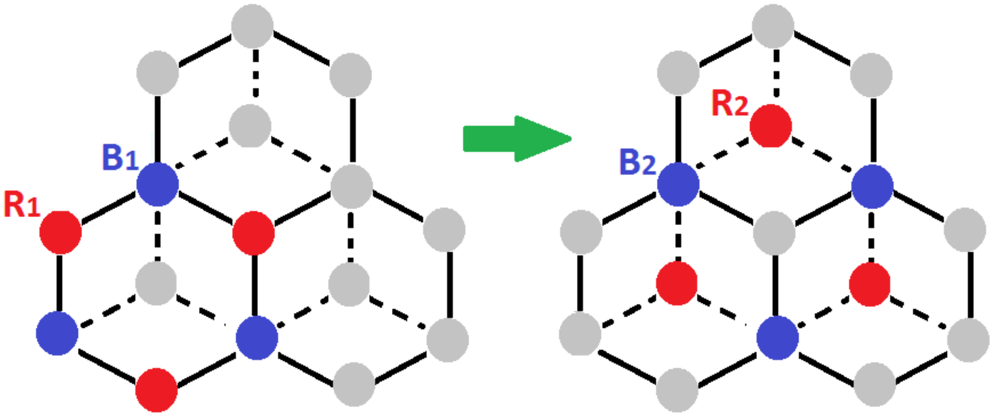


Figure (20): a) Top layer A *Figure (20): b) Bottom layer B*

Figure (20): shows Bilayer graphene it shows how the atoms in the top and bottom are arranged relative to each other. The blue and red colored circles are atoms from B- and R-sublattices respectively and the gray are empty spaces shows locations of other atoms from both layers, B1-sublattice is above B2-sublattice. (First kind of labeling)

The procedure is almost identical to the bulk monolayer case; only for the bilayer we have four coupled equations and the Schrödinger equation in k-space becomes:

$$\begin{pmatrix} \langle B_{1k}|\widehat{H}_0|B_{1k}\rangle & \langle B_{1k}|\widehat{H}_0|R_{1k}\rangle & \langle B_{1k}|\widehat{H}_0|B_{2k}\rangle & \langle B_{1k}|\widehat{H}_0|R_{2k}\rangle \\ \langle R_{1k}|\widehat{H}_0|B_{1k}\rangle & \langle R_{1k}|\widehat{H}_0|R_{1k}\rangle & \langle R_{1k}|\widehat{H}_0|B_{2k}\rangle & \langle R_{1k}|\widehat{H}_0|R_{2k}\rangle \\ \langle B_{2k}|\widehat{H}_0|B_{1k}\rangle & \langle B_{2k}|\widehat{H}_0|R_{1k}\rangle & \langle B_{2k}|\widehat{H}_0|B_{2k}\rangle & \langle B_{2k}|\widehat{H}_0|R_{2k}\rangle \\ \langle R_{2k}|\widehat{H}_0|B_{1k}\rangle & \langle R_{2k}|\widehat{H}_0|R_{1k}\rangle & \langle R_{2k}|\widehat{H}_0|B_{2k}\rangle & \langle R_{2k}|\widehat{H}_0|R_{2k}\rangle \end{pmatrix} \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} = E(k) \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} \tag{430}$$

The procedure of finding the explicit Hamiltonian in k-space is also very similar to what we did for the one layer graphene in the previous section; the only difference is that we get more terms; otherwise all the non-constant terms involve the function $g(k)$ (or its complex conjugate) we found in equation **(341)** , which could easily be seen geometrically; the main difference is that interaction coefficients are weaker when there is a hop between different layers as they are farther away. The terms that are hops between atoms in different layers that lie directly above each other (R1-B2), those give only a constant γ_1; so the Schrödinger becomes:

$$\begin{pmatrix} 0 & \varepsilon_0 g(k) & \gamma_4 g(k) & \gamma_3 g(k)^* \\ \varepsilon_0 g(k)^* & 0 & \gamma_1 & \gamma_4 g(k) \\ \gamma_4 g(k)^* & \gamma_1 & 0 & \varepsilon_0 g(k) \\ \gamma_3 g(k) & \gamma_4 g(k)^* & \varepsilon_0 g(k)^* & 0 \end{pmatrix} \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} = E(k) \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} \tag{431}$$

4.2 Bilayer nearest neighbor interlayer hops Approximation

Let us first neglect all higher energy terms, which is simply the nearest neighbor approximation between layers i.e. the only overlap between states of different layers come from the (R1-B2) hops and we get:

$$\begin{pmatrix} 0 & \varepsilon_0 g(k) & 0 & 0 \\ \varepsilon_0 g(k)^* & 0 & \gamma_1 & 0 \\ 0 & \gamma_1 & 0 & \varepsilon_0 g(k) \\ 0 & 0 & \varepsilon_0 g(k)^* & 0 \end{pmatrix} \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} = E(k) \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} \tag{432}$$

The solution for the eigenvalue equation above is:

$$\mathrm{E}(\vec{\mathrm{k}}) = \pm\frac{\gamma_1}{2} \pm \frac{1}{2}\sqrt{\gamma_1^2 + 4\varepsilon_0^4 \left|\mathrm{g}(\vec{\mathrm{k}})\right|^4} \tag{433}$$

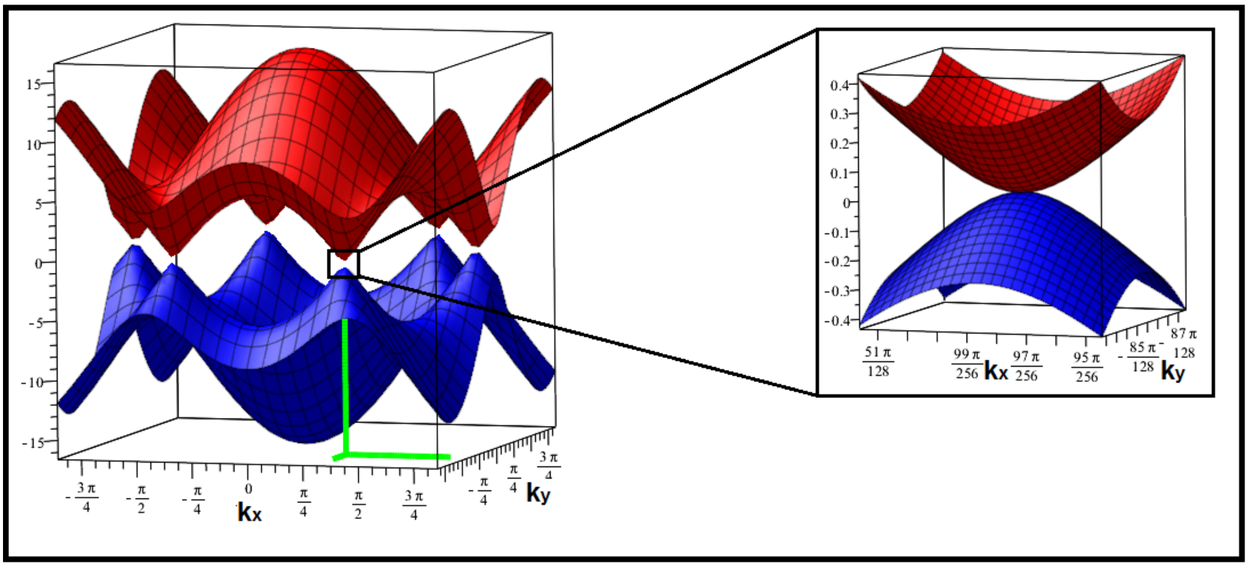


Figure (21): left: shows the two interesting solutions of equation **(433)** *that touch each other* $E = \pm 0.5\left(\gamma_1 - \sqrt{\gamma_1^2 + 4\varepsilon_0^4 \left|g(\vec{k})\right|^4}\right)$*, right the area near Dirac's point* $\vec{K}_+$ *shown in large which is parabolic for the bilayer case.*

We already have looked at the function $g(\vec{k})$ near Dirac points; so using equation **(375)** for the function near Dirac's point $\vec{K}_+$ with $(\hbar = 1)$; equation **(432)** above becomes **[17]**:

$$\begin{pmatrix} 0 & v_f\left(q_x - iq_y\right) & 0 & 0 \\ v_f\left(q_x + iq_y\right) & 0 & \gamma_1 & 0 \\ 0 & \gamma_1 & 0 & v_f\left(q_x - iq_y\right) \\ 0 & 0 & v_f\left(q_x + iq_y\right) & 0 \end{pmatrix}\begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} = E\begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} \qquad \textbf{(434)}$$

The solution is similar to equation **(433)** with $v_F q$ instead of $\varepsilon_0\left|g(\vec{k})\right|$ nevertheless let us solve the eigenvalue equation **(434)** in detail to see the algebra; with $H(\vec{k})$ being the square matrix in the above equation; we have $det\left(H(\vec{k}) - EI\right)$:

$$\begin{vmatrix} -E & v_F\left(q_x - iq_y\right) & 0 & 0 \\ v_F\left(q_x + iq_y\right) & -E & \gamma_1 & 0 \\ 0 & \gamma_1 & -E & v_F\left(q_x - iq_y\right) \\ 0 & 0 & v_F\left(q_x + iq_y\right) & -E \end{vmatrix} = 0 \qquad \textbf{(435)}$$

The determinant above gives the following 4th degree (quartic) polynomial equation:

$$E^4-\left(\gamma_1^2+2v_F^2q^2\right)E^2+v_F^4q^4=0 \tag{436}$$

We rearrange the above equation in a little more convenient way for solving:

$$\begin{aligned}&E^4-\left(\gamma_1^2+2v_F^2q^2\right)E^2+v_F^4q^4=0\\&E^4-2v_F^2q^2E^2+v_F^4q^4-\gamma_1^2E^2=0\\&\left(E^2-v_F^2q^2\right)^2-\gamma_1^2E^2=0\end{aligned} \tag{437}$$

We first solve it for E as a function of E and get two quadratic equations:

$$E=\pm\frac{1}{\gamma_1}\left(E^2-v_F^2q^2\right)=0 \tag{438}$$

We rewrite them in more familiar quadratic equations:

$$E^2\pm\gamma_1E-v_F^2q^2=0 \tag{439}$$

So the four solutions of the quartic equation **(436)** are:

$$E=\pm\frac{\gamma_1}{2}\pm\frac{1}{2}\sqrt{\gamma_1^2+4v_F^2q^2} \tag{440}$$

Now remember that q is small, we only look at the energy spectrum near Dirac's points; so can expand the solution to the least order in q; and get the dispersion relations:

$$\begin{aligned}E&=\pm\frac{\gamma_1}{2}\pm\frac{\gamma_1}{2}\left(1+2\frac{v_F^2q^2}{\gamma_1^2}+O\left(q^4\right)\right)\\&\approx\pm\frac{\gamma_1}{2}\pm\frac{\gamma_1}{2}\left(1+2\frac{v_F^2q^2}{\gamma_1^2}\right)\end{aligned} \tag{441}$$

The solutions above are four parabolic equations; two of them touch each other at $q=0,\ E=0$ and have two extremal points at $E=\pm\gamma_1$ (look at Figure (21) above), the first two solutions are:

$$E=\pm\frac{v_F^2}{\gamma_1^2}q^2 \tag{442}$$

And the other two solutions are:

$$E=\pm\left(\gamma_1+\frac{v_F^2}{\gamma_1}q^2\right) \tag{443}$$

The two equations above the approximate solutions near Dirac's points which already have seen in Figure (21) in the graph of the exact solution, never the less it is nice to them algebraically and see the coefficients in more detail. In conclusion the bilayer graphene behaves like a zero gap semiconductor.

4.3 Effective Hamiltonian for Bilayer Graphene

We can write an effective Hamiltonian for the first two solutions **(442)** of the bilayer graphene; let us write the equations from **(434)** explicitly one by one:

$$v_f\left(q_x - iq_y\right)B_1 = E(k)B_1 \tag{444}$$

$$v_f\left(q_x + iq_y\right)A_1 + \gamma_1 A_2 = E(k)R_1 \tag{445}$$

$$\gamma_1 B_1 + v_f\left(q_x - iq_y\right)B_2 = E(k)B_2 \tag{446}$$

$$v_f\left(q_x + iq_y\right)A_2 = E(k)R_2 \tag{447}$$

The second and third equations above **(445)** and **(446)** involve interactions between the two layers; we can take the terms involving γ_1 to the right hand side of the equations and then write them as 2x2 matrix equation:

$$\begin{pmatrix} 0 & v_f\left(q_x - iq_y\right) \\ v_f\left(q_x + iq_y\right) & 0 \end{pmatrix}\begin{pmatrix} B_2 \\ R_1 \end{pmatrix} = \begin{pmatrix} E & -\gamma_1 \\ -\gamma_1 & E \end{pmatrix}\begin{pmatrix} B_2 \\ R_1 \end{pmatrix} \tag{448}$$

We can also write the first and fourth equations **(444)** and **(447)** as another 2x2 matrices:

$$E\begin{pmatrix} B_1 \\ R_2 \end{pmatrix} = \begin{pmatrix} 0 & v_f\left(q_x - iq_y\right) \\ v_f\left(q_x + iq_y\right) & 0 \end{pmatrix}\begin{pmatrix} B_2 \\ R_1 \end{pmatrix} \tag{449}$$

We can use the first matrix equation **(448)** to eliminate B_2 and R_1:

$$\begin{pmatrix} B_2 \\ R_1 \end{pmatrix} = \begin{pmatrix} E & -\gamma_1 \\ -\gamma_1 & E \end{pmatrix}^{-1}\begin{pmatrix} 0 & v_f\left(q_x - iq_y\right) \\ v_f\left(q_x + iq_y\right) & 0 \end{pmatrix}\begin{pmatrix} B_1 \\ R_2 \end{pmatrix} \tag{450}$$

With the inverse

$$\begin{pmatrix} E & -\gamma_1 \\ -\gamma_1 & E \end{pmatrix}^{-1} = \frac{1}{E^2 - \gamma_1^2}\begin{pmatrix} E & \gamma_1 \\ \gamma_1 & E \end{pmatrix} \approx \frac{1}{-\gamma_1^2}\begin{pmatrix} E & \gamma_1 \\ \gamma_1 & E \end{pmatrix} \approx \begin{pmatrix} 0 & -1/\gamma_1 \\ -1/\gamma_1 & 0 \end{pmatrix} \tag{451}$$

The last two equalities in the above equation are because $E \ll \gamma_1$.

We put the expression from **(450)** into the second matrix equation **(449)** and use the inverse **(451)**; we get:

$$E\begin{pmatrix} B_1 \\ R_2 \end{pmatrix} = \begin{pmatrix} 0 & v_f\left(q_x - iq_y\right) \\ v_f\left(q_x + iq_y\right) & 0 \end{pmatrix}\begin{pmatrix} 0 & -\gamma_1^{-1} \\ -\gamma_1^{-1} & 0 \end{pmatrix}\begin{pmatrix} 0 & v_f\left(q_x - iq_y\right) \\ v_f\left(q_x + iq_y\right) & 0 \end{pmatrix}\begin{pmatrix} B_1 \\ R_2 \end{pmatrix} \quad \textbf{(452)}$$

We multiply the matrices on the RHS and finally get the effective Hamiltonian for Bilayer graphene **[17]**:

$$E\begin{pmatrix} B_1 \\ R_2 \end{pmatrix} = -\frac{v_F^2}{\gamma_1}\begin{pmatrix} 0 & \left(q_x - iq_y\right)^2 \\ \left(q_x + iq_y\right)^2 & 0 \end{pmatrix}\begin{pmatrix} B_1 \\ R_2 \end{pmatrix} \quad \textbf{(453)}$$

4.4 Next-nearest neighbor interlayer hops and trigonal warping:

Now let us study a little the bilayer graphene when we also consider second nearest neighbor term which are hops between (B1-R2) sublattices, they are terms involving γ_3. The matrix equation (Schrödinger equation) in k-space near Dirac's point is then:

$$\begin{pmatrix} 0 & v_f\left(q_x - iq_y\right) & 0 & \frac{3a}{2}\gamma_3\left(q_x + iq_y\right) \\ v_f\left(q_x + iq_y\right) & 0 & \gamma_1 & 0 \\ 0 & \gamma_1 & 0 & v_f\left(q_x - iq_y\right) \\ \frac{3a}{2}\gamma_3\left(q_x - iq_y\right) & 0 & v_f\left(q_x + iq_y\right) & 0 \end{pmatrix}\begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} = E(k)\begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} \quad \textbf{(454)}$$

Doing similar procedure as we did for the nearest neighbor approximation in the previous section; we find the effective Hamiltonian in for bilayer including the nearest neighbor terms to be:

$$\begin{pmatrix} 0 & -\frac{v_F^2}{\gamma_1}q_-^2 + \frac{3a}{2}\gamma_3 q_+ \\ -\frac{v_F^2}{\gamma_1}q_+^2 + \frac{3a}{2}\gamma_3 q_- & 0 \end{pmatrix}\begin{pmatrix} B_1 \\ R_2 \end{pmatrix} = E\begin{pmatrix} B_1 \\ R_2 \end{pmatrix} \quad \textbf{(455)}$$

The symbols q_- and q_+ in the equation above are $q_- = q_x - iq_y$ and $q_+ = q_x + iq_y$ simply to write the answer shorter just as we did for the monolayer graphene.

The next nearest neighbor terms will change the band at low energies; it is quite interesting what happens when we include this extra term. The next nearest neighbor term introduces a trigonal distortion **[15]**, **[18]**; we get three extra sets of linear bands Dirac's points (look at figure (22) below), one at $E=0$ and $\mathrm{k}=0$, and three points where $\mathrm{E}=0$ but with $\mathrm{k}\neq 0$. When we include the next nearest neighboring term, the electron and symmetry is preserved.

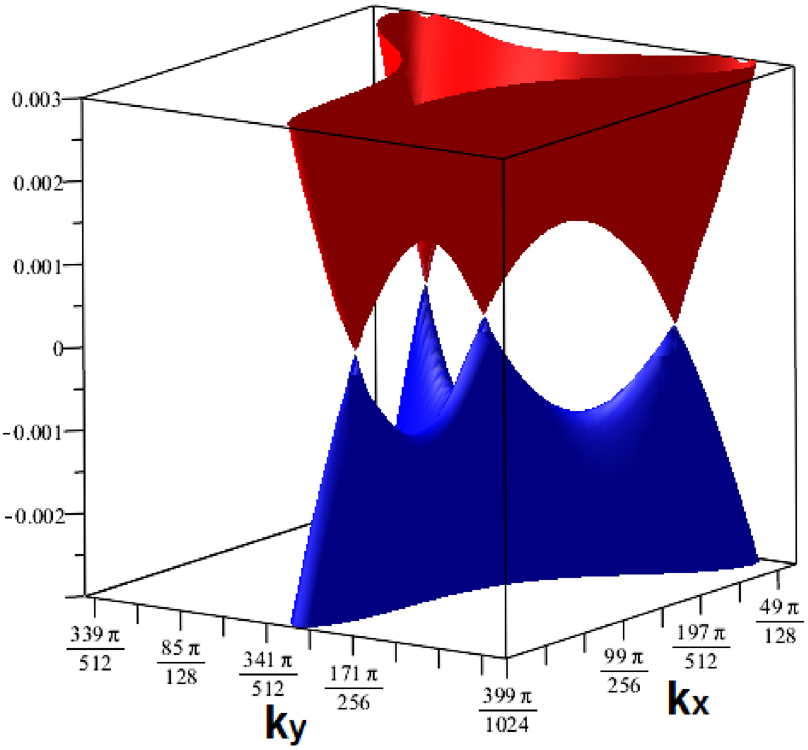


Figure (22): shows the two energy bands of bilayer graphene that touch each other near Fermi energy(Dirac's points) ; we see that once we include the next nearest neighboring term γ_3 *in our calculation; we get three extra linear band near but not exactly at Dirac's points.*

4.5 Bilayer graphene in an external electric field:

Now we look at the bilayer graphene an electric field is applied to it which is called the biased bilayer; it could have interesting consequences practically and can be useful in technology. Mathematically we express the effect of applying an external electric field by adding a new term $\hat{H}_V$ to the total Hamiltonian from equation **(427)** for the bilayer graphene **[19]**:

$$\hat{H}_V = V\sum_{n}^{N}\left(-\left(a_{1,n}^{\dagger}a_{1,n} + b_{1,n}^{\dagger}b_{1,n}\right) + \left(a_{2,n}^{\dagger}a_{2,n} + b_{2,n}^{\dagger}b_{2,n}\right)\right) \qquad \textbf{(456)}$$

When we only consider nearest neighbor approximation; the Hamiltonian in k-space near Dirac's point K_+ is:

$$\begin{pmatrix} -V & v_f\left(q_x - iq_y\right) & 0 & 0 \\ v_f\left(q_x + iq_y\right) & -V & \gamma_1 & 0 \\ 0 & \gamma_1 & V & v_f\left(q_x - iq_y\right) \\ 0 & 0 & v_f\left(q_x + iq_y\right) & V \end{pmatrix}\begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} = E(k)\begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \end{pmatrix} \qquad \textbf{(457)}$$

The four solutions of the energy eigenvalue equation **(457)** for bilayer in a constant potential (look at Figure (23) below) are:

$$E = \pm\sqrt{V^2 + v_F^2k^2 + \frac{\gamma_1^2}{2} \pm \frac{1}{2}\sqrt{16V^2v_F^2k^2 + 4\gamma_1^2v_F^2k^2 + \gamma_1^4}} \qquad \textbf{(458)}$$

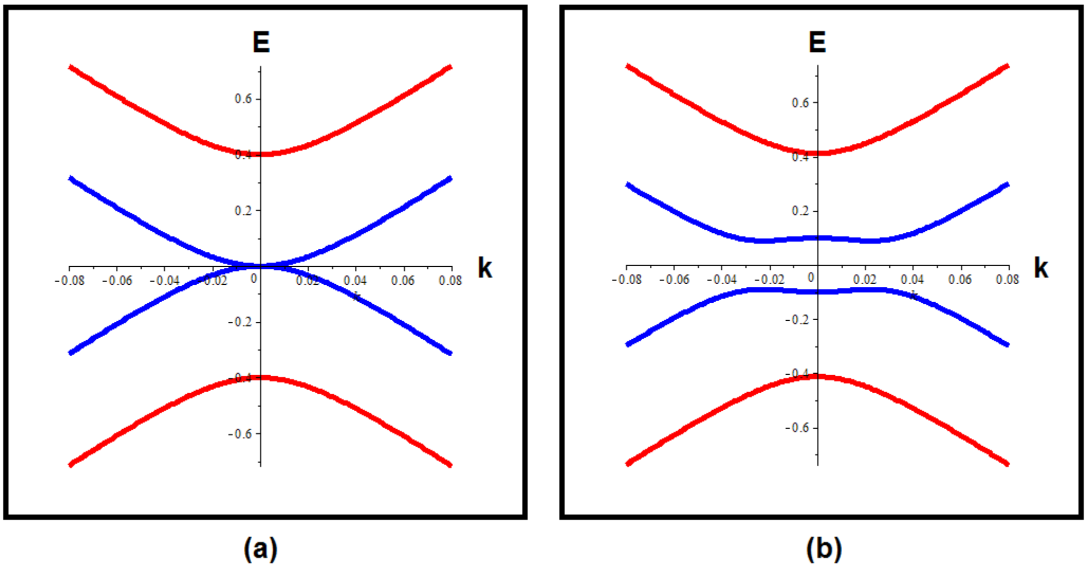


Figure (23): Right the energy band for graphene bilayer graphene nearest neighbor approximation near Diracs point without applied electric field. Left the same approximation but applied electrical field; we see that the applied field opens a gap **[15]**.

We can find the gap points easily from in this case since it is a simple function; we put the derivative of the dispersion relation above equal to zero and we find all the extremal points of the solutions which they make a total of six solutions:

$$\frac{dE(k)}{dk}=\pm\frac{1}{2E(k)}\left(2v_F^2k\pm\frac{1}{2}\frac{\left(8V^2+2\gamma_1^2\right)v_F^2k}{\sqrt{\left(4V^2+v_F^2\right)k^2+\frac{\gamma_1^2}{4}}}\right)=0 \tag{459}$$

We solve for k and get two solutions at $k=0$ for electrons and holes. The other four interesting solutions are two gap points for electrons and two gap points for holes at the points:

$$K_{gap\pm}=\pm\frac{V}{v_F}\sqrt{1+\frac{\gamma_1^2}{\gamma_1^2+4V^2}} \tag{460}$$

The height of the gap is of course $E\left(K_{gap\pm}\right)$ which is not exactly at Dirac point. For small values of V; the gap points are at **[15]**:

$$K_{gap\pm}\approx\pm\frac{\sqrt{2}V}{v_F} \tag{461}$$

The gap is dependent on the applied field which means that the gap can be regulated and also can be measured experimentally. It is a remarkable property that the bilayer is opening a gap in the energy band when an electric field is applied to it; we switch on and off the field and a gap opens; the bilayer has a lot of potential for future technology in carbon electronics. This property has been shown experimentally, it is the first semiconductor with an externally tunable gap.

5 N-layer graphene:

5.1 General lattices for multilayer graphene:

The multilayer graphene has a lot of interesting properties; in fact each number of layers of graphene has its own interesting properties. In the previous section; we looked at the bilayer graphene and as saw that half of the atoms (R1-sublattice) in one sublattice in the top layer were directly above half of the atoms (B2-sublattice) of the bottom layer (look at Figures (18) and (19)) while the other half (B1) of the top layer were located in the empty space in the center of the hexagonal cells of the bottom layer.

When considering the third layer, then we have more possibilities: One possibility is that the atoms of the third layer lie exactly in the same positions as the first layer; that is all the atoms be directly under all the atoms of the first layer; that is B3 under B1 one and R3 under R1 sublattices, they are better known as ABA stacked or **Bernal stacking** (look at Figure (24) below): The ABA stacked multilayer is when it repeats itself with ABABAB….. graphene layers on top of each other; this is the more common stacking in nature in graphite **[15]**.

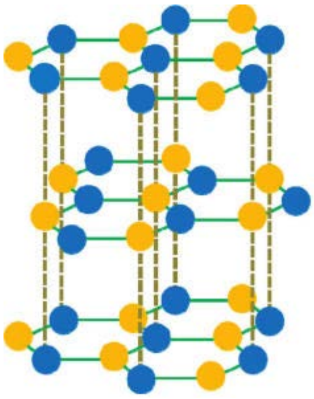


*Figure (24): shows **ABA** orientation of three graphene layers, the blue colored balls are the B-sublattice and the yellow colored are atoms of the R-sublattice, as you see the first and third layers are identical in orientation. The sublattices that are directly in line are B1-R2-B3* **[21]**.

The third layer can also have another orientation; the third layer could have half of the atoms lie directly under the first layer (R3 under B1) and the other half under the second layer (B3 under R2) which means a new distinct position. This orientation is better known as **Rhombohedral** stacking or ABC stacked graphene (look at figure (25) below). The ABC stacked N-layer is when the ABC repeats itself; ABCABC…. Graphene layers on top of each other. Graphene layers with ABC stacking order are less occurring in natural graphite than ABA but also are a natural orientation found in graphite **[15]**.

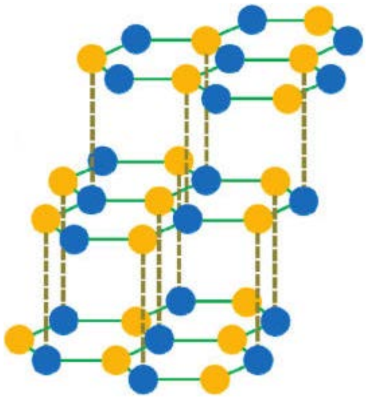


*Figure (25): shows **ABC** orientation of three graphene layers, the blue colored balls are the B-sublattice and the yellow colored are atoms of the R-sublattice, as you see each layer has one sublattice(R-sublattice) directly above the layer under it (R1 over B2 and R2 over B3), while the second sublattice in the empty space of the hexagonal cell of the layer under it* **[21]**.

There are no more inequivalent positions graphene layers can have relative to each other than A, B and C; however in multilayer graphene the stacking could also be more random than Bernal and Rhombohedral (turbostratic graphite).

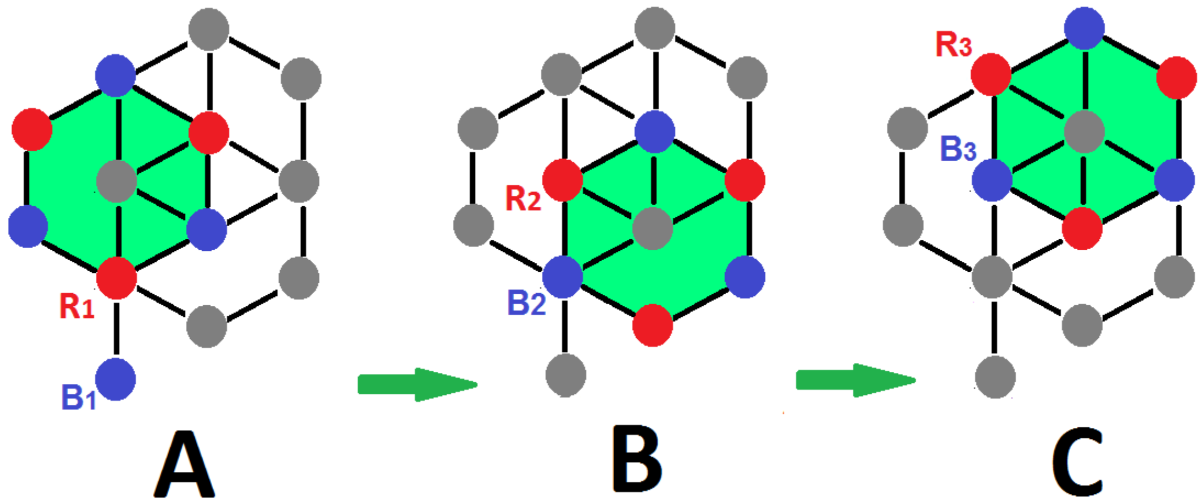


Figure (26): shows ABC orientation of three graphene layers, the blue colored are the B-sublattice and the yellow colored are atoms of the R-sublattic. There are no lines that consist of sublattices from three layers in line with each other; there are only sublattices in line between each two; R1-B2 and R2-B3.

Finally graphene layers can also rotate relative to each other by a random angle due to the weak interactions between planes. Rotations of layers relative to each other are of course also observed in graphite and give rise to Moiré interference patterns that is observed in STM (scanning tunneling michroscopy) **[15]**.

Let us now study the vectors and distances of carbon atoms in the multilayer case in detail. . The shortest distance between two atoms in two nearest neighboring planes(two graphene layers) is $D = 3.4\text{Å}$ (look at Figure (27) below); so the distance between two atoms of different layers is $\Delta S = \sqrt{Z^2D^2 + d_{plane}^2}$; where $Z = 0,1,2....$ is the number of layers the two atoms are a part from each other and d_{plane} is the distance of the horizontal component (on plane component).

We start by writing the general vectors for the atomic positions in multilayer graphene with our knowledge for the monolayer graphene: as we explained earlier that there are only three distinct positions for graphene layers could have relative to each other; that give three inequivalent sublattices that could describe any number of graphene layers. Each layer has two of these three distinct sublattices. The first one is what we already had in equation**(310)** and called B-sublattice:

$$\vec{B}_{mn} = m\vec{e}_1 + n\vec{e}_2 \tag{462}$$

The other ones could be described by 60 degrees.

However when we are considering infinite (or almost infinite to use block form); we can identify all the sublatties by a translation vector $\vec{d} = (0.1)$: the translation operator T^+ when operated on the set of position vectors of the B-sublattice; $\{\vec{B}_{mn}\}$ it simply adds the vector $\vec{d}$ to each vector:

$$T^+\vec{B}_{mn} = \vec{B}_{mn} + \vec{d} = m\vec{e}_1 + n\vec{e}_2 + \vec{d} \tag{463}$$

The above set of vectors is exactly those of what we called the R-sublattice when we worked on monolayer graphene (look at equation**(311)**).

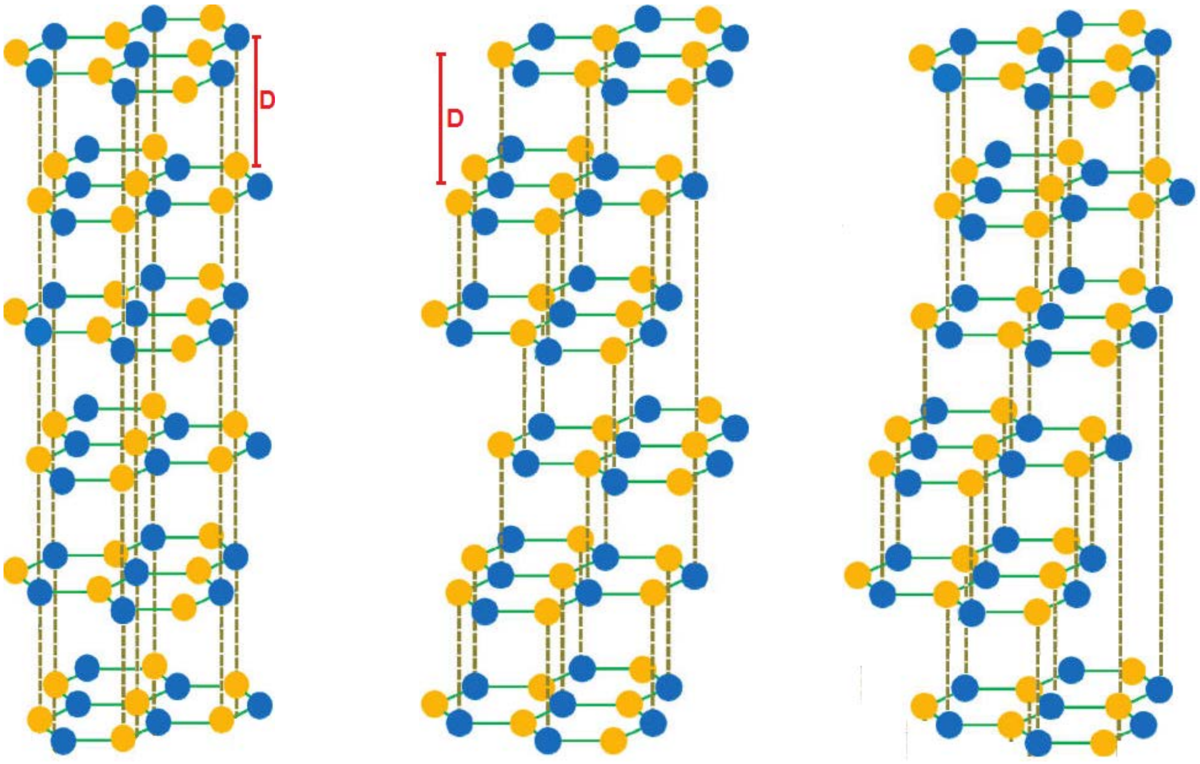
In order to get the final inequivalent sublattice; we operate the set of vectors of the B-sublattice by the inverse translation operator T^{-} which simply subtracts a vector $\vec{\mathrm{d}}$ from each vector of the B-sublattice:

$$\begin{aligned}\mathrm{T}^{-}\vec{\mathrm{B}}_{\mathrm{mn}} &= \vec{\mathrm{B}}_{\mathrm{mn}} - \vec{\mathrm{d}} \\ &= \mathrm{m}\vec{\mathrm{e}}_1 + \mathrm{n}\vec{\mathrm{e}}_2 - \vec{\mathrm{d}}\end{aligned} \tag{464}$$

The three sublattices create a cyclic group of three elements; so there are no more new sets of vectors and further translations give back on of the three sets of vectors $\left\{\vec{\mathrm{B}}_{\mathrm{mn}}\right\}$, $\left\{\mathrm{T}^{+}\vec{\mathrm{B}}_{\mathrm{mn}}\right\}$ and $\left\{\mathrm{T}^{-}\vec{\mathrm{B}}_{\mathrm{mn}}\right\}$.

Let us proof that algebraically: We need to write the following identity:

$$\vec{\mathrm{e}}_1 + \vec{\mathrm{e}}_2 = \left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right) + \left(-\frac{\sqrt{3}}{2}, \frac{3}{2}\right) = (0,3) = 3(0,1) = 3\vec{\mathrm{d}} \tag{465}$$



a) Bernal stacking *b) Rhombohedral Stacking* *c) Mixed (turbostratic)*

Figure (27): a) shows Bernal stacking; ABAB…, b) shows rhombohedral stacking; ABCABC and c) an example of a mixed (turbostratic) stacking; in this case ABABCABC. The distance D is the shortest distance between two parallel graphene planes **[21]**.

If we operate the set of vectors $\{\vec{B}_{mn}\}$ by the translation operator T^+ a number of times; $N = 0,1,2....$ that is $(T^+)^N$; we have:

$$(T^+)^N \vec{B}_{mn} = \vec{B}_{mn} + N\vec{d} \\ = m\vec{e}_1 + n\vec{e}_2 + N\vec{d} \tag{466}$$

According to the division theorem; the positive number N could be one of the three forms:

$$1) N = 3M \\ 2) N=3M+1 \\ 3) N=3M+2=3(M+1)-1 \tag{467}$$

In the above equation; we have $M = 0,1,2.....$ Those three forms above are the only three unique form of writing an integer as multiplicative of three plus some remainder.

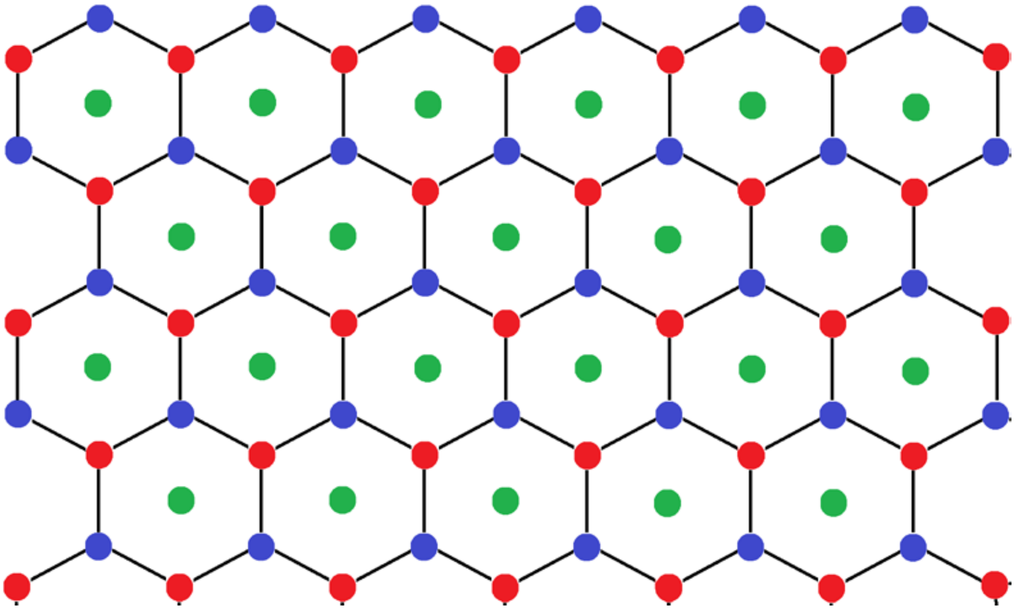


Figure (28): show the three inequivalent sublattices on top of each other each in different color; blue, red and green. Each layer in multilayer graphene has two of these sublattices.

Then for each of the three cases of equation **(467)**; we have:

$$1)\ (T^+)^{3M} \vec{B}_{mn} = \vec{B}_{mn} + 3M\vec{d} = (m+M)\vec{e}_1 + (n+M)\vec{e}_2 \in \{\vec{B}_{mn}\} \\ 2)\ (T^+)^{3M+1} \vec{B}_{mn} = \vec{B}_{mn} + 3M\vec{d} + \vec{d} = (m+M)\vec{e}_1 + (n+M)\vec{e}_2 + \vec{d} \in \{T^+\vec{B}_{mn}\} \\ 3)\ (T^+)^{3M+2} \vec{B}_{mn} = \vec{B}_{mn} + 3M\vec{d} + 2\vec{d} = \vec{B}_{mn} + 3(M+1)\vec{d} - \vec{d} \\ = (m+M+1)\vec{e}_1 + (n+M+1)\vec{e}_2 - \vec{d} \in \{T^-\vec{B}_{mn}\} \tag{468}$$

In the above equation; we have used the identity from equation **(465)** to write $3M\vec{d} = M\vec{e}_1 + M\vec{e}_2$. The position vectors of the three inequivalent orientations of graphene layers of the multilayer case can now be specified in detail: Each of the inequivalent layers have the following two sublattices: $A:\{\vec{B}_{mn},\ T^{+}\vec{B}_{mn}\}$, $B:\{T^{+}\vec{B}_{mn},\ T^{-}\vec{B}_{mn}\}$ and $C:\{T^{-}\vec{B}_{mn}, \vec{B}_{mn}\}$. This means that the distance between two atoms that belong to any layer (same layer or different layers) is:

$$\Delta S = \sqrt{Z^2 D^2 + \left\| \vec{X}_{m_1,m_2} - \vec{Y}_{n_1,n_2} \right\|^2} \tag{469}$$

In the above equation; the vectors $\vec{X}_{m_1,m_2}, \vec{Y}_{n_1,n_2} \in \{\vec{B}_{mn}, T^{+}\vec{B}_{mn}, T^{-}\vec{B}_{mn}\}$ and as earlier mentioned $Z = 0,1,2,.....$ is the number of layers the two carbon atoms are apart from each other and finally D is the shortest distance between two nearest neighboring planes(two graphene layers).

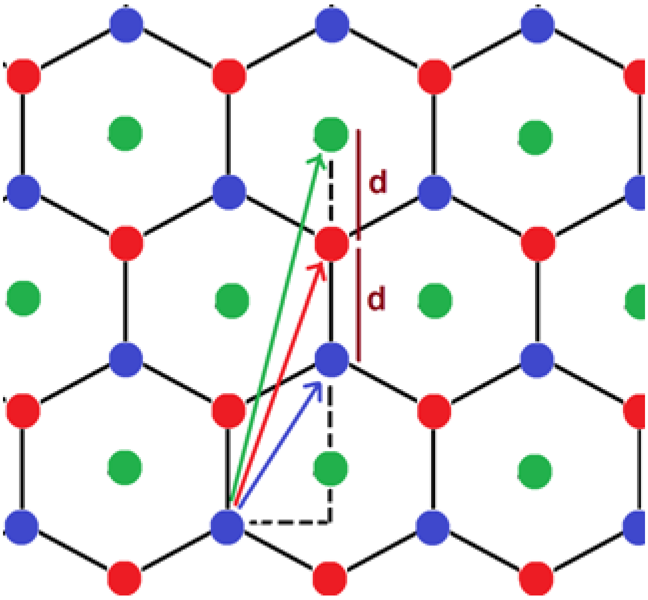


Figure (29): shows the inequivalent sublatties and their vectors which are separated by simple vector translations of magnitude $\vec{d}$.

The general state vector of all layers just like we did for the bilayer and monolayer is a superposition of all state vectors of all layers:

$$|\psi_k\rangle = \sum_{L=1}^{M} B_L |B_{k,L}\rangle + R_L |R_{k,L}\rangle \tag{470}$$

In the above equation; L runs over all the layers of the multilayer system with total number of layers M. The vectors $|B_{k,L}\rangle$ and $|R_{k,L}\rangle$ are the state vectors of each individual layers for the two sublattices B and R.

Finally B_L and R_L are the complex numbers multiplying the vectors of each single layer vectors. The general Hamiltonian $\hat{H}_M$ for multilayer system with total number of layers equal to M can be written as:

$$\hat{H}_M = \hat{H}_{\text{onlayer}} + \hat{H}_{\text{int.layer}} \tag{471}$$

The first term of the above equation in $\hat{H}_{\text{plane}}$ is the sum of all hops between atoms of the same layer:

$$\hat{H}_{\text{onlayer}} = \sum_{L=1}^{M}\sum_{\vec{n},\vec{m}}\left(\varepsilon_{\vec{n},\vec{m}}\left(a^{\dagger}_{\vec{n},L}b_{\vec{m},L} + b^{\dagger}_{\vec{m},L}a_{\vec{n},L}\right) + \tilde{\varepsilon}_{\vec{n},\vec{m}}\left(a^{\dagger}_{\vec{n},L}a_{\vec{m},L} + b^{\dagger}_{\vec{n},L}b_{\vec{m},L}\right)\right)$$

(472)

In the above equation; $\varepsilon_{\vec{n},\vec{m}}$ and $\tilde{\varepsilon}_{\vec{n},\vec{m}}$ are hopping energies of in-plane hops.

The second term of the total Hamiltonian from equation **(471)** is the sum of interlayer hops between layers u and v and atomic:

$$\hat{H}_{\text{int.layer}} = \sum_{\substack{u,v=1\\ u\neq v}}^{M}\sum_{\vec{n},\vec{m}}\left(\varepsilon^{u,v}_{\vec{n},\vec{m}}\left(a^{\dagger}_{\vec{n},u}a_{\vec{m},v} + b^{\dagger}_{\vec{n},u}b_{\vec{m},v}\right) + \tilde{\varepsilon}^{u,v}_{\vec{n},\vec{m}}\left(a^{\dagger}_{\vec{n},u}b_{\vec{m},v} + b^{\dagger}_{\vec{m},v}a_{\vec{n},u}\right)\right) \tag{473}$$

In the above equations; $\varepsilon^{u,v}_{\vec{n},\vec{m}}$ and $\tilde{\varepsilon}^{u,v}_{\vec{n},\vec{m}}$ are hopping energies for hops between atomic sites of different layers. The reason we have single terms like $a^{\dagger}_{\vec{n},u}a_{\vec{m},v}$, $a^{\dagger}_{\vec{n},L}a_{\vec{m},L}$ etc. of each hop without their hermitian conjugates in equations **(472)** and **(473)** is of Corse because the indices $u, v, \vec{m}$ and $\vec{n}$ are all free and run over the whole lattices and total number of layers, so they include all hops and also hopping back too.

The Schrödinger equation for the multilayer graphene is:

$$\hat{H}_M\left|\psi_k\right\rangle = E\left|\psi_k\right\rangle \tag{474}$$

If we multiply the above equation by a random bra of a statevector of a random layer and random sublattice that belongs to the system for example say; $\left\langle B_{k,L}\right|$; we get a coupled equation:

$$\left\langle B_{k,L}\right|\hat{H}_M\left|\psi_k\right\rangle = \sum_{L=1}^{M}\left\langle B_{k,L}\right|\hat{H}_M\left|B_{k,L}\right\rangle B_L + \left\langle B_{k,L}\right|\hat{H}_M\left|R_{k,L}\right\rangle R_L \tag{475}$$

For each multiplication of Schrödinger equation by a bra vector $\left\langle B_{k,L}\right|$ or $\left\langle R_{k,L}\right|$; we get a coupled equation.

Finally just as we had for the monolayer and bilayer; we get a total set of 2M coupled equations. We can write the equations as a large (depending on the number of layers M) 2Mx2M matrix equation:

$$\begin{pmatrix} \langle B_{k,1}|\hat{H}_M|B_{k,1}\rangle & \langle B_{k,1}|\hat{H}_M|R_{k,1}\rangle & \langle B_{k,1}|\hat{H}_M|B_{k,2}\rangle & \langle B_{k,1}|\hat{H}_M|R_{k,2}\rangle & .\ .\ .\ . \\ \langle R_{k,1}|\hat{H}_M|B_{k,1}\rangle & \langle R_{k,1}|\hat{H}_M|R_{k,1}\rangle & \langle R_{k,1}|\hat{H}_M|B_{k,2}\rangle & . & .\ .\ .\ . \\ \langle B_{k,2}|\hat{H}_M|B_{k,1}\rangle & \langle B_{k,2}|\hat{H}_M|R_{k,1}\rangle & . & . & .\ .\ .\ . \\ \langle R_{k,2}|\hat{H}_M|B_{k,1}\rangle & . & . & . & .\ .\ .\ . \\ . & . & . & . & .\ .\ .\ . \\ . & . & . & . & .\ .\ .\ . \\ . & . & . & . & .\ .\ .\ . \\ . & . & . & . & .\ .\ .\ . \end{pmatrix} \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \\ B_3 \\ R_3 \\ . \\ . \\ . \end{pmatrix} = E \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \\ B_3 \\ R_3 \\ . \\ . \\ . \end{pmatrix} \quad \textbf{(476)}$$

The results we got for general lattice in multilayer graphene in the previuos section means that the functions for hops between different layers of atomic sites with spesific distances would involve the functions similar to $G(\vec{k})$ and $F(\vec{k})$ from equations **(401)** and **(403)**; the only difference is that the hopping energies $\varepsilon^{u,v}_{\vec{n},\vec{m}}$ and $\tilde{\varepsilon}^{u,v}_{\vec{n},\vec{m}}$ are weaker than the hopping energies for the onlayer hopping energies $\varepsilon_{\vec{n},\vec{m}}$ and $\tilde{\varepsilon}_{\vec{n},\vec{m}}$; the reason for that we can see from equation **(469)** the distance ΔS between carbon atoms are larger between two different layers than onlayers, considering of course that we are talking about same indices $\vec{n}$ and $\vec{m}$ for two atoms from the same layer and two atoms from different layers).

5.2 ABA stacked trilayer and M-layer graphene

Let start with some applications so it would be more clear; For the trilayer with ABA orientation we have M=3; so the matrix equation(2Mx2M) is 6x6 matrix. If we only consider the nearest neighboring hops between atoms of the same layer and also only nearest neighboring interlayer hops which we already know from the bilayer case that it is just a constant $\gamma_1 \approx 0.4\text{eV}$; so the matrix equation becomes:

$$\begin{pmatrix} 0 & \varepsilon_0 g(\vec{k}) & 0 & 0 & 0 & 0 \\ \varepsilon_0 g(\vec{k})^* & 0 & \gamma_1 & 0 & 0 & 0 \\ 0 & \gamma_1 & 0 & \varepsilon_0 g(\vec{k}) & 0 & \gamma_1 \\ 0 & 0 & \varepsilon_0 g(\vec{k})^* & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_0 g(\vec{k}) \\ 0 & 0 & \gamma_1 & 0 & \varepsilon_0 g(\vec{k})^* & 0 \end{pmatrix} \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \\ B_3 \\ R_3 \end{pmatrix} = E \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \\ B_3 \\ R_3 \end{pmatrix} \quad (477)$$

The above Equation near Dirac's point $\vec{K}_{+}$ is:

$$\begin{pmatrix} 0 & v_F k & 0 & 0 & 0 & 0 \\ v_F k^* & 0 & \gamma_1 & 0 & 0 & 0 \\ 0 & \gamma_1 & 0 & v_F k & 0 & \gamma_1 \\ 0 & 0 & v_F k^* & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & v_F k \\ 0 & 0 & \gamma_1 & 0 & v_F k^* & 0 \end{pmatrix} \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \\ B_3 \\ R_3 \end{pmatrix} = E \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \\ B_3 \\ R_3 \end{pmatrix} \qquad (478)$$

The above equation gives four parabolic bands of which two touch each other just like in bilayer graphene, in addition to the four parabolic bands; the trilayer ABA gives two linear Dirac like bands that each other at k equal zero just like the monolayer graphene (look at figure (30)).

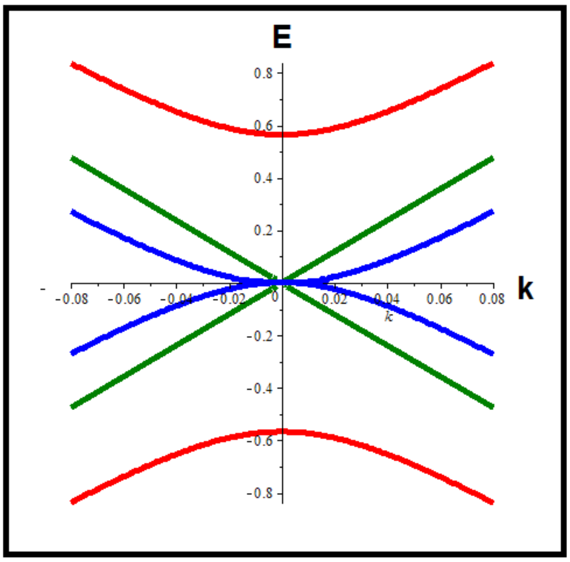
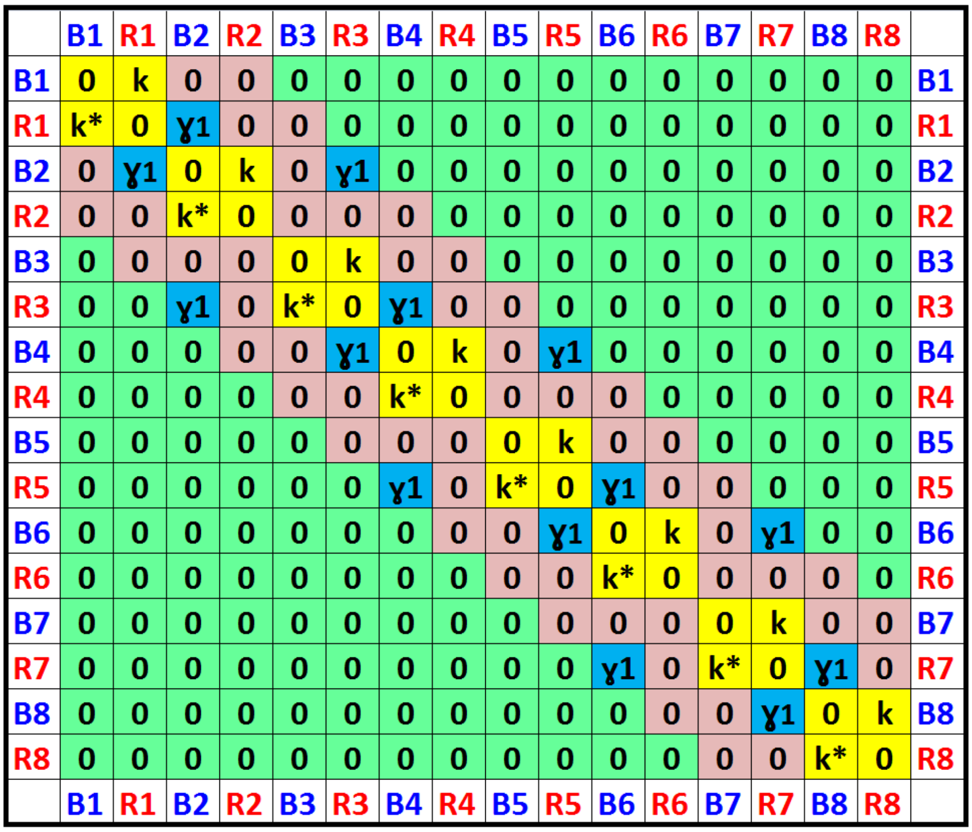


Figure (30): shows the dispersion relation for trilayer ABA stacked graphene near high symmetry Dirac point $\vec{K}_{+}$*; as we see there are four parabolic bands and two linear bands* **[15]**.

The Hamiltonians for ABA stacked graphene layers with random number of layers have some similar patterns with each other and one can study the matrix mathematically and see the consequences physically.

For multilayer ABA we have the following Hamiltonian which is drawn in figure (31) below with labeling to which hop each term represents:



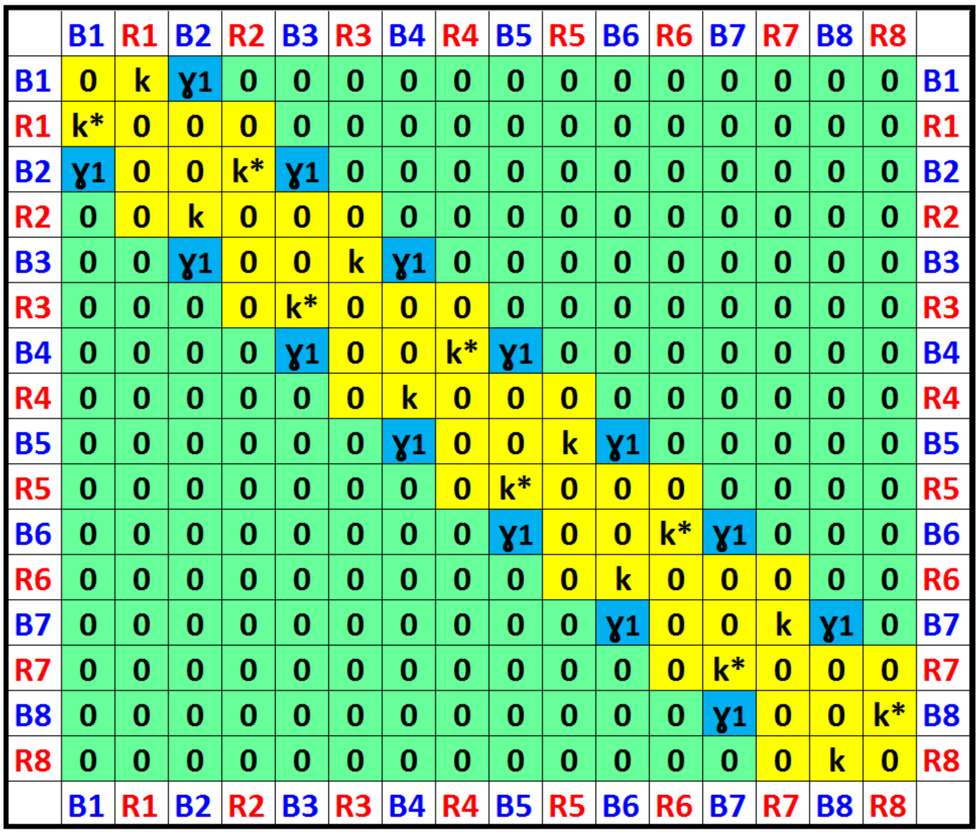
	B1	R1	B2	R2	B3	R3	B4	R4	B5	R5	B6	R6	B7	R7	B8	R8	
B1	0	k	0	0	0	0	0	0	0	0	0	0	0	0	0	0	B1
R1	k*	0	γ1	0	0	0	0	0	0	0	0	0	0	0	0	0	R1
B2	0	γ1	0	k	0	γ1	0	0	0	0	0	0	0	0	0	0	B2
R2	0	0	k*	0	0	0	0	0	0	0	0	0	0	0	0	0	R2
B3	0	0	0	0	0	k	0	0	0	0	0	0	0	0	0	0	B3
R3	0	0	γ1	0	k*	0	γ1	0	0	0	0	0	0	0	0	0	R3
B4	0	0	0	0	0	γ1	0	k	0	γ1	0	0	0	0	0	0	B4
R4	0	0	0	0	0	0	k*	0	0	0	0	0	0	0	0	0	R4
B5	0	0	0	0	0	0	0	0	0	k	0	0	0	0	0	0	B5
R5	0	0	0	0	0	0	γ1	0	k*	0	γ1	0	0	0	0	0	R5
B6	0	0	0	0	0	0	0	0	0	γ1	0	k	0	γ1	0	0	B6
R6	0	0	0	0	0	0	0	0	0	0	k*	0	0	0	0	0	R6
B7	0	0	0	0	0	0	0	0	0	0	0	0	0	k	0	0	B7
R7	0	0	0	0	0	0	0	0	0	0	γ1	0	k*	0	γ1	0	R7
B8	0	0	0	0	0	0	0	0	0	0	0	0	0	γ1	0	k	B8
R8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	k*	0	R8
	B1	R1	B2	R2	B3	R3	B4	R4	B5	R5	B6	R6	B7	R7	B8	R8	

Figure (31): show the form of the Hamiltonian of multilayer graphene with Bernal (ABA) stacking, the Hamiltonian is for 8 layers, but the pattern could be extended to any number.

Since the Hamiltonian for the ABA stacked graphene with a random number of layers has some special pattern, the energy band can also have a simpler and some pattern too: If the number of layers M is an even number, the energy band shows M/2 electron-like and M/2 hole-like bands. If M is an odd number; it will show an extra linear Dirac like band just as we have seen earlier for the trilayer ABA. In the presence of an electric field; the multilayer with ABA stacking order would not have a big change unlike the ABC stacking which opens a gap.

We can make a matrix transformation of the Hamiltonian in the above figure and get a matrix with a more clear form for the pattern; the transformation could be done by simply exchanging the labeling of some of the sublattices of the system (B to R or R to B) which of course should not have any physical effect when we are still preserving the ABA form and count for the interactions of the system.

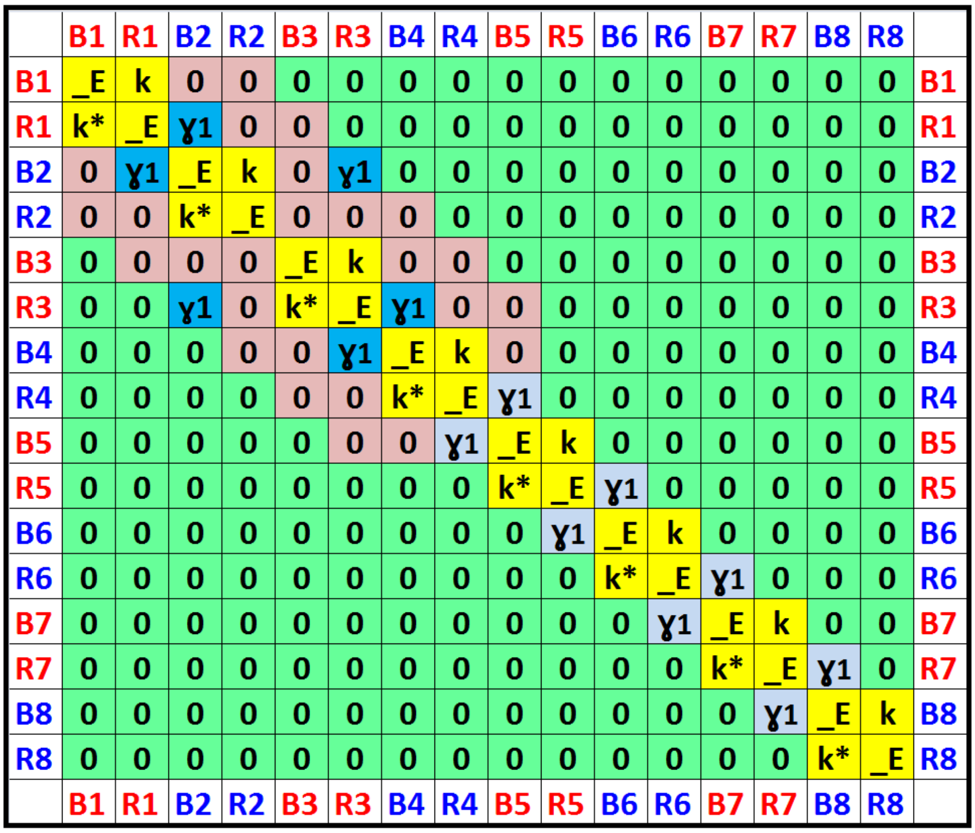
The transformed matrix and its form is drawn in the following figure (32) below:



	B1	R1	B2	R2	B3	R3	B4	R4	B5	R5	B6	R6	B7	R7	B8	R8	
B1	0	k	γ1	0	0	0	0	0	0	0	0	0	0	0	0	0	B1
R1	k*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	R1
B2	γ1	0	0	k*	γ1	0	0	0	0	0	0	0	0	0	0	0	B2
R2	0	0	k	0	0	0	0	0	0	0	0	0	0	0	0	0	R2
B3	0	0	γ1	0	0	k	γ1	0	0	0	0	0	0	0	0	0	B3
R3	0	0	0	0	k*	0	0	0	0	0	0	0	0	0	0	0	R3
B4	0	0	0	0	γ1	0	0	k*	γ1	0	0	0	0	0	0	0	B4
R4	0	0	0	0	0	0	k	0	0	0	0	0	0	0	0	0	R4
B5	0	0	0	0	0	0	γ1	0	0	k	γ1	0	0	0	0	0	B5
R5	0	0	0	0	0	0	0	0	k*	0	0	0	0	0	0	0	R5
B6	0	0	0	0	0	0	0	0	γ1	0	0	k*	γ1	0	0	0	B6
R6	0	0	0	0	0	0	0	0	0	0	k	0	0	0	0	0	R6
B7	0	0	0	0	0	0	0	0	0	0	γ1	0	0	k	γ1	0	B7
R7	0	0	0	0	0	0	0	0	0	0	0	0	k*	0	0	0	R7
B8	0	0	0	0	0	0	0	0	0	0	0	0	γ1	0	0	k*	B8
R8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	k	0	R8
	B1	R1	B2	R2	B3	R3	B4	R4	B5	R5	B6	R6	B7	R7	B8	R8	

Figure (32): Show the Transformed matrix for the multilayer graphene with 8 layers in the ABA stacked graphene, after the transformation, it is clearer how the pattern the matrix continues for a larger number of layers

The ABC stacking also share the interesting properties with the monolayer and bilayer and could have a lot of applications in modern electronics as we shall see in the next section, so we will study it in full detail in the next section. As for multilayers with random stacking, they could be arbitrary complex and they don’t necessarily have a pattern.



	B1	R1	B2	R2	B3	R3	B4	R4	B5	R5	B6	R6	B7	R7	B8	R8	
B1	_E	k	0	0	0	0	0	0	0	0	0	0	0	0	0	0	B1
R1	k*	_E	ɣ1	0	0	0	0	0	0	0	0	0	0	0	0	0	R1
B2	0	ɣ1	_E	k	0	ɣ1	0	0	0	0	0	0	0	0	0	0	B2
R2	0	0	k*	_E	0	0	0	0	0	0	0	0	0	0	0	0	R2
B3	0	0	0	0	_E	k	0	0	0	0	0	0	0	0	0	0	B3
R3	0	0	ɣ1	0	k*	_E	ɣ1	0	0	0	0	0	0	0	0	0	R3
B4	0	0	0	0	0	ɣ1	_E	k	0	0	0	0	0	0	0	0	B4
R4	0	0	0	0	0	0	k*	_E	ɣ1	0	0	0	0	0	0	0	R4
B5	0	0	0	0	0	0	0	ɣ1	_E	k	0	0	0	0	0	0	B5
R5	0	0	0	0	0	0	0	0	k*	_E	ɣ1	0	0	0	0	0	R5
B6	0	0	0	0	0	0	0	0	0	ɣ1	_E	k	0	0	0	0	B6
R6	0	0	0	0	0	0	0	0	0	0	k*	_E	ɣ1	0	0	0	R6
B7	0	0	0	0	0	0	0	0	0	0	0	ɣ1	_E	k	0	0	B7
R7	0	0	0	0	0	0	0	0	0	0	0	0	k*	_E	ɣ1	0	R7
B8	0	0	0	0	0	0	0	0	0	0	0	0	0	ɣ1	_E	k	B8
R8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	k*	_E	R8
	B1	R1	B2	R2	B3	R3	B4	R4	B5	R5	B6	R6	B7	R7	B8	R8	

Figure (33): illustrating random stacking; it shows an example of multilayer graphene with random stacking, in this case we have ABABCABC.

5.3 Rhombohedral Stacking ABC-Orientation:

Let us start with the Hamiltonian for trilayer ABC in k-space, if we only consider the nearest neighboring interactions between different layers and near Dirac's point K_+ ; we get:

$$\begin{pmatrix} 0 & \mathrm{v_F k} & 0 & 0 & 0 & 0 \\ \mathrm{v_F k^*} & 0 & \gamma_1 & 0 & 0 & 0 \\ 0 & \gamma_1 & 0 & \mathrm{v_F k} & 0 & 0 \\ 0 & 0 & \mathrm{v_F k^*} & 0 & \gamma_1 & 0 \\ 0 & 0 & 0 & \gamma_1 & 0 & \mathrm{v_F k} \\ 0 & 0 & 0 & 0 & \mathrm{v_F k^*} & 0 \end{pmatrix} \begin{pmatrix} \mathrm{B_1} \\ \mathrm{R_1} \\ \mathrm{B_2} \\ \mathrm{R_2} \\ \mathrm{B_3} \\ \mathrm{R_3} \end{pmatrix} = \mathrm{E} \begin{pmatrix} \mathrm{B_1} \\ \mathrm{R_1} \\ \mathrm{B_2} \\ \mathrm{R_2} \\ \mathrm{B_3} \\ \mathrm{R_3} \end{pmatrix} \qquad \textbf{(479)}$$

The equation above gives the following band drawn in figure (34) below:

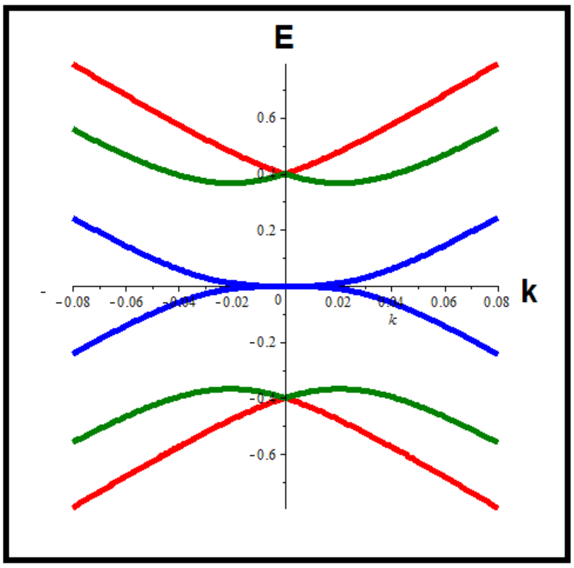


Figure (34): shows the energy band for trilayer graphene with ABC stacking order, for the ABC case; only two bands touch each other at the Fermi energy.

Let us derive the effective Hamiltonian for the trilayer ABC from equation **(479)**, we simply find the effective Hamiltonian when k is small; that is when $E, v_F k \ll \gamma_1$, the effective Hamiltonian is the approximate solution for the chiral terms(the two bands that touch zero, see figure () above). We define three 2x2 matrices that help us with calculations: one for k-dependece:

$$\tilde{H} \equiv \begin{pmatrix} 0 & v_F k \\ v_F k^* & 0 \end{pmatrix} \qquad (480)$$

Another one for the energy which is just the identity matrix multiplied by a constant:

$$\tilde{\mathrm{E}} \equiv \begin{pmatrix} \mathrm{E} & 0 \\ 0 & \mathrm{E} \end{pmatrix} \qquad (481)$$

The last involves γ_1 for the interlayer hops between two neighboring layers:

$$\tilde{\gamma}_1 \equiv \begin{pmatrix} 0 & \gamma_1 \\ \gamma_1 & 0 \end{pmatrix} \tag{482}$$

Now let us look a bit more at the last matrix above $\tilde{\gamma}_1$; it is a constant and large matrix relative to the other two; so if we had a small 2x2 matrix $\tilde{\varepsilon}$ defined as:

$$\tilde{\varepsilon} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} \\ \varepsilon_{21} & \varepsilon_{22} \end{pmatrix} \tag{483}$$

By small matrix $\tilde{\varepsilon}$ we mean its entries are very small relative to γ_1; then the inverse of the sum or the difference of the matrices $\tilde{\varepsilon}$ and $\tilde{\gamma}_1$ can be approximated to:

$$\begin{aligned}(\tilde{\gamma}_1 \pm \tilde{\varepsilon})^{-1} &= \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} \pm \gamma_1 \\ \varepsilon_{21} \pm \gamma_1 & \varepsilon_{22} \end{pmatrix}^{-1} = \frac{1}{\varepsilon_{11}\varepsilon_{22} - (\varepsilon_{12} \mp \gamma_1)(\varepsilon_{21} \mp \gamma_1)} \begin{pmatrix} \varepsilon_{22} & -\gamma_1 \mp \varepsilon_{12} \\ -\gamma_1 \mp \varepsilon_{21} & \varepsilon_{11} \end{pmatrix} \\ &\approx -\frac{1}{\gamma_1^2} \begin{pmatrix} \varepsilon_{22} & -\gamma_1 \mp \varepsilon_{12} \\ -\gamma_1 \mp \varepsilon_{21} & \varepsilon_{11} \end{pmatrix} \approx \begin{pmatrix} 0 & 1/\gamma_1 \\ 1/\gamma_1 & 0 \end{pmatrix} = \tilde{\gamma}_1^{-1}\end{aligned} \tag{484}$$

The above result is all we need to carry on to derive the effective Hamiltonian.

Now we can use the above three matrices to rewrite the eigenvalue equation for trilayer graphene **(479)** as three 2x2 matrix equations each involving only two components of the general vector for the system; the first equation involves the two terms with least interactions; B_1 and R_3 (the first and last equation of the **(479)**), we have:

$$\tilde{H} \begin{pmatrix} B_3 \\ R_1 \end{pmatrix} = \tilde{E} \begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{485}$$

The second equation is:

$$\tilde{H} \begin{pmatrix} B_1 \\ R_3 \end{pmatrix} + \tilde{\gamma}_1 \begin{pmatrix} B_2 \\ R_2 \end{pmatrix} = \tilde{E} \begin{pmatrix} B_3 \\ R_1 \end{pmatrix} \tag{486}$$

And at last we have the following equation:

$$\tilde{H} \begin{pmatrix} B_2 \\ R_2 \end{pmatrix} + \tilde{\gamma}_1 \begin{pmatrix} B_3 \\ R_1 \end{pmatrix} = \tilde{E} \begin{pmatrix} B_2 \\ R_2 \end{pmatrix} \tag{487}$$

Now we try to write the three equations above as one 2x2 equation by simply eliminating some of the components of the general vector for trilayer graphene ABC stacked. From equation **(487)** we get:

$$\begin{pmatrix} B_3 \\ R_1 \end{pmatrix} = \tilde{\gamma}_1^{-1} (\tilde{E} - \tilde{H}) \begin{pmatrix} B_2 \\ R_2 \end{pmatrix} \tag{488}$$

Rewriting equation **(486)** and putting it in the above equation we get:

$$\begin{pmatrix} B_3 \\ R_1 \end{pmatrix} = \tilde{\gamma}_1^{-1}\left(\tilde{E}-\tilde{H}\right)\tilde{\gamma}_1^{-1}\left(\tilde{E}\begin{pmatrix} B_3 \\ R_1 \end{pmatrix} - \tilde{H}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix}\right) \tag{489}$$

Rearranging the above equation a little bit; we get :

$$\begin{pmatrix} B_3 \\ R_1 \end{pmatrix} = \left(I - \tilde{\gamma}_1^{-1}\left(\tilde{E}-\tilde{H}\right)\tilde{\gamma}_1^{-1}\right)^{-1}\left(-\tilde{\gamma}_1^{-1}\left(\tilde{E}-\tilde{H}\right)\tilde{\gamma}_1^{-1}\tilde{H}\right)\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{490}$$

Finally if we put the result from the above equation into equation **(485)** we get a 2x2 equation for the ABC trilayer graphene as we wanted:

$$\tilde{H}\begin{pmatrix} B_3 \\ R_1 \end{pmatrix} = -\tilde{H}\left(I - \tilde{\gamma}_1^{-1}\left(\tilde{E}-\tilde{H}\right)\tilde{\gamma}_1^{-1}\right)^{-1}\left(\tilde{\gamma}_1^{-1}\left(\tilde{E}-\tilde{H}\right)\tilde{\gamma}_1^{-1}\tilde{H}\right)\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} = \tilde{E}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{491}$$

Until now we have the exact solution of equation **(479)**; we simply eliminated four equations and only two left with components of the general vector for trilayer ABC; B1 and R3 i.e. the two components with least interactions. In the first parenthesis in the second equality of the above equation; the identity matrix is the largest term, the second term is small; so we can make the following approximation:

$$\left(I - \tilde{\gamma}_1^{-1}\left(\tilde{E}-\tilde{H}\right)\tilde{\gamma}_1^{-1}\right)^{-1} \approx I \tag{492}$$

Using the above approximation and putting all diagonal terms on the left hand side of the equation; we get:

$$\tilde{H}\tilde{\gamma}_1^{-1}\tilde{H}\tilde{\gamma}_1^{-1}\tilde{H}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} = \left(\tilde{H}\tilde{\gamma}_1^{-1}\right)^2\tilde{H}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} = \left(\tilde{E}+\tilde{H}\tilde{\gamma}_1^{-1}\tilde{E}\tilde{\gamma}_1^{-1}\tilde{H}\right)\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{493}$$

Now in the right hand side of the above equation; the energy matrix $\tilde{E}$ is small, but the second term is much smaller; so we can do last approximation:

$$\left(\tilde{E}+\tilde{H}\tilde{\gamma}_1^{-1}\tilde{E}\tilde{\gamma}_1^{-1}\tilde{H}\right) \approx \tilde{E} \tag{494}$$

Using the above approximation; we come to our final answer or the effective Hamiltonian for the chiral terms when k is small or near Dirac’s points:

$$\left(\tilde{H}\tilde{\gamma}_1^{-1}\right)^2\tilde{H}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} = \tilde{E}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{495}$$

Writing the above result explicitly; we have **[22]**:

$$\hat{H}_{eff,3} \equiv \left(\tilde{H}\tilde{\gamma}_1^{-1}\right)^2\tilde{H} = \frac{v_F^3}{\gamma_1^2}\begin{pmatrix} 0 & (k)^3 \\ (k^*)^3 & 0 \end{pmatrix} \tag{496}$$

So the trilayer excitation energy would scale like k^3 near Dirac's points. This is a general property of multilayer graphene with ABC stacking; the dispersion goes as k^{M} where M is the total number of layers. We will come back to it.

Now let us look include the next nearest neighbor γ_3 term in the trilayer Schrödinger equation In k-space; the equation near Dirac's point K_+ now is:

$$\begin{pmatrix} 0 & v_F k & 0 & v_3 k^* & 0 & 0 \\ v_F k^* & 0 & \gamma_1 & 0 & 0 & 0 \\ 0 & \gamma_1 & 0 & v_F k & 0 & v_3 k^* \\ v_3 k & 0 & v_F k^* & 0 & \gamma_1 & 0 \\ 0 & 0 & 0 & \gamma_1 & 0 & v_F k \\ 0 & 0 & v_3 k & 0 & v_F k^* & 0 \end{pmatrix} \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \\ B_3 \\ R_3 \end{pmatrix} = E \begin{pmatrix} B_1 \\ R_1 \\ B_2 \\ R_2 \\ B_3 \\ R_3 \end{pmatrix} \tag{497}$$

In the above equation; we have $v_3 = \frac{3a\gamma_3}{2}$; it is simply the additional term get when we consider next nearest neighboring hops between two neighboring layers. We can write the above equation as set of three 2x2 matrix equations just as we did for the nearest neighboring approximation for hops between layers earlier; we have:

$$\tilde{H}\begin{pmatrix} B_3 \\ R_1 \end{pmatrix} + \tilde{\gamma}_3 \begin{pmatrix} B_2 \\ R_2 \end{pmatrix} = \tilde{E}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{498}$$

The second one:

$$\tilde{H}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} + \tilde{\gamma}_1 \begin{pmatrix} B_2 \\ R_2 \end{pmatrix} = \tilde{E}\begin{pmatrix} B_3 \\ R_1 \end{pmatrix} \tag{499}$$

And the last equation:

$$\tilde{H}\begin{pmatrix} B_2 \\ R_2 \end{pmatrix} + \tilde{\gamma}_1 \begin{pmatrix} B_3 \\ R_1 \end{pmatrix} + \tilde{\gamma}_3 \begin{pmatrix} B_1 \\ R_3 \end{pmatrix} = \tilde{E}\begin{pmatrix} B_2 \\ R_2 \end{pmatrix} \tag{500}$$

In the above three equations we have defined the new matrix $\tilde{\gamma}_3$ representing nearest neighbor hops:

$$\tilde{\gamma}_3 \equiv \begin{pmatrix} 0 & v_3 k^* \\ v_3 k & 0 \end{pmatrix} = \begin{pmatrix} 0 & \frac{3a\gamma_3}{2} k^* \\ \frac{3a\gamma_3}{2} k & 0 \end{pmatrix} \tag{501}$$

Doing similar procedure as we did earlier; the effective Hamiltonian in this case is:

$$E\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \approx \left(\tilde{H}\tilde{\gamma}_1^{-1}\right)^2 \tilde{H}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} - 2\tilde{H}\tilde{\gamma}_1^{-1}\tilde{\gamma}_3 \begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{502}$$

Writing the above equation explicitly; we have:

$$E\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} = \frac{v_F^3}{\gamma_1^2}\begin{pmatrix} 0 & (k)^3 \\ (k^*)^3 & 0 \end{pmatrix}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} - 2\frac{v_F v_3}{\gamma_1}\begin{pmatrix} 0 & |k|^2 \\ |k|^2 & 0 \end{pmatrix}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{503}$$

5.4 The effective Hamiltonian for ABC stacked mulitilayer graphene:

If we use a similar technique to eliminate components of four layers ABC stacked graphene and keep only the terms B1 from first layer and R4 from the fourth layer; the exact answer is:

$$\left(\tilde{E} + \tilde{H}M^{-1}\tilde{E}\tilde{\gamma}^{-1}\tilde{H}\right)\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} = \tilde{H}M^{-1}\tilde{H}\left(\tilde{E} - \tilde{\gamma}\right)^{-1}\tilde{H}\tilde{\gamma}^{-1}\tilde{H}\begin{pmatrix} B_1 \\ R_3 \end{pmatrix} \tag{504}$$

In the above equation; the matrix M is:

$$M = \tilde{\gamma} - \tilde{E}\tilde{\gamma}^{-1}\tilde{E} + \tilde{H}\left(\tilde{E} - \tilde{\gamma}\right)^{-1}\tilde{H}\tilde{\gamma}^{-1}\tilde{E} \tag{505}$$

The matrix $\tilde{\gamma}$ is the only large term of the matrix M, the other two are small which can just be called $\tilde{\varepsilon}$ so we can use equation **(484)** to do the following approximation:

$$\begin{aligned} M^{-1} &= \left(\tilde{\gamma} - \tilde{E}\tilde{\gamma}^{-1}\tilde{E} + \tilde{H}\left(\tilde{E} - \tilde{\gamma}\right)^{-1}\tilde{H}\tilde{\gamma}^{-1}\tilde{E}\right)^{-1} \\ &\equiv \left(\tilde{\gamma} - \tilde{\varepsilon}\right)^{-1} \approx \tilde{\gamma}^{-1} \end{aligned} \tag{506}$$

We do the same with the following term on the right hand side of equation **(504)**:

$$\left(\tilde{E} - \tilde{\gamma}\right)^{-1} \approx \tilde{\gamma}^{-1} \tag{507}$$

And similarly for the right hand side of equation **(504)** we have the following approximation:

$$\left(\tilde{E} + \tilde{H}M^{-1}\tilde{E}\tilde{\gamma}^{-1}\tilde{H}\right) \approx \tilde{E} \tag{508}$$

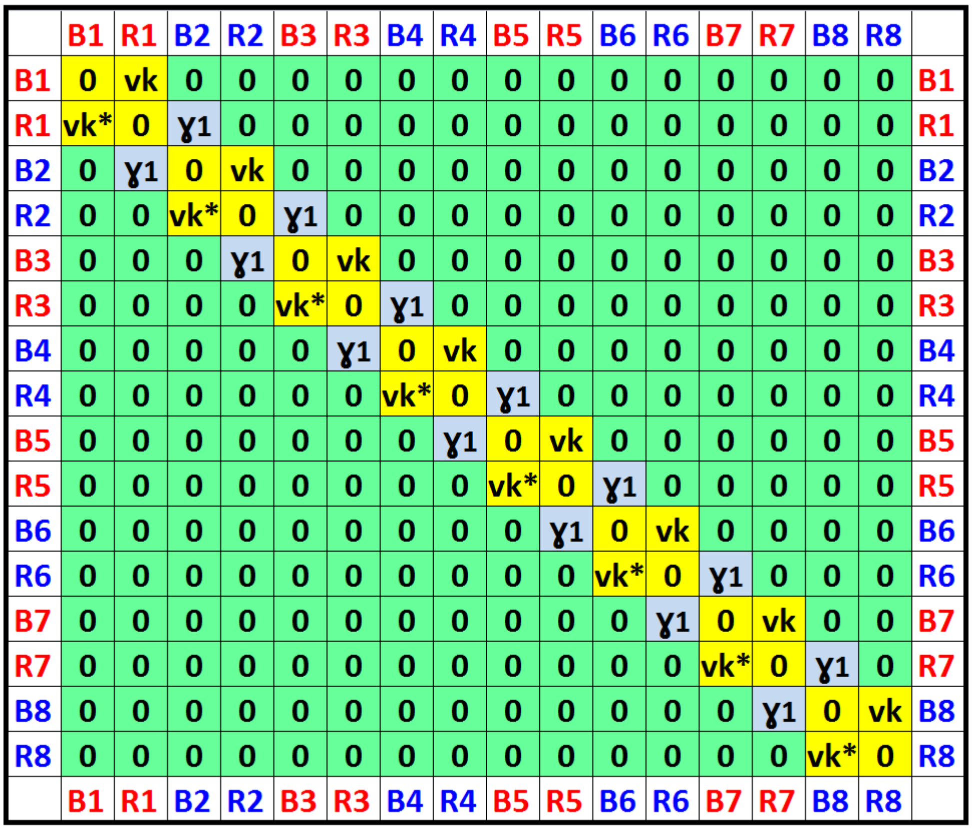
Finally with the approximations done above; we can get the effective Hamiltonian from the right hand side of equation **(504)**:

$$\begin{aligned} &\tilde{H}M^{-1}\tilde{H}\left(\tilde{E} - \tilde{\gamma}\right)^{-1}\tilde{H}\tilde{\gamma}^{-1}\tilde{H} \\ &\approx \tilde{H}\tilde{\gamma}^{-1}\tilde{H}\tilde{\gamma}^{-1}\tilde{H}\tilde{\gamma}^{-1}\tilde{H} = \left(\tilde{H}\tilde{\gamma}^{-1}\right)^3\tilde{H} \equiv \hat{H}_{eff,4} \end{aligned} \tag{509}$$

The full Schrödinger equation with the effective Hamiltonian is:

$$\hat{H}_{eff,4}\begin{pmatrix}B_1\\ R_3\end{pmatrix}=-\frac{v_F^4}{\gamma_1^3}\begin{pmatrix}0 & (k)^4\\ \left(k^*\right)^4 & 0\end{pmatrix}\begin{pmatrix}B_1\\ R_3\end{pmatrix}=\tilde{E}\begin{pmatrix}B_1\\ R_3\end{pmatrix} \qquad (510)$$

Let us now study the general case for ABC stacked graphene with any number of layers: If we consider the nearest neighboring term between different layers and only interactions between nearest neighboring layers; we get a large matrix equation with a simple pattern, simpler than for the ABA from previous section; for example the Hamiltonian for 8 layers graphene with ABC stacking order is drawn in figure (35) below:



	B1	R1	B2	R2	B3	R3	B4	R4	B5	R5	B6	R6	B7	R7	B8	R8	
B1	0	vk	0	0	0	0	0	0	0	0	0	0	0	0	0	0	B1
R1	vk*	0	ɣ1	0	0	0	0	0	0	0	0	0	0	0	0	0	R1
B2	0	ɣ1	0	vk	0	0	0	0	0	0	0	0	0	0	0	0	B2
R2	0	0	vk*	0	ɣ1	0	0	0	0	0	0	0	0	0	0	0	R2
B3	0	0	0	ɣ1	0	vk	0	0	0	0	0	0	0	0	0	0	B3
R3	0	0	0	0	vk*	0	ɣ1	0	0	0	0	0	0	0	0	0	R3
B4	0	0	0	0	0	ɣ1	0	vk	0	0	0	0	0	0	0	0	B4
R4	0	0	0	0	0	0	vk*	0	ɣ1	0	0	0	0	0	0	0	R4
B5	0	0	0	0	0	0	0	ɣ1	0	vk	0	0	0	0	0	0	B5
R5	0	0	0	0	0	0	0	0	vk*	0	ɣ1	0	0	0	0	0	R5
B6	0	0	0	0	0	0	0	0	0	ɣ1	0	vk	0	0	0	0	B6
R6	0	0	0	0	0	0	0	0	0	0	vk*	0	ɣ1	0	0	0	R6
B7	0	0	0	0	0	0	0	0	0	0	0	ɣ1	0	vk	0	0	B7
R7	0	0	0	0	0	0	0	0	0	0	0	0	vk*	0	ɣ1	0	R7
B8	0	0	0	0	0	0	0	0	0	0	0	0	0	ɣ1	0	vk	B8
R8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	vk*	0	R8
	B1	R1	B2	R2	B3	R3	B4	R4	B5	R5	B6	R6	B7	R7	B8	R8	

Figure (35): show the form of the Hamiltonian of multilayer graphene with Rhombohedral (ABC) stacking, the Hamiltonian is for 8 layers, but the pattern could be extended to any number.

The Schrödinger equation for the M layer Hamiltonian in the form of figure above is as already mentioned an eigenvalue equation with 2Mx2M matrix. The first equation for the M-layers graphene is simply the interactions between the B1-sublattice and the R1-sublattice of the first layer system (top layer):

$$\mathrm{v_F k R_1 = E B_1} \qquad (511)$$

The last equation for the M-layers is interactions between BM-sublattice and the RM-sublattice of the last layer in the system (bottom layer):

$$v_F k^* B_M = E R_M \tag{512}$$

The two equations above are the equations at the boundaries of the multilayer system under study. The effective Hamiltonian will eventually involve these two boundary components (B_1 and R_M) of the general eigenvector of the system. All the equations between have the interlayer interactions with the hopping energy γ_1: we have two coupled recurrence relations; the first is:

$$v_F k^* B_m + \gamma_1 B_{m+1} - E R_m = 0 \tag{513}$$

And we have a second recurrence relation is:

$$v_F k R_{m+1} + \gamma_1 R_m - E B_{m+1} = 0 \tag{514}$$

The result for the effective Hamiltonian in the case of three layers had the relation between energy and the momentum k ($\hbar = 1 \Rightarrow p = k$) is $E \sim |k|^3$ and for the case of four layers; $E \sim |k|^4$. This suggests that the energy for the ABC stacked graphene with total number M layers in the lowest order is $E \sim |k|^M$; so make the assumption that the terms ER_m and EB_{m+1} in equations **(513)** and **(514)** are negligible and check what we get, once we do neglect those terms we can solve the two recurrence relations very easily; for the first one equation **(513)** after the neglect we have:

$$B_{m+1} = \left(\frac{v_F k^*}{-\gamma_1} \right) B_m \tag{515}$$

The above equation at the boundary (for the component B_M) gives the solution:

$$B_M = \left(\frac{v_F k^*}{-\gamma_1} \right)^{M-1} B_1 \tag{516}$$

The second recurrence relation from equation **(514)** after the neglect we have:

$$R_m = \left(\frac{v_F k}{-\gamma_1} \right) R_{m+1} \tag{517}$$

Finally from the above equation we get a solution for R_1:

$$R_1 = \left(\frac{v_F k}{-\gamma_1} \right)^{M-1} R_M \tag{518}$$

Now we have found the important results; we use the expression we got in equations **(516)** and **(518)**, and we put them into the boundary equations **(511)** and **(512)**, and we get the two desired coupled equations which only involves the weak interactions between B_1 and R_M :

$$v_F k \left(\frac{v_F k}{-\gamma_1} \right)^{M-1} R_M = B_1 \tag{519}$$

And the second equation is:

$$v_F k^* \left(\frac{v_F k^*}{-\gamma_1} \right)^{M-1} B_1 = E R_M \tag{520}$$

We can the two equations above as an eigenvalue equation with 2x2 matrix which looks familiar to what we got for the three and four layers **[22]**:

$$\hat{H}_{eff,M} \begin{pmatrix} B_1 \\ R_M \end{pmatrix} = \frac{v_F^M}{(-\gamma_1)^{M-1}} \begin{pmatrix} 0 & (k)^M \\ (k^*)^M & 0 \end{pmatrix} \begin{pmatrix} B_1 \\ R_M \end{pmatrix} = E \begin{pmatrix} B_1 \\ R_M \end{pmatrix} \tag{521}$$

The solution for the energy in the equation above is:

$$E = \pm \frac{v_F^M}{\gamma_1^{M-1}} |k|^M \sim \pm |k|^M \tag{522}$$

As we see that the energy E is proportional to $|k|^M$ and is symmetric in respect to electrons and holes. The bands we found in the above equation are the two flat bands of the ABC stacked graphene that touch each other near Dirac's point K_+; the rest of the ABC bands are all divided equally electron-like and hole-like with distance γ_1 from zero (Dirac's point). It remains to verify that the terms EB_{m+1} and ER_m we neglected in equations **(513)** and **(514)** are indeed small relative to the ones we kept.

Let us use the solution for the energy in equation **(522)** above and put it back into equation **(521)** to find the components B_1, R_M and from them the rest of the components of the general eigenvector of the ABC stacked graphene in this approximation; the solution is:

$$\begin{pmatrix} B_1 \\ R_M \end{pmatrix} = \begin{pmatrix} 1 \\ \dfrac{\mp (k^*)^M}{|k|^M} \end{pmatrix} \tag{523}$$

The solutions for the energy and the components B_m and R_m show that our assumption that the terms EB_{m+1} and ER_m in equations **(513)** and **(514)** to negligible was reasonable; we have:

$$EB_{m+1} = \left(\pm\frac{v_F^M}{\gamma_1^{M-1}}|k|^M\right)\left(\frac{v_F k^*}{-\gamma_1}\right)^{m-1} \approx 0 \tag{524}$$

And the same for the second term that we neglected:

$$ER_m = \left(\pm\frac{v_F^M}{\gamma_1^{M-1}}|k|^M\right)\left(\frac{v_F k}{-\gamma_1}\right)^{M-m}\left(\frac{\mp\left(k^*\right)^M}{|k|^M}\right) \approx 0 \tag{525}$$

The terms that we neglected are maximum equal to one and the energy is proportional $|k|^M$ which is very small relative to the absolute value $|k|$,which already small itself.

The solutions for the band near Dirac's points without making approximation to the effective Hamiltonian give two bands that touch each other exactly at Dirac's points and they become flatter and flatter bands as the number of layers increases; so the results we got using the effective Hamiltonian is a valid one (look at figure(36) below).

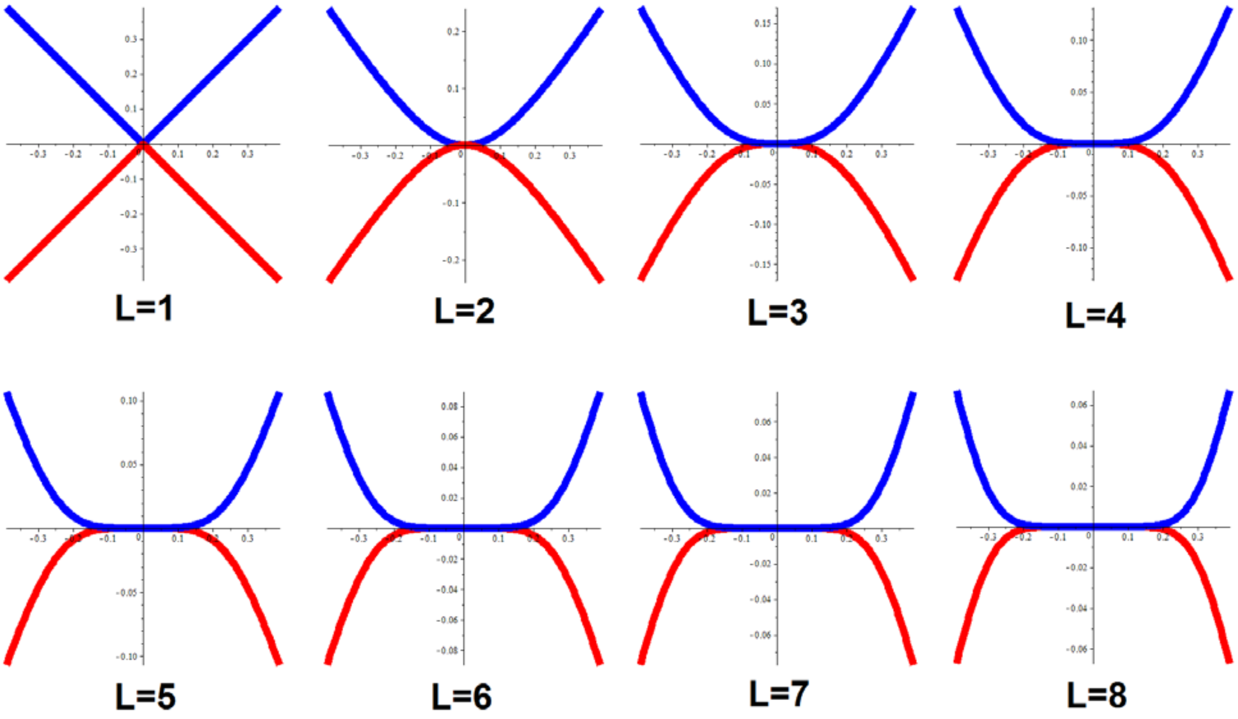


Figure (36): E(k) vertical axis, and k horizontal axis) shows the energy dispersion relation E(k) for the monolayer, the two bands of the bilayer that touch each other and from three to eight layers two bands that touch each other for ABC stacking for the Hamiltonian, and as we see, the bands become flatter and flatter; it confirms that equation **(521)** *for the effective Hamiltonian is valid near Dirac's point* K_+.

When an external electric field is applied to a multilayer graphene system with ABC orientation; unlike the ABA stacked graphene a gap will open with appreciable size i.e. the ABC stacked graphene becomes more insulating in the presence of an external electric field in similarity to the bilayer case we studied earlier. Also we can control it easily with our adjustment to the external electric field we apply on the system. These properties make ABC stacked multilayer graphene systems useful for future technology in electronics.

6 Graphene in a magnetic field

6.1 Dirac-like Equation in a magnetic field

The effective Hamiltonian of graphene near Dirac points is similar to ultrarelativistic fermions; that is the quasiparticles behave linear just as in the Dirac equation. Now we will study graphene in a magnetic field; we solve the effective Hamiltonian (The Dirac equation in 2D) in a constant magnetic field and study the energy spectrum. We include the field interaction by minimum coupling:

$$\mathrm{p_n} \rightarrow \mathrm{p_n} - \mathrm{qA_n} \tag{526}$$

One simple choice of the vector potential is

$$\vec{\mathrm{A}} = \left(-\mathrm{By}, 0, 0\right) \tag{527}$$

Then the coupled equation becomes $\hbar = 1$:

$$v_F \begin{pmatrix} 0 & \frac{\partial}{\partial x} + eBy - \frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + eBy + \frac{\partial}{\partial y} & 0 \end{pmatrix} \begin{pmatrix} \psi_B \\ \psi_R \end{pmatrix} = E \begin{pmatrix} \psi_B \\ \psi_R \end{pmatrix} \tag{528}$$

The eigenvector for the x-direction is just a plane wave; $\psi_B = e^{ikx}\varphi_B(y)$ and $\psi_R = e^{ikx}\varphi_R(y)$ so the derivative with respect to x gives the eigenvalue $\mathrm{p_x}$:

$$v_F \begin{pmatrix} 0 & p_x + eBy - \frac{\partial}{\partial y} \\ p_x + eBy + \frac{\partial}{\partial y} & 0 \end{pmatrix} \begin{pmatrix} \psi_B \\ \psi_R \end{pmatrix} \equiv v_F \begin{pmatrix} 0 & D^\dagger \\ D & 0 \end{pmatrix} \begin{pmatrix} \psi_B \\ \psi_R \end{pmatrix} = \tag{529}$$

The operators $D^\dagger$ and D in the above equation are defined as:

$$D^\dagger = \left(p_x + eBy - \frac{\partial}{\partial y} \right) \quad \text{and} \quad D = p_x + eBy + \frac{\partial}{\partial y} \tag{530}$$

If we multiply the second equation for of the matrix equation **(528)** by the operator $D^{\dagger}$ and put it into the first equation; we get:

$$v_F^2 D^{\dagger}\left(D\psi_B\right) = E\left(D^{\dagger}\psi_R\right) = E^2\psi_B \tag{531}$$

Multiplying the operators $\mathrm{D}^{\dagger}\mathrm{D}$ and doing a little rearranging; we get:

$$\begin{aligned} \mathrm{D}^{\dagger}\mathrm{D} &= \mathrm{p}_x^2 + (\mathrm{qB})^2\mathrm{y}^2 - \frac{\partial^2}{\partial \mathrm{y}^2} + \mathrm{qB}\left[\mathrm{y}, \frac{\partial}{\partial \mathrm{y}}\right] + 2\mathrm{p}_x\mathrm{qBy} \\ &= (\mathrm{qB})^2\left(\frac{\mathrm{p}_x}{\mathrm{qB}} + \mathrm{y}\right)^2 - \frac{\partial^2}{\partial \mathrm{y}^2} + \mathrm{qB}\left[\mathrm{y}, \frac{\partial}{\partial \mathrm{y}}\right] \end{aligned} \tag{532}$$

We make the substitution $\tilde{\mathrm{y}} = \left(\frac{\mathrm{p}_x}{\mathrm{qB}} + \mathrm{y}\right)$; we get:

$$\mathrm{v}_F^2\mathrm{D}^{\dagger}\mathrm{D}\psi_B = \mathrm{v}_F^2\left((\mathrm{qB})^2\tilde{\mathrm{y}}^2 - \frac{\partial^2}{\partial \tilde{\mathrm{y}}^2} - \mathrm{qB}\right)\psi_B = \mathrm{E}^2\psi_B \tag{533}$$

This is simply the harmonic oscillator:

$$\left((\mathrm{qB})^2\tilde{\mathrm{y}}^2 - \frac{\partial^2}{\partial \tilde{\mathrm{y}}^2} - \mathrm{qB}\right)\psi_B = \mathrm{E}^2\psi_B \tag{534}$$

The appropriate ladder operators for the above equation are:

$$\mathrm{a} = \sqrt{\frac{\mathrm{qB}}{2}}\mathrm{y} + \frac{1}{\sqrt{2\mathrm{qB}}}\frac{\partial}{\partial \mathrm{y}} \quad \text{and} \quad \mathrm{a}^{\dagger} = \sqrt{\frac{\mathrm{qB}}{2}}\mathrm{y} - \frac{1}{\sqrt{2\mathrm{qB}}}\frac{\partial}{\partial \mathrm{y}} \tag{535}$$

The commutator between the ladder operators in the above equation is equal to 1 exactly as we had for the Harmonic oscillator in equation **(140)** so the procedure is very similar for solving the energies of the system; the only difference is that we have different set of constants otherwise the same. That means we get the familiar harmonic oscillator expressed in ladder operators, only we don’t have the extra half added:

$$\hat{\mathrm{H}}_B = \left(2\mathrm{v}_F^2\mathrm{qB}\right)\mathrm{a}^{\dagger}\mathrm{a} \tag{536}$$

That means the solution is exactly like equation **(162)** only we have E^2 instead of E on the left hand side of the equation and we don’t have the extra half as mentioned earlier, so we can use similar method to find the energy and we get:

$$\mathrm{E}^2 = \left(2\mathrm{v}_F^2\mathrm{qB}\right)\mathrm{N} \tag{537}$$

Where $N = 0,1,2.....$ in the above equation, using the value for $\omega_B = 2v_F^2 qB$; the energy levels (look at figure (37) below) then are **[15]**:

$$E = \pm\left(2v_F^2 qB\right)^{1/2} \sqrt{N} \tag{538}$$

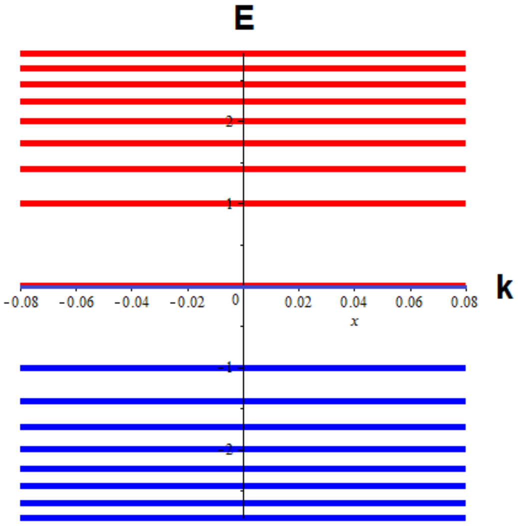


Figure (37): shows the energy levels for graphene in a perpendicular magnetic near Dirac's points; we have put the physical factor $\left(2v_F^2 qB\right)^{1/2} = 1$

Notice the interesting solution for energy levels in equation **(538)**; we have a zero-energy state at $N = 0$. This state is responsible for the experimental anomalies in quantum hall effect. Further, if we did the same procedure for the other inequivalent Dirac's point K_-; we obtain exactly the same result. That means that the energy levels are double degenerate. The hall conductivity in graphene is:

$$\sigma_{xy} = 4\frac{e^2}{h}\left(N + \frac{1}{2}\right) \tag{539}$$

The extra factor 4 in the equation above comes from spin up and down, but in addition because we have two inequivalent Dirac points. Notice in the equation above the anomalous quantum hall effect; that we have the extra $1/2$ shifted from the sequence of N steps **[2]**.

Another interesting result in graphene is that near the Dirac point where the two bands meet, the carrier concentration should be zero and that means the conductivity is zero, however in graphene there is a minimal conductivity of the order of $4\frac{e^2}{h}$.

Last we see from equation **(538)** for the energy levels; that the cyclotron energy scales like $E \sim \sqrt{B}$ different from non-relativistic fermions. This property is very important, since it implies that we can measure the quantum hall effect in graphene at room temperature. If we apply a magnetic field to a single layer graphene of the order of 10T; then the cyclotron energy scales like 1000K, which remarkably are two orders of magnitude higher than for an electron gas in 2D which is about 10K.

6.2 ABC Stacked Multilayer graphene in a magnetic field:

Let us start with looking at the commutator of the operators D and its hermitian conjugate $D^{\dagger}$ from equation **(530)**:

$$\left[D, D^{\dagger}\right] = DD^{\dagger} - D^{\dagger}D = 2qB \tag{540}$$

That means we can write the operators and in terms of the ladder operators a and $a^{\dagger}$ we defined in equation **(535)** for the monolayer case in a magnetic field:

$$D = \sqrt{2qB}a \qquad \text{and} \qquad D^{\dagger} = \sqrt{2qB}a^{\dagger} \tag{541}$$

The Schrödinger equation for the bilayer AB and multilayer ABC stacked graphene with a random M layers near Dirac's point K_{+} in a magnetic field when we are considering the effective Hamiltonian is:

$$\frac{v_F^M}{(-\gamma_1)^{M-1}} \begin{pmatrix} 0 & \left(D^{\dagger}\right)^M \\ (D)^M & 0 \end{pmatrix} \begin{pmatrix} B_1 \\ R_M \end{pmatrix} = E \begin{pmatrix} B_1 \\ R_M \end{pmatrix} \tag{542}$$

We use the second coupled equation from the above matrix equation to get one equation involving only the one for component B_1:

$$\frac{v_F^{2M}}{\gamma_1^{2M-2}} \left(D^{\dagger}\right)^M (D)^M B_1 = E^2 B_1 \tag{543}$$

We write the above equation in terms of the ladder operators with the use of equation **(541)**:

$$\begin{aligned} \hat{H}_M B_1 &\equiv \left(D^{\dagger}\right)^M (D)^M B_1 = \frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}} \left(a^{\dagger}\right)^M (a)^M B_1 \\ &= \frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}} \left(a^{\dagger}\right)^M (a)^M B_1 = E^2 B_1 \end{aligned} \tag{544}$$

It is easier to use the ladder operators because the commutator between them is simply equal to one and also we could easily compare the multilayer problem to the single layer one where we had the harmonic oscillator.

We need to do simple calculations of commutators and use commutations relations to find the energy of a multilayer ABC stacked graphene in a magnetic field. We start with a simple commutation relation that will be important in the calculations of the energy; for two scalars α and β we have:

$$\left(a^\dagger a-\alpha\right)\left(a^\dagger a-\beta\right)=a^\dagger a\ a^\dagger a-\left(\alpha+\beta\right)a^\dagger a+\alpha\beta=\left(a^\dagger a-\beta\right)\left(a^\dagger a-\alpha\right) \tag{545}$$

Writing the above equation as a commutator:

$$\left[\left(a^\dagger a-\alpha\right),\left(a^\dagger a-\beta\right)\right]=0 \tag{546}$$

Next we need to prove the following formula:

$$\left[a^\dagger,a^M\right]=-Ma^{M-1} \tag{547}$$

We prove the above equation by induction; we first verify it for $M=2$ by doing the calculation:

$$\left[a^\dagger,a^2\right]=\left[a^\dagger,a\,a\right]=\left[a^\dagger,a\right]+a\left[a^\dagger,a\right]=-2a \tag{548}$$

Next if we assume that it is true for M and prove that it to be also true for $M+1$:

$$\begin{aligned}\left[a^\dagger,a^{M+1}\right]&=\left[a^\dagger,a\,a^M\right]=\left[a^\dagger,a\right]a^M+a\left[a^\dagger,a^M\right]\\&=-a^M+a\left(-\left(M\right)a^{M-1}\right)=-a^M-Ma^M=-\left(M+1\right)a^M\end{aligned} \tag{549}$$

The above equation gives us:

$$\begin{aligned}a^\dagger\left(a\right)^{M-1}&=\left[a^\dagger,\left(a\right)^{M-1}\right]+\left(a\right)^{M-1}a^\dagger\\&=-\left(M-1\right)\left(a\right)^{M-2}+\left(a\right)^{M-1}a^\dagger\end{aligned} \tag{550}$$

Now we use the expression for n the above equation to find the a recurrence relation between $\hat{H}_M$; we start with a polynomial $P_M\left(a,a^\dagger\right)$:

$$P_M\left(a,a^\dagger\right)=\left(a^\dagger\right)^M\left(a\right)^M \tag{551}$$

Then we use the result for $a^\dagger\left(a\right)^{M-1}$ from equation **(550)** above to find the following recurrence relation:

$$\begin{aligned}&P_M\left(a,a^\dagger\right)=\left(a^\dagger\right)^M\left(a\right)^M=\left(a^\dagger\right)^{M-1}a^\dagger\left(a\right)^{M-1}a\\&\left(a^\dagger\right)^{M-1}\left(-\left(M-1\right)\left(a\right)^{M-2}+\left(a\right)^{M-1}a^\dagger\right)a\\&=\left(a^\dagger\right)^{M-1}\left(a\right)^{M-1}\left(a^\dagger a-M+1\right)=P_{M-1}\left(a,a^\dagger\right)\left(a^\dagger,a\right)\left(a^\dagger a-M+1\right)\end{aligned} \tag{552}$$

By repeating the calculations we did in the above equation; we can find an explicit solution for the polynomial $P_M\left(a,a^\dagger\right)$ in terms the number operator; $a^\dagger a$ and that would make our calculations for the energy levels for multilayer ABC stacked graphene very easy to find. Finally we have the following solution for the polynomial $P_M\left(a,a^\dagger\right)$:

$$P_M\left(a,a^\dagger\right)=a^\dagger a\left(a^\dagger a-1\right)\left(a^\dagger a-2\right).....\left(a^\dagger a-M+1\right) \tag{553}$$

Then we can course find an expression for the operator $\hat{H}_M$ which is the above expression multiplied by an appropriate constant:

$$\begin{aligned}\hat{H}_M&=\frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}}\prod_{m=1}^{M}\left(a^\dagger a-m+1\right)\\&=\frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}}a^\dagger a\left(a^\dagger a-1\right)\left(a^\dagger a-2\right).....\left(a^\dagger a-M+1\right)\end{aligned} \tag{554}$$

Using equation **(546)** we find that $\hat{H}_M$ commutes with the operator $\hat{H}_B$ from equation **(536)** for monolayer:

$$\begin{aligned}\hat{H}_M\hat{H}_B&=\frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}}a^\dagger a\left(a^\dagger a-1\right).....\left(a^\dagger a-M+1\right)\hat{H}_B\\&=\frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}}a^\dagger a\left(a^\dagger a-1\right).....\hat{H}_B\left(a^\dagger a-M+1\right)\\&=.....=\hat{H}_B\frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}}a^\dagger a\left(a^\dagger a-1\right).....\left(a^\dagger a-M+1\right)\\&=\hat{H}_B\hat{H}_M\end{aligned} \tag{555}$$

In the above equation we simply $\beta=0$ and $\alpha=-m+1$ for the commutator in equation **(546)**, so each term in the product **(554)** will commute with $\hat{H}_B$ which means of course $\hat{H}_M$ would commute with it too. Writing the above equation as a commutator :

$$\left[\hat{H}_B,\hat{H}_M\right]=0 \tag{556}$$

The result in the above equation is our final condition to solve for energies: We worked with commutators and anticommutators in section (1.5) and we saw that if two operators commute, then the eigenvectors of the one operator are automatically eigenvectors of the other operator. This means that the eigenvectors for $\hat{H}_B$ which were simply the harmonic oscillator are also eigenvectors of the operator we are interested in and that is $\hat{H}_M$.

We can find the eigenvalues or the energies by simply operating $\hat{H}_M$ on the eigenvector of $\hat{H}_B$ which in this case as mentioned earlier; they are the eigenvectors of the harmonic oscillator. We know already from harmonic oscillator that the operator (called the number operator) $a^\dagger a$ acted on an eigenvector $|N\rangle$ will simply give the number N:

$$a^\dagger a|N\rangle = N|N\rangle \tag{557}$$

That means when the operator $\hat{H}_M$ acting on the eigenvector $|N\rangle$; then each parenthesis in the product will contain the number N:

$$\begin{aligned} E^2|N\rangle = \hat{H}_M|N\rangle &= \frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}} \prod_{m=1}^{M}\left(a^\dagger a - m + 1\right)|N\rangle = \frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}} \prod_{m=1}^{M}\left(N - m + 1\right)|N\rangle \\ &= \frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}} N(N-1)(N-2).....(N-M+1)|N\rangle \end{aligned} \tag{558}$$

And of course from the above equation; we have that the energy eigenvalues of a multilayer graphene with ABC stacking order in a magnetic field are **[23]**:

$$E = \pm\frac{\left(v_F^2 2qB\right)^M}{\gamma_1^{2M-2}}\sqrt{N(N-1)(N-2).....(N-M+1)} \tag{559}$$

All the states $|0\rangle, |1\rangle, |2\rangle, ...$ up to $|M-1\rangle$ give zero when acted on by the operator $\hat{H}_M$ of the m-layer system; so the zero energy is degenerate with 4M states; the factor 4 in front of M is due to the fact that we have two spin states and we also have two Dirac points.

Part III: Appendix and sources

7 Appendix:

7.1 Calculations of Energy band for Graphene in the Tight Binding Model

Let us carry out the calculations for the general Hamiltonian for the monolayer graphene explicitly; we know the Hamiltonian for the hops of the whole lattice for graphene as we have seen section (3.1) is:

$$\begin{aligned}\hat{H}_{gen} &= \sum_{\vec{m},\vec{n}} \varepsilon_{m,n} \left(a^{\dagger}_{\vec{m}} b_{\vec{n}} + b^{\dagger}_{\vec{n}} a_{\vec{m}} \right) + \sum_{\vec{m},\vec{n}} \tilde{\varepsilon}_{m,n} \left(\left(a^{\dagger}_{\vec{m}} a_{\vec{n}} + a^{\dagger}_{\vec{n}} a_{\vec{m}} \right) + \left(b^{\dagger}_{\vec{m}} b_{\vec{n}} + b^{\dagger}_{\vec{n}} b_{\vec{m}} \right) \right) \\ &= \hat{H}_{gen,0} + \hat{H}_{gen,1}\end{aligned} \tag{560}$$

We get two coupled equations by multiplying the Schrödinger equation by the ket of the general statevectors for each of the sublattices $\left\langle B_k \right|$ and $\left\langle R_k \right|$ in monolayer graphene lattice:

$$\left\langle B_k \right| \hat{H}_{gen} \left| \psi_k \right\rangle = \left\langle B_k \right| \hat{H}_{gen} \left| B_k \right\rangle B + \left\langle B_k \right| \hat{H}_{gen} \left| R_k \right\rangle R = EB \tag{561}$$

And another coupled equation by multiplying with $\left\langle R_k \right|$:

$$\left\langle R_k \right| \hat{H}_{gen} \left| \psi_k \right\rangle = \left\langle R_k \right| \hat{H}_{gen} \left| B_k \right\rangle B + \left\langle R_k \right| \hat{H}_{gen} \left| R_k \right\rangle R = ER \tag{562}$$

We write the above two coupled equation as a matrix equation to see the terms more clearly:

$$\begin{pmatrix} \left\langle B_k \right| \hat{H}_{gen} \left| B_k \right\rangle & \left\langle B_k \right| \hat{H}_{gen} \left| R_k \right\rangle \\ \left\langle R_k \right| \hat{H}_{gen} \left| B_k \right\rangle & \left\langle R_k \right| \hat{H}_{gen} \left| R_k \right\rangle \end{pmatrix} \begin{pmatrix} B \\ R \end{pmatrix} = E \begin{pmatrix} B \\ R \end{pmatrix} \tag{563}$$

Let us start calculating the off-diagonal elements of the matrix in the equation above; we know the Hamiltonian is a sum of two terms, so for the term $\left\langle B_k \right| \hat{H}_{gen} \left| R_k \right\rangle$ we have:

$$\left\langle B_k \right| \hat{H}_{gen} \left| R_k \right\rangle = \left\langle B_k \right| \hat{H}_{gen,0} \left| R_k \right\rangle + \left\langle B_k \right| \hat{H}_{gen,1} \left| R_k \right\rangle \tag{564}$$

The second term on the right hand of the above equation is zero; $\left\langle B_k \right| \hat{H}_{gen,1} \left| R_k \right\rangle = 0$, while the first term is not, we start by operating $\hat{H}_{gen,0}$ on the eigenvector $\left| R_k \right\rangle$:

$$\begin{aligned}\hat{H}_{gen,0} \left| R_k \right\rangle &= \frac{1}{\sqrt{N}} \sum_{\vec{v},\vec{m},\vec{n}}^{N} e^{i\vec{k}\bullet\vec{R}_{\vec{v}}} \left(a^{\dagger}_{\vec{m}} b_{\vec{n}} + b^{\dagger}_{\vec{n}} a_{\vec{m}} \right) b^{\dagger}_{\vec{v}} \left| 0 \right\rangle \\ &= \frac{1}{\sqrt{N}} \sum_{\vec{v},\vec{m},\vec{n}}^{N} e^{i\vec{k}\bullet\vec{R}_{\vec{v}}} \left(a^{\dagger}_{\vec{m}} \left(\delta_{\vec{n}\vec{v}} - b^{\dagger}_{\vec{v}} b_{\vec{n}} \right) + \left(b^{\dagger}_{\vec{m}} b^{\dagger}_{\vec{v}} \right) a_{\vec{m}} \right) \left| 0 \right\rangle \\ &= \frac{1}{\sqrt{N}} \sum_{\vec{m},\vec{n}}^{N} \varepsilon_{\vec{m},\vec{n}} e^{i\vec{k}\bullet\vec{R}_{\vec{n}}} a^{\dagger}_{\vec{m}} \left| 0 \right\rangle\end{aligned} \tag{565}$$

In the above equation we have used the anticommmutation relations from equations **(315)-(317)** to get the final result. Now we multiply the equation above by the ket vector $\left\langle B_k \right|$ to calculate the first term in on the right hand side of equation **(564)**:

$$\begin{aligned}\left\langle B_k \middle| \hat{H}_{gen,0} \middle| R_k \right\rangle &= \frac{1}{N}\sum_{\vec{w}}^{N} e^{-i\vec{k}\bullet\vec{B}_{\vec{w}}} \left\langle 0 \right| a_{\vec{w}} \sum_{\vec{m},\vec{n}}^{N} \varepsilon_{\vec{m},\vec{n}} e^{i\vec{k}\bullet\vec{R}_{\vec{n}}} a^{\dagger}_{\vec{m}} \left| 0 \right\rangle \\ &= \frac{1}{N}\sum_{\vec{m},\vec{n}}^{N} \varepsilon_{\vec{m},\vec{n}} e^{i\vec{k}\bullet\vec{R}_{\vec{n}}} e^{-i\vec{k}\bullet\vec{B}_{\vec{w}}} \left\langle 0 \middle| a_{\vec{w}} a^{\dagger}_{\vec{m}} \middle| 0 \right\rangle\end{aligned} \tag{566}$$

The hopping energies $\varepsilon_{\vec{m},\vec{n}}$ are only dependent on the distance between atoms; $\varepsilon_{\vec{m},\vec{n}} = \varepsilon_{\vec{m}-\vec{n}}$ and we also make the substitution $\vec{q} = \vec{n} - \vec{m} \Rightarrow \vec{n} = \vec{q} + \vec{m}$ and we get the function $G(\vec{k})$ we had in section () for general symmetry for graphene:

$$\begin{aligned}\left\langle B_k \middle| \hat{H}_{gen,0} \middle| R_k \right\rangle &= \sum_{\vec{m},\vec{n}}^{N} \varepsilon_{\vec{n}-\vec{m}} e^{i\vec{k}\bullet\vec{R}_{\vec{n}-\vec{w}}} \delta_{\vec{w}\vec{m}} \\ &= \sum_{\vec{m},\vec{n}}^{N} \varepsilon_{\vec{n}-\vec{m}} e^{i\vec{k}\bullet\vec{R}_{\vec{n}-\vec{m}}} = \frac{1}{N}\sum_{\vec{q},\vec{m}}^{N} \varepsilon_{\vec{q}} e^{i\vec{k}\bullet\vec{R}_{\vec{q}}} \equiv G(\vec{k})\end{aligned} \tag{567}$$

The second off-diagonal $\left\langle R_k \middle| \hat{H}_{gen} \middle| B_k \right\rangle$ is of course the complex conjugate of the result from the above equation:

$$\left\langle R_k \middle| \hat{H}_{gen} \middle| B_k \right\rangle = G^{*}\left(\vec{k}\right) \tag{568}$$

Now let us calculate the diagonal of the matrix from equation (563) and just as we had two terms for the off-diagonal elements; we have two terms for diagonal elements, we start with $\left\langle B_k \middle| \hat{H}_{gen} \middle| R_k \right\rangle$:

$$\left\langle B_k \middle| \hat{H}_{gen} \middle| B_k \right\rangle = \left\langle B_k \middle| \hat{H}_{gen,0} \middle| B_k \right\rangle + \left\langle B_k \middle| \hat{H}_{gen,1} \middle| B_k \right\rangle \tag{569}$$

The first term on the right hand side of the equation above is zero: $\left\langle B_k \middle| \hat{H}_{gen,0} \middle| B_k \right\rangle = 0$, so we start by operating $\hat{H}_{gen,1}$ on $\left| B_k \right\rangle$; we get:

$$\begin{aligned}\hat{H}_{gen,1}\left| B_{\vec{k}} \right\rangle &= \frac{1}{\sqrt{N}}\sum_{\vec{m},\vec{n}} \tilde{\varepsilon}_{m,n} e^{i\vec{k}\bullet\vec{B}_{\vec{u}}} \left(\left(a^{\dagger}_{\vec{m}} a_{\vec{n}} + a^{\dagger}_{\vec{n}} a_{\vec{m}}\right) + \left(b^{\dagger}_{\vec{m}} b_{\vec{n}} + b^{\dagger}_{\vec{n}} b_{\vec{m}}\right)\right) a^{\dagger}_{\vec{u}} \left| 0 \right\rangle \\ &= \frac{1}{\sqrt{N}}\sum_{\vec{m},\vec{n}} \tilde{\varepsilon}_{m,n} e^{i\vec{k}\bullet\vec{B}_{\vec{u}}} \left(a^{\dagger}_{\vec{m}} a_{\vec{n}} + a^{\dagger}_{\vec{n}} a_{\vec{m}}\right) a^{\dagger}_{\vec{u}} \left| 0 \right\rangle = \frac{1}{\sqrt{N}}\sum_{\vec{m},\vec{n}} \tilde{\varepsilon}_{m,n} e^{i\vec{k}\bullet\vec{B}_{\vec{u}}} \left(a^{\dagger}_{\vec{m}} \delta_{\vec{n}\vec{u}} + a^{\dagger}_{\vec{n}} \delta_{\vec{m}\vec{u}}\right) \left| 0 \right\rangle \\ &= \frac{1}{\sqrt{N}}\sum_{\vec{m},\vec{n}} \tilde{\varepsilon}_{m,n} \left(e^{i\vec{k}\bullet\vec{B}_{\vec{n}}} a^{\dagger}_{\vec{m}} + e^{i\vec{k}\bullet\vec{B}_{\vec{m}}} a^{\dagger}_{\vec{n}}\right) \left| 0 \right\rangle\end{aligned} \tag{570}$$

In the equation above we again used the anticommmutation relations from equations **(315)-(317)** to get the final result and had the send term $\hat{H}_{gen,1}$ give zero. Now we multiply the result from the above equation by the ket eigenvector $\langle B_{\vec{k}}|$ in order to find the diagonal element from equation **(569)**:

$$\begin{aligned}\left\langle B_{\vec{k}}\middle|\hat{H}_{gen,1}\middle|B_{\vec{k}}\right\rangle &= \frac{1}{N}\sum_{\vec{w}}^{N} e^{-i\vec{k}\bullet\vec{B}_{\vec{w}}}\sum_{\vec{m},\vec{n}}^{N}\tilde{\varepsilon}_{\vec{m},\vec{n}}\left(e^{i\vec{k}\bullet\vec{B}_{\vec{n}-\vec{w}}}\left\langle 0\middle|a_{\vec{w}}a_{\vec{m}}^{\dagger}\middle|0\right\rangle + e^{i\vec{k}\bullet\vec{B}_{\vec{m}-\vec{w}}}\left\langle 0\middle|a_{\vec{w}}a_{\vec{n}}^{\dagger}\middle|0\right\rangle\right)\\ &= \frac{1}{N}\sum_{\vec{m},\vec{n}}^{N}\tilde{\varepsilon}_{\vec{m},\vec{n}}\left(e^{i\vec{k}\bullet\vec{B}_{\vec{n}-\vec{w}}}\delta_{\vec{w}\vec{m}} + e^{i\vec{k}\bullet\vec{B}_{\vec{m}-\vec{w}}}\delta_{\vec{w}\vec{n}}\right)\\ &= \frac{1}{N}\sum_{\vec{m},\vec{n}}^{N}\tilde{\varepsilon}_{\vec{m},\vec{n}}\left(e^{i\vec{k}\bullet\vec{B}_{\vec{n}-\vec{m}}} + e^{-i\vec{k}\bullet\vec{B}_{\vec{n}-\vec{m}}}\right)\end{aligned} \tag{571}$$

And just as we used earlier that hopping energies $\varepsilon_{\vec{m},\vec{n}}$ are only dependent on the distance between atoms; $\varepsilon_{\vec{m},\vec{n}} = \varepsilon_{\vec{m}-\vec{n}}$ and we also make the substitution $\vec{q} = \vec{n} - \vec{m} \Rightarrow \vec{n} = \vec{q} + \vec{m}$ and get $F\left(\vec{k}\right)$ just as we had in section (3.4):

$$\begin{aligned}\left\langle B_k\middle|\hat{H}_{gen,1}\middle|B_k\right\rangle &= \frac{1}{N}\sum_{\vec{m},\vec{n}}^{N}\tilde{\varepsilon}_{\vec{m}-\vec{n}}\left(e^{i\vec{k}\bullet\vec{B}_{\vec{n}-\vec{m}}} + e^{-i\vec{k}\bullet\vec{B}_{\vec{n}-\vec{m}}}\right)\\ &= \frac{1}{N}\sum_{\vec{q},\vec{m}}^{N}\tilde{\varepsilon}_{\vec{q}}\left(e^{i\vec{k}\bullet\vec{B}_{\vec{q}}} + e^{-i\vec{k}\bullet\vec{B}_{\vec{q}}}\right) = \sum_{\vec{q}}^{N}\tilde{\varepsilon}_{\vec{q}}\left(e^{i\vec{k}\bullet\vec{B}_{\vec{q}}} + e^{-i\vec{k}\bullet\vec{B}_{\vec{q}}}\right) \equiv F(\vec{k})\end{aligned} \tag{572}$$

Notice that $F\left(\vec{k}\right)$ is real just as it supposes to be for the matrix from equation **(563)** to be hermitian. The final element in the matrix in equation **(563)** is exactly the same as the result above:

$$\left\langle R_k\middle|\hat{H}_{gen}\middle|R_k\right\rangle = F(\vec{k}) \tag{573}$$

Writing the matrix explicitly which is simply the Hamiltonian of all hops in the lattice of one graphene layer in k-space; we get the result we had in equation**(406)**:

$$\begin{pmatrix}\left\langle B_k\middle|\hat{H}_{gen}\middle|B_k\right\rangle & \left\langle B_k\middle|\hat{H}_{gen}\middle|R_k\right\rangle\\ \left\langle R_k\middle|\hat{H}_{gen}\middle|B_k\right\rangle & \left\langle R_k\middle|\hat{H}_{gen}\middle|R_k\right\rangle\end{pmatrix} = \begin{pmatrix}F(\vec{k}) & G(\vec{k})\\ G(\vec{k})^{*} & F(\vec{k})\end{pmatrix} \tag{574}$$

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