

Quantum Hall Effect
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Lec 12: Electronic structure of Graphene

We shall be talking about quantum Hall effect in graphene. As I told you that it will serve two sort of purpose. One of them is doing the quantum Hall effect or rather rewinding the story of quantum Hall effect in a crystal lattice structure. We have seen that in a square lattice how magnetic field enters into the problem and now we will see it for graphene. One of the more important things in this context is that in square lattice the dispersion is the low energy or rather the long wavelength dispersion is that of a k square type whereas here it is a relativistic dispersion which we call it a pseudo relativistic and in order to do that we will have to know the electronic structure of graphene and so our first sort of activity would be understanding the electronic structure particularly the low energy dispersion of graphene. Just wanted to remind you that there are different allotropes of carbon graphene is one of them and some of the allotropes such as diamond.

Diamond	—	4 000 B.C.
Graphite	—	16 th century.
C_{60}	—	1985
MWCNT (nanotube).	—	1991.
SWCNT	—	1993
Graphene	—	2005.

Diamond was known for a very long time I mean 4000 BC so that's even before Christ

and the graphite which is a well-known form of carbon this is basically what you find in your pencil tips. So, this is discovered in 16th century then there are other allotropes such as carbon 60 which is called as a buckyball. So, this was in 1985 and single wall carbon nanotube okay. So, it's a nanotube form was there in 1991 initially it was I think so 1991 was so this is multi-walled carbon nanotube.

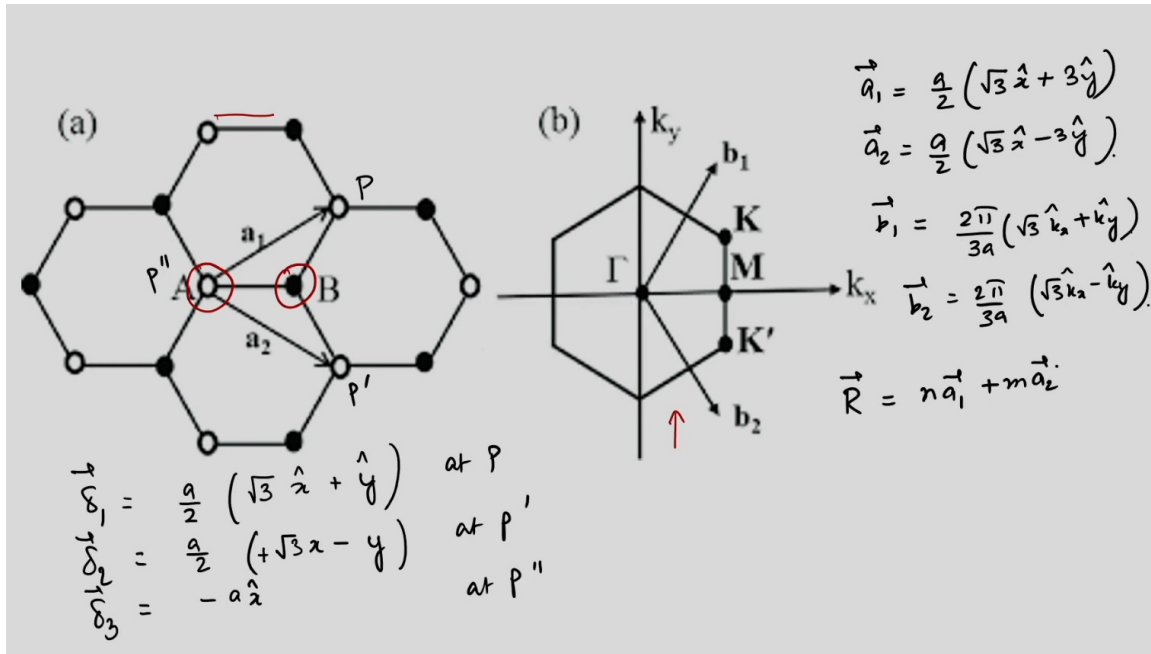
So, this was 1991 then single walled carbon nanotube was in 1993. So, these are like one-dimensional structures C 60 is like a zero-dimensional structure and graphene was there in at the end around 2004-2005 okay. So, this is how the history unfolded of carbon and its allotropes okay. So, let's go to study graphene and so this structure has already been told to you that this is the structure where these open atoms that you see here. So, there is an open atom and then there is a closed atom there okay.

So, each open atom and closed atom would be called as A and B atoms or A and B sub lattices there is the sub lattice actually contains these two atoms. So, the unit cell has these two atoms and this is the Brillouin zone. So, if you have a flat top just like what you see here like here there is a flat top. So, this will have a hexagon with of this shape and if you have the real space of this shape that is of this the momentum space structure that you see here if the real space atoms are arranged in this fashion then the momentum space would be like what the real space looks like. So, the important thing is that in a real space you have a honeycomb structure and also in the momentum space you have a honeycomb structure these a_1 and a_2 are called as the unit cell vectors or the primitive lattice vectors and b_1 and b_2 are called as a reciprocal lattice vectors and these there are some points in the Brillouin zone that are shown here on the right picture where you see a gamma point and then there are K and K prime points and then the M point and so on these are quite important as the subsequent discussions will show.

And so, this a_1 and a_2 are the primitive lattice vectors or this unit cells are given by these a_1 and a_2 . So, let me write down the nearest neighbor vectors. So, each B atom has a nearest neighbor as A atoms as you can see. So, this is the A atom here there is one A atom here there is one A atom here and hence the three nearest neighbors which will write it with a δ_1 which is $a/2 + \sqrt{3}y/2$. So, this is δ_1 which is this one which you see it here let us call it as some point say p and a p prime and a p double prime.

So, a δ_1 connects the B atom to p point and similarly one can write down the δ_2 which is $-a/2 + \sqrt{3}x/2$ and a δ_3 which is $-a/2 - \sqrt{3}y/2$ because it is below that and then the last one is actually a δ_3 which is equal to $-a/2 - \sqrt{3}x/2$ at the point. So, at p at p prime and at p double prime and we can write down the a_1 and a_2 vectors as $a_1 = a/2 + \sqrt{3}x/2$ and $a_2 = -a/2 + \sqrt{3}y/2$.

plus $3y$ cap and a_2 equal to a by $2\sqrt{3}x$ cap minus $3y$ cap and similarly the b_1 which are the reciprocal lattice vectors can be written as 2π over $3a$ and $\sqrt{3}k_x$ cap plus k_y cap and b_2 would be 2π over $3a$ and $\sqrt{3}k_x$ minus k_y cap. Now, these are all the vectors that are important for our discussion and any point on the lattice can be or any position of any of the atoms can be obtained by doing this that is $a_1n + a_2m$ where n and m are integers and a_1, a_2 are shown here okay. So, n, m are integers.



So, this is again the thing shown in color. So, these A and B just for your benefit are shown as blue and red atoms and then the Brillouin zone is shown okay. Alright, we will come to this discussion in just a while okay. So, let me write down the tight binding dispersion and the tight binding dispersion is say written as so, the Hamiltonian and the Hamiltonian is first let us write it in the real space which is the nearest neighbor hopping. So, each carbon atom has one electron per atom.

So, it is like half filled system where the entire valence band is filled okay. So, this is like a i sigma dagger b_j sigma plus a Hermitian conjugate of that and sigma. So, I am using the second quantized notation where a i sigma creates an electron with spin sigma at the i th site which belongs to the a sub lattice and it destroys an electron with spin sigma at the j th site in b sub lattice and just to make sure that these a_i and b_j are nearest neighbors there is an angular bracket that is shown and this sigma actually denotes the spin of the electrons. However, the spin here carries no meaning. So, in the subsequent discussions the spin will be dropped will only include spin as and when it is needed that

is when there is a spin orbit coupling that is present.

So, we write down this a little more elaborately and so, this is a minus t that is the tight binding Hamiltonian we are doing and why we are doing a tight binding Hamiltonian because these t is of the order of 2.7 electron volt which is very large and also that each carbon atom has one electron. So, the interaction between the electrons is completely neglected. So, we write it as r and δ and this is like I am writing it slightly differently, but they mean the same thing δ i where δ i 's are those nearest neighbor this is a generic form for any tight binding Hamiltonian now I am writing it for graphene. So, that is why we are using these δ i 's δ 1 δ 2 δ 3 are defined earlier and so, this is equal to a of r where r is as I said is a general point which connects any atom starting from some chosen origin.

So, this is a dagger r br plus δ i these are all vectors. So, this is a Hermitian conjugate and Hamiltonian needs a Hermitian conjugate to be considered as real that means, for the hermiticity of the Hamiltonian. So, that it gives real eigenvalues you need to add the Hermitian conjugate. So, this is basically the Hermitian conjugate and again in keeping with the notation that we have talked about earlier that is a b a b dagger will create an electron at the b site with b sub lattice with the site r plus δ i and a r will annihilate an electron at site r belonging to the a sub lattice and just to make sure that each a sub lattice has a neighbor as a b sub lattice and vice versa and there is a sum over all these δ i and there are three neighbors as we have said. So, now, because this Hamiltonian has translational invariance we can do a Fourier transform and why I mention about translational invariance because k is a good quantum number or a k is a conserved quantity which can be used to denote the basis for the problem.

So, a k is equal to now these are all vectors sometimes I would not write them as vectors, but they are all vectors. So, this is a a of r . So, this k is a vector r is a vector and e to the power minus i k dot r and you have a sum over r . So, if you do that so, there are these Hamiltonian takes the form minus t over n because this root over of n that this n denotes the number of sites. So, this is equal to now there are you are multiplying two operators here b and a .

So, they will come with different wave vectors maybe k and k prime or let us see what we use here. So, we use a k and q and of course, there is a r which is coming from the this Fourier transform and then δ i where you know i is equal to 1 2 and 3. So, with that so, we have a exponential i k minus q dot r now remember because there is a dagger there. So, if you want to write a dagger. So, a k dagger will come with a 1 by root n exactly everything remains same excepting that you have a a dagger r and exponential i k dot r and these are column vectors each of these vectors a and b because they are column vectors when you write them you have to use different notations otherwise it will mean

that you are using only the like terms like $a_1 b_1 a_2 b_2$ and so on because they are not simply just algebraic quantities they involve a column vector.

$$\begin{aligned}
 & \boxed{H = -t \sum_{\langle ij \rangle, \sigma} (a_{i\sigma}^\dagger b_{j\sigma} + h.c.)} \quad t = 2.7 \text{ eV.} \\
 & H = -t \sum_{\vec{R}, \delta_i} \left[b^\dagger(\vec{R} + \vec{\delta}_i) a(\vec{R}) + \underbrace{a^\dagger(\vec{R}) b(\vec{R} + \vec{\delta}_i)}_{h.c.} \right] \\
 & \text{Fourier transform,} \\
 & a_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} a(\vec{R}) e^{-i\vec{k} \cdot \vec{R}} \quad a_{\vec{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_{\vec{R}} a^\dagger(\vec{R}) e^{i\vec{k} \cdot \vec{R}} \\
 & H = -\frac{t}{N} \sum_{\vec{k}, \vec{q}} \sum_{\vec{R}} \sum_{\vec{\delta}_i, i=1,2,3} \left[e^{i(\vec{k}-\vec{q}) \cdot \vec{R}} e^{i\vec{q} \cdot \vec{\delta}_i} b_{\vec{q}} a_{\vec{k}} + e^{i(\vec{k}-\vec{q}) \cdot \vec{R}} e^{-i\vec{q} \cdot \vec{\delta}_i} a_{\vec{k}}^\dagger b_{\vec{q}} \right] \\
 & \delta_{\vec{k}, \vec{q}} = \frac{1}{N} \sum_{\vec{R}} e^{i(\vec{k}-\vec{q}) \cdot \vec{R}}
 \end{aligned}$$

So, the first term is that and then exponential $i \vec{q} \cdot \vec{\delta}_i$ these and then $b_{\vec{q}}^\dagger a_{\vec{k}}$. So, we can write it down here as plus exponential $i \vec{k} \cdot \vec{R}$ exponential minus $i \vec{q} \cdot \vec{\delta}_i$ and $a_{\vec{q}}^\dagger b_{\vec{k}}$. So, that is the two terms that we have written above and now a little bit of simplification will have to be done, but now notice one thing that the definition of the Kronecker delta which is usually written as $\delta_{\vec{k}, \vec{q}}$ this is equal to 1 by N summation over $\vec{R}$ and it is a exponential $\vec{k} \cdot \vec{R}$ minus $\vec{q} \cdot \vec{R}$. So, you see that there is a sum over $\vec{R}$ and then there are these exponential factors which are there and these exponential factors will give you nothing, but just the Kronecker delta which means that it will make $\vec{k}$ and $\vec{q}$ to be same and with that what one gets is a following. the Hamiltonian is written as minus t sum over $\vec{k}$ and then these delta's will go from 1 to 3 which we have said and there is a minus $\vec{k} \cdot \vec{\delta}_i$ because $\vec{k}$ and $\vec{q}$ have become same.

So, it is $i \vec{k} \cdot \vec{\delta}_i b_{\vec{k}}^\dagger a_{\vec{k}}$ and a plus exponential $i \vec{k} \cdot \vec{\delta}_i a_{\vec{k}}^\dagger b_{\vec{k}}$. This you need to do it once in order to get used to this and then we can write this as minus t then there is a sum over $\vec{k}$ and you again have this delta i equal to 1 2 3 and I can write it just like a matrix where $a_{\vec{k}}^\dagger b_{\vec{k}}^\dagger$. So, this is like a row vector and this is a 0 and exponential minus $i \vec{k} \cdot \vec{\delta}_i$ exponential $i \vec{k} \cdot \vec{\delta}_i$ and then 0 and then you have $a_{\vec{k}}$ and $b_{\vec{k}}$ okay. Now you see that there is no term that contains $a_{\vec{k}}^\dagger a_{\vec{k}}$ because there is no hopping from a atom to a atom. So, it is the hopping is between a atom to b atom because we are talking about nearest neighbour

model nearest neighbour tight binding model.

Actually there is no term which is $b_k^\dagger b_k$ that is why this matrix that you see at the middle sandwich between the row vector and the column vector actually does not have any diagonal elements, but it only has off diagonal elements. So, this can be written as a sum over k and again a δ_i equal to I may forget these vectors, but please put it. So, this is a $k^\dagger b_k^\dagger$ and then let us write this as h_k and a $k b_k$ that is your Hamiltonian and what is the form of h_k ? Now h_k involves a sum of 3 terms with the δ_1 and δ_2 and δ_3 that we have mentioned earlier that is δ_1 , δ_2 and δ_3 which are written here ok. So, once when you put that then h_k becomes a sum of 3 terms let me also take this minus t here. So, that I do not write the minus t here.

So, I take it with h_k . So, that this becomes like a 0 exponential $i k \cdot \delta_1$ plus exponential $i k \cdot \delta_2$ plus exponential $i k \cdot \delta_3$ okay. And so, and then there will be a term like the similar kind of term, but with the Hermitian conjugate. So, it is a minus $i k \cdot \delta_1$ plus exponential minus $i k \cdot \delta_2$ plus exponential minus $i k \cdot \delta_3$ and this and a 0 here and if we want to diagonalize this we just have to find the eigenvalues of this matrix H of k okay. Now the difference between this δ_1 and δ_2 or δ_2 and δ_3 or δ_1 and δ_3 must give you a lattice vector which is r . So, one can do in order to you know achieve more simplification one can do a transformation of like a_k can be changed to $e^{i k \cdot \delta_3} a_k$ and $a_k^\dagger$ will be exponential minus $i k \cdot \delta_3$ and $a_k^\dagger$ okay.

$$\begin{aligned}
 H &= -t \sum_{\vec{k}} \sum_{\delta_i=1}^3 \left[e^{-i\vec{k} \cdot \vec{\delta}_i} b_k^\dagger a_k + e^{i\vec{k} \cdot \vec{\delta}_i} a_k^\dagger b_k \right] \\
 &= -t \sum_{\vec{k}} \sum_{\delta_i=1}^3 \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} 0 & e^{-i\vec{k} \cdot \vec{\delta}_i} \\ e^{i\vec{k} \cdot \vec{\delta}_i} & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \\
 &= \sum_{\vec{k}} \sum_{\delta_i=1}^3 \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} h(\vec{k}) \begin{pmatrix} a_k \\ b_k \end{pmatrix} \\
 h(\vec{k}) &= -t \begin{pmatrix} 0 & (e^{i\vec{k} \cdot \vec{\delta}_1} + e^{i\vec{k} \cdot \vec{\delta}_2} + e^{i\vec{k} \cdot \vec{\delta}_3}) \\ (e^{-i\vec{k} \cdot \vec{\delta}_1} + e^{-i\vec{k} \cdot \vec{\delta}_2} + e^{-i\vec{k} \cdot \vec{\delta}_3}) & 0 \end{pmatrix}
 \end{aligned}$$

This is not required, but if you make this then at one term becomes equal to 1 and that is

what is intended here. So, we will write this H_k , but now because we made this transformation let us write it with a $\tilde{H}$ it is equal to $-\tau$ and 0 here and $\exp(i k \delta_1 - \delta_3)$ plus $\exp(i k \delta_2 - \delta_3)$ plus 1 and then you have a . So, this is a term there and then one can actually have $\exp(-i k \delta_1 - \delta_3)$ plus $\exp(-i k \delta_2 - \delta_3)$ plus 1 and there is a 0 here and that becomes the matrix. If we use the definitions of δ_1 and δ_2 so, you see now that one term has become equal to 1 just for the simplicity now we put δ_1 and δ_2 and δ_3 and then one gets this H of k to be rather $\tilde{H}$ of k to be $-\tau$ and it is a 0 $\exp(i k \cdot a_1)$ plus $\exp(i k \cdot a_2)$ and a plus 1 and there is a minus there is a minus sign $\exp(-i k \cdot a_1)$ plus $\exp(-i k \cdot a_2)$ plus 1 and this is a 0 . So, this is one term and the off diagonal term there and now one can actually verify that this $\tilde{H}$ obeys this equal to $\tilde{H} \cdot k$ plus G where G is the proper reciprocal lattice vector which is defined as.

So, this is defined as p of b_1 plus q of b_2 and again p, q alright. So, this is the form and then let us write a little more neatly where we write this as $-\tau f(k)$ and $f^*(k)$ and 0 where $f(k)$ is equal to this just the simplified form of this 2 by 2 matrix where this is equal to $-\tau \exp(-i k_x a) + 2 \exp(i k_x a)$ by 2 and a cosine of $k_y \sqrt{3} a$ by 2 okay. That is the form for $f(k)$ and we can now diagonalize this matrix $\tilde{H}$ of k and get the energy dispersion for the tight binding problem of for graphene. So, this is equal to $\pm \tau \sqrt{f(k)^2}$ and this is equal to $\pm \tau \sqrt{4 \cos^2(k_y \sqrt{3} a / 2) + 4 \cos^2(k_x a / 2)}$. Ideally this should have been the end of the problem because we have found out there are 2 bands one correspond to plus sign and the other other correspond to minus sign and there are 2 bands because there are 2 atoms per unit cell.

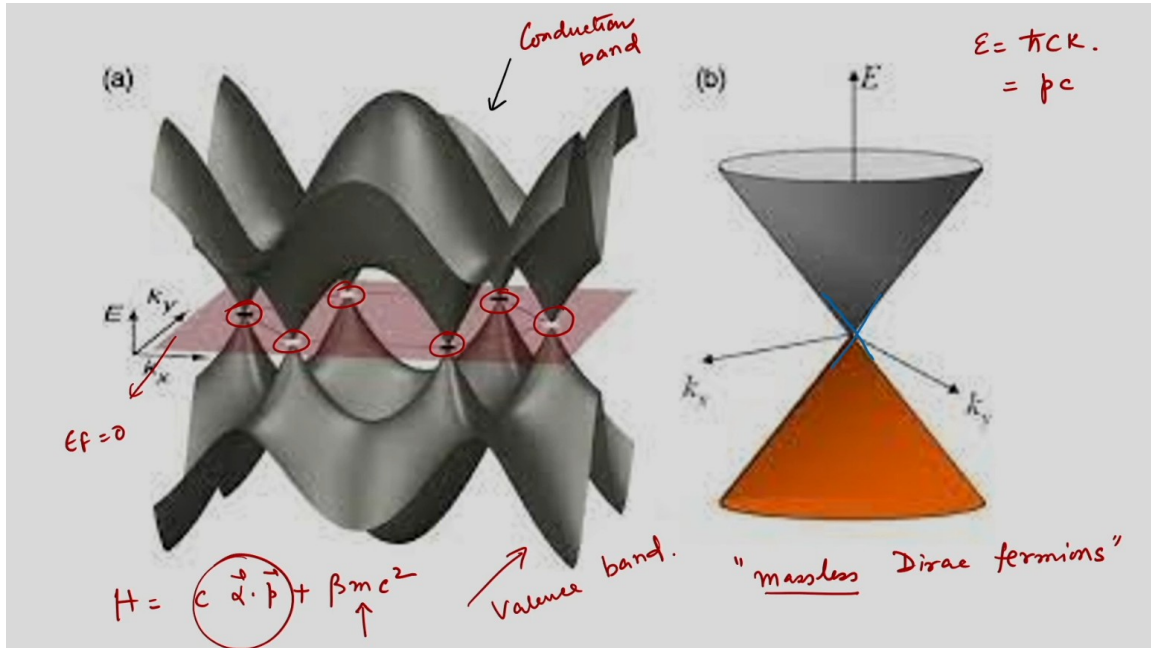
$$\begin{aligned}
a_k &\rightarrow e^{i\vec{k}\cdot\vec{\delta}_3} a_k & a_k^\dagger &\rightarrow e^{-i\vec{k}\cdot\vec{\delta}_3} a_k^\dagger \\
\tilde{h}(k) &= -t \begin{pmatrix} 0 & (e^{i\vec{k}\cdot(\vec{\delta}_1-\vec{\delta}_3)} + e^{i\vec{k}\cdot(\vec{\delta}_2-\vec{\delta}_3)} + 1) \\ e^{-i\vec{k}\cdot(\vec{\delta}_1-\vec{\delta}_3)} + e^{-i\vec{k}\cdot(\vec{\delta}_2-\vec{\delta}_3)} + 1 & 0 \end{pmatrix} \\
\tilde{h}(k) &= -t \begin{pmatrix} 0 & (e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2} + 1) \\ -(e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2} + 1) & 0 \end{pmatrix} \\
\tilde{h}(k) &= \tilde{h}(\vec{k} + \vec{G}) \quad \text{where } \vec{G} = p\vec{b}_1 + q\vec{b}_2 \quad p, q \in \mathbb{N} \\
\tilde{h}(k) &= -t \begin{pmatrix} 0 & f(k) \\ f^*(k) & 0 \end{pmatrix} \quad \text{where } f(k) = -t \left(e^{-ik_x a} + 2e^{ik_x a/2} \cos\left(\frac{k_y \sqrt{3}a}{2}\right) \right)
\end{aligned}$$

So, it is like a diatomic lattice and that is why there are 2 bands we have seen this in while doing the phonons or the crystal vibrations monoatomic lattice would give rise to 1 band and diatomic would give rise to 2 and if you have more atoms per unit cell such as a Kagome lattice you will have 3 bands etcetera. So, this is the dispersion k_x and k_y both go from minus π to π in the Brillouin zone and one can actually plot this dispersion and one gets the how the bands look like and when we do that let me show you the pictures. So, this is the picture of the bands you see there are 2 bands. So, this is the top band which is called as a conduction band and this is known as a valence band. However, they are not separated you see that there are these points which are denoted by white and black dots here and they are touching at the 6 points on the Fermi sheet.

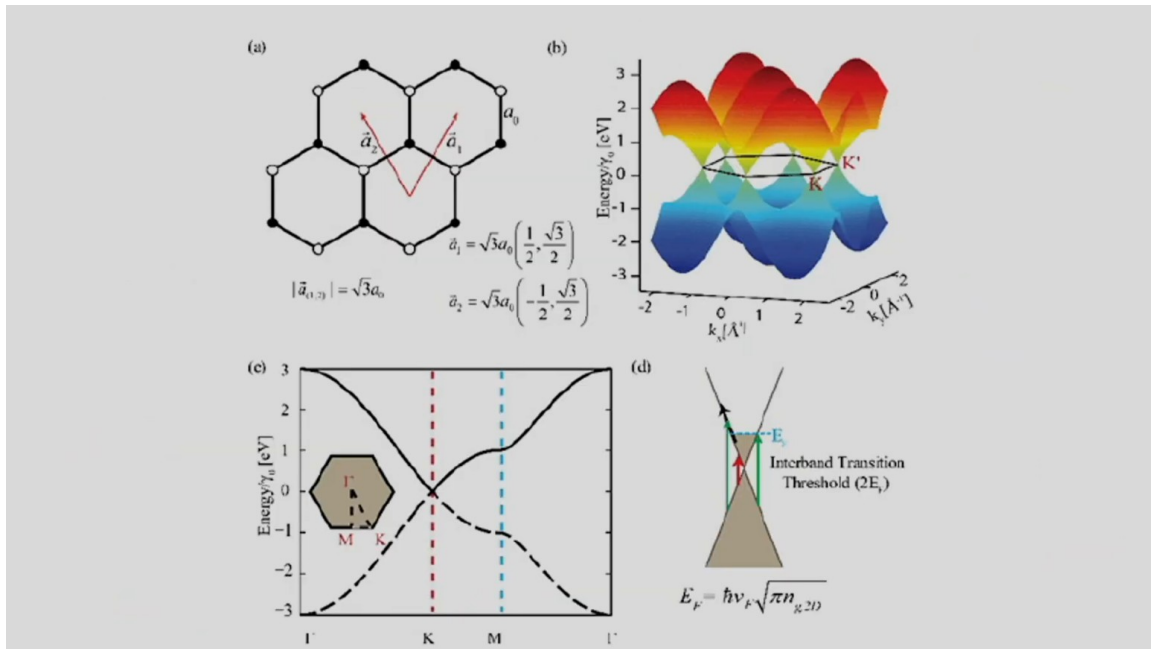
So, this is the Fermi sheet or you can call it ϵ_f equal to 0 or if suppose the chemical potential is fixed there then these bands 2 bands just barely touch at these 6 points and not only that they touch they touch like a light cone as is shown here you see that this is like a light cone. So, it is like a linear dispersion and linear dispersion is equated to the behavior of photons. So, photons have a behavior which is like which is PC which is like a extreme relativistic limit of a particle or you can call it a massless particle. So, that is why the electrons in graphene they show character of a massless Dirac fermions. So, these word is very common and why are they called as massless Dirac fermions let me tell you that the Dirac equation is written as this is equal to $C \alpha \cdot p + \beta m c^2$ where α and β are matrices and p is the momentum and $m c^2$ is the energy the rest mass energy and C is the speed of light.

However, this dispersion that we will see in a while looks like only this term being present and this term is absent and that is why it is called as a massless and why it is

called a Dirac because it is you can see that the energy is linear in p or k as it is shown here because. So, this is the conical dispersion that you see there it is been also seen in experiments angular resolve photo emission spectroscopy shows this formation of Dirac cones.



Now we need to understand because condensed matter physics deals with low energy properties of systems we need to understand that what is a low energy property for this particular Hamiltonian and in order to understand that before we go there let me show you a colored picture of this again you see that this is the energy plotted in e v and there is a k_x and a k_y and so on and then these red colored red and yellowish that corresponds to the conduction band and then blue and greenish tinge that corresponds to valence band and we have said that it is one electron per site per carbon atom. So, it is half filled which means that all the states in the valence band is full. Now we need to find the Dirac point so that we can expand the energy which we have just obtained about those Dirac points I told you why they are called Dirac points because dispersion is that of a ultra relativistic or a massless relativistic particle and that is why they are called Dirac.



So, there is no scale the velocity scale here is only the fermionic velocity at the Fermi level not the velocity of light. So, the fermionic velocity is typically about three orders of magnitude lower. So, that is why it is called as massless Dirac fermions, but they are called pseudo massless fermions that is the pseudo Dirac fermions or pseudo relativistic fermions. So, you know how now the dispersion looks like and so on and then let us find out the Dirac points and that is not too difficult what you can do is that you can put the real part and imaginary part of this dispersion equal to 0. Here of course, you do not see that you go to this f of k which has real part and an imaginary part and you put them separately to be equal to 0 because you want to see where it meets epsilon equal to 0 which is the Fermi energy or the Fermi sheet or the chemical potential.

So, we will put these f of k equal to 0 to find out what are the coordinates of k_x and k_y for which the dispersion vanishes and that can be found out easily if you do that exercise of putting the real and imaginary parts to be equal to 0. So, let me write down this as finding the Dirac points that is the exercise. So, putting the real and imaginary parts. We get two equations one from the real part one from the imaginary part and let us write down these equations as you can check them. So, it is a $\cos k_x a$ by 2 $\cos \sqrt{3} k_y a$ by 2 equal to 0 and $-\sin k_x a$ plus 2 $\sin k_x a$ by 2 $\cos \sqrt{3} k_y a$ by 2 equal to 0.

So, this one of them is from the real part the top one and the bottom one is from the imaginary part putting that equal to 0 and I hope I have been able to communicate why I am putting them equal to 0 because I want to see these points of touching which I have shown here that these red circle points are what I am trying to determine and because the dispersion gives you 0 value. So, that is why the f of k has to be it has to

vanish and from those conditions we have found out these two equations. And the so, if you manipulate the first one then what you get is so, from 1 its $\sin k_x a/2$ and a minus $\cos k_x a/2$ plus a $\cos k_y a/\sqrt{3}$ by 2 this is equal to 0. So, that is from 1 we get from this let us call this as 3 and we are left with two options in which there is a product of these two terms equal to 0 which means either the $\sin k_x a/2$ is 0 or these bracketed square bracket is 0 and we will see both of them separately. So, one of them gives so, option 1 is let us call them as option.

$$\epsilon_k = \pm t \sqrt{|f(k)|^2}$$

$$= \pm t \sqrt{3 + 2\cos(\sqrt{3}ak_y) + 4\cos(\frac{k_x a}{2})\cos(\frac{\sqrt{3}ak_x}{2})}$$

Finding the Dirac points.

Putting the real and imaginary parts of $f(k) = 0$.

$$\cos(k_x a) + 2\cos(\frac{k_x a}{2})\cos(\frac{\sqrt{3}k_y a}{2}) = 0 \quad (1)$$

$$-\sin(k_x a) + 2\sin(\frac{k_x a}{2})\cos(\frac{\sqrt{3}k_y a}{2}) = 0 \quad (2)$$

from (1)

$$\sin(\frac{k_x a}{2}) \left[-\cos(\frac{k_x a}{2}) + \cos(\frac{k_y a \sqrt{3}}{2}) \right] = 0 \quad (3)$$

Option 1 its $\sin k_x a/2$ equal to 0 which also means that cosine of $k_x a/2$ is either plus 1 or minus 1. So, sine vanishes and cosine just either phase leads or phase lags. So, that is why it is a plus or minus 1 or option 2 is when the bracket is equal to 0 which means that a cosine $k_x a/2$ equal to cosine $k_y a/\sqrt{3}$ by 2. So, this is equal to a cosine $k_x a/2$ and equal to cosine $\sqrt{3}k_y a/2$.

So, we look at option 1. So, let us write it as equation number 4 and equation number 5. So, from equation 4 what one gets is we get a condition that $1 + 2\cos k_y a/\sqrt{3}$ is equal to 0 option 1 gives this equal to 0 and then what you can do is that you can this gives a position of the points as so, these are the points which are 0 plus minus 4π by $3\sqrt{3}a$. So, these are the so, this k_x and these are k_y . So, I get 2 points 0 and 4π by $3\sqrt{3}a$ another is 0 minus 4π by $3\sqrt{3}a$ these are the 2 points that we get from these option 1 and from option 2 we get from equation 5 one gets the other option which is

equal to the cosine of $k_y a \sqrt{3}$ which is plus a 2 cosine square $k_y a \sqrt{3}$ by 2. So, where we have used this equation that we get from here.

So, we have used 6 and 7 I mean we have used 6 here and then we get a 4 more points from this equation and these points are plus minus 2π by $3a$ and a by $\sqrt{3}$ and plus minus 2π by $3a$ minus a by $\sqrt{3}$. So, we get 2 points here and 4 points it is like 2 more points here and 2 more points here. So, that becomes 6 points. So, 2 points 2 Dirac points this is 2 Dirac points and these are 2 more Dirac points. So, that makes it 6 Dirac points which is what we have seen in the dispersion.

option (i) $\sin \frac{k_x a}{2} = 0 \Rightarrow \cos \left(\frac{k_x a}{2} \right) = \pm 1.$ (4)

(ii) $\cos \frac{k_x a}{2} = \cos \left(\frac{\sqrt{3} k_y a}{2} \right).$ (5)

from Eq (4) (6)

$$1 + 2 \cos \left(k_y \frac{\sqrt{3} a}{2} \right) = 0.$$

$\left(0, \pm \frac{4\pi}{3\sqrt{3}a} \right)$

2 Dirac points

from Eq (5) (7)

$$\cos \left(k_y a \sqrt{3} \right) + 2 \cos^2 \left(k_y a \frac{\sqrt{3}}{2} \right) = 0.$$

$\pm \frac{2\pi}{3a} \left(1, \frac{1}{\sqrt{3}} \right)$

$\pm \frac{2\pi}{3a} \left(1, -\frac{1}{\sqrt{3}} \right)$

2 Dirac points

2 Dirac points

So, we have these 6 Dirac points however, it can actually be checked that all the 6 points are not independent. In fact, there are relationships such as the let us take the first one with the positive sign and these $3\sqrt{3}a$ plus a by $2b$ has been defined earlier if you see that b has been defined here b_1 and b_2 . So, once you add b_1 or b_2 to this the first point you get a 1 other Dirac point which is 1 minus a by $\sqrt{3}$ which is here the plus 1 with a minus sign inside and so on between them. So, this is 1 and we have a 0 4π by $3\sqrt{3}a$ plus or minus a by 1 that gives another 1 which is 2π by $3a$ minus 1 minus a by $\sqrt{3}$.

So, these are the 2 relations. So, that cut down the relationship or rather the independent Dirac points and there are other relations that connect the other 2 Dirac points. So, we are left with only 2 independent Dirac points, and these are called as k and k' okay. They are also referred to as valleys. Now, whenever I write it a big k and a k' they

mean the Dirac points that we are referring to. So, they are 2 independent Dirac points and they can be anything, but what is usually done is that you can write it down as 2π by $3a$ 1 by $\sqrt{3}$ and the k prime is equal to 2π by $3a$ 1 minus 1 by $\sqrt{3}$ okay.

$$\begin{aligned} \left(0, \frac{4\pi}{3\sqrt{3}a}\right) + \vec{b}_2 &= \frac{2\pi}{3a} \left(1, -\frac{1}{\sqrt{3}}\right) \\ \left(0, \frac{4\pi}{3\sqrt{3}a}\right) - \vec{b}_1 &= \frac{2\pi}{3a} \left(-1, -\frac{1}{\sqrt{3}}\right) \end{aligned}$$

We are left with 2 independent Dirac points

$$\vec{K}, \vec{K}' : 2 \text{ independent Dirac points.}$$

$$\vec{K} = \frac{2\pi}{3a} \left(1, \frac{1}{\sqrt{3}}\right), \quad \vec{K}' = \frac{2\pi}{3a} \left(1, -\frac{1}{\sqrt{3}}\right)$$

So, these are the usual choices, but it does not matter you can have other choices as well that is you can work with any 2 of them the other 4 become dependent on these 2 and they also refer to as valleys as I told. So, these are the k and k prime points that you have seen earlier in that dispersion you see here. So, there is a k point here and a k prime point in between that is called as a m point the center of the Brillouin zone is called as a gamma point and so on okay. So, at these points one has massless Dirac kind of dispersion for the electrons of graphene okay. Now, since we have found these points the Dirac points we can expand the electronic dispersion about these points okay.

And when we do that so, what we have to do is we now get the low energy dispersion. And in order to do that what we do is we basically expand f of k about a k or k prime in principle it is we will do it around both. So, let us write down a momentum say q which is equal to k minus k okay. Now this is a momentum variable okay, this is runs in the Brillouin zone this is fixed this is a Dirac point. And this q is actually also a variable, but it is a low energy variable because you are expanding the dispersion about the k point.

So, we write now f of q and in order to do that let us take the derivative of that that is f prime of q which is $\frac{\partial f}{\partial k_x}$ at the k point and this is like k_x minus k_x okay. This is the x component of the Dirac point in the Brillouin zone and this small k_x is actually a variable plus $\frac{\partial f}{\partial k_y}$ at the k point and k_y minus k_y okay. So, if you do that then this yields a spectrum which is $3\hbar v_F$ divided by $2q_x$ plus i

q y, okay, where a is the lattice constant which is 1.42 angstrom which we have said earlier t is of course, the hopping strength hopping amplitude.

And these are the wave vectors q x and q y i is of course, the imaginary number. This dispersion at k the low energy dispersion is $\hbar \text{ cross } v_f$ where v_f is the scale and this is equal to q x plus i q y. Now, if you repeat this for the other k point which is k prime at q this will give a $\hbar \text{ cross } v_f$ and q x minus i q y where v_f is nothing, but $3 a t$ divided by $2 \hbar$ cross and this has a value which is like 10 to the power 6 meters per second as opposed to 10 to the power 8 meters per second etcetera for that is for the light. So, this is called as a Fermi velocity okay. These is very important this gives the low energy dispersion of graphene.

Low energy dispersion of Graphene

$f(k)$ about $\vec{k}$ or $\vec{k}'$ $\vec{q} = \vec{k} - \vec{K}$ ← a Dirac point variable.

$$f'(\vec{q}) = \left. \frac{\partial f(\vec{k})}{\partial k_x} \right|_{\vec{k}} (k_x - K_x) + \left. \frac{\partial f(\vec{k})}{\partial k_y} \right|_{\vec{k}} (k_y - K_y)$$

$$= \frac{3at}{2} (\tau_x + i\tau_y)$$

$a = \text{lattice const.}$
 $t = \text{hopping amplitude.}$

$$\epsilon_{\vec{k}}(\tau) = \hbar v_f (\tau_x + i\tau_y)$$

$$\epsilon_{\vec{k}'}(\tau) = \hbar v_f (\tau_x - i\tau_y)$$

$v_f = \frac{3at}{2\hbar} \approx 10^6 \text{ m s}^{-1}$
Fermi velocity.

← Low energy dispersion.

So, if we forget that we have done all these exercise and we want to write down a dispersion for this graphene for the low energy dispersion and we can write it as a k and k prime just combined is equal to a $\hbar \text{ cross } v_f \text{ q dot sigma}$ where q is a 2 dimensional wave vector and this sigma is they denote the Pauli matrices. So, this is like sigma x sigma y and sigma z of course, but sigma z is not important because q itself is a 2 dimensional vector. So, q couples with sigma. So, this will be like a q x sigma x and q y sigma y okay and it can also be checked that epsilon at k prime is the epsilon at k and its complex conjugate. So, this 2 Dirac points the electronic dispersion are related and if one just get the scalar form of energy then this is equal to a plus minus $\hbar \text{ cross } v_f$ and a q.

So, that explains the dispersion like this which is what we have seen. So, because there is a mode of q. So, there is a term that you know it there is a conical kind of dispersion that you get and so, it looks like relativistic like photons, but of course, we are not

talking about photons we are talking about electrons and that is why these electrons are called as the massless Dirac electrons or Dirac fermions okay. The discussion throws up one small anomaly which we want to point out and that anomaly is about the effective mass of electrons and the anomaly arises from the fact that this the effective mass is defined as $\hbar^2$ cross square divided by $\nabla^2 \epsilon$ say $q \nabla^2 q$ square okay or you can write it with k , k is just a wave vector.

$$\epsilon_{\vec{k}, \vec{k}'} = \hbar v_f \vec{z} \cdot \vec{\sigma}$$

$$\epsilon_{\vec{k}'}^* = \epsilon_{\vec{k}}^*$$

$$\epsilon(z) = \pm \hbar v_f |z|$$

"Massless" Dirac fermions.

$$\vec{z} = (z_x, z_y)$$

$$\vec{\sigma} = (\sigma_x, \sigma_y)$$

Now you see here the dispersion is linear. So, $\epsilon(q)$ is like $\hbar v_f q$ or you can neglect this and just say it is linear in q . So, this is a universe of that. Now this is equal to it will go to 0 because there is no dependence there is no curvature and this will go to 0. So, m^* goes to infinity because this inverse of 0 would be infinity, but that is not true and we are on the other hand we are saying that there are these massless Dirac fermions. So, how do we actually reconcile these definition of the effective mass and what we have just said so far okay.

For that we have to use a formula m^* is equal to $\hbar^2$ cross square $k \nabla^2 E \nabla^2 k$ inverse. So, it is not a double derivative, but it is a single derivative and if you want to understand where it comes from simple a semi classical argument would be good enough. So, we have p is equal to $\hbar k$ which is nothing, but the m^* into v_g where v_g denotes a groove velocity okay. So, this v_g has a form which is equal to like 1 by $\hbar$ cross $\nabla^2 E \nabla^2 k$ that is the groove velocity and which is obtained from the slope of the dispersion and if you put it back into this.

So, let us call this as equation 1. So, 1 apparently throws up a controversy and so, we are reconciling that by introducing a new definition and trying to understand whether that new definition holds. So, v_g equal to $1/\hbar$ cross $\nabla E / \nabla k$. So, if you put 4 in 3. So, your p becomes equal to m^* by $\hbar \nabla E / \nabla k$ and that gives you m^* equal to $\hbar$ cross $p / \nabla E / \nabla k$ inverse and if you put p equal to $\hbar$ cross k this becomes $\hbar$ cross square $k / \nabla E / \nabla k$ inverse ok. So, this is the definition that we wish to use and if we use this definition then of course, we get a finite mass of these things because your $\nabla E / \nabla k$ here it is of course, v_g we have sort of been a little casual in talking about the wave vector, but this v_g . So, this is a linear in v_g . So, we have we can save the definition it is some finite thing which is related to the electron I mean which is close to the bare mass of the electron or at least it is related to the bare mass of the electron.

Effective mass of Dirac fermions in graphene

$$m^* = \hbar^2 \left(\frac{\partial^2 \epsilon_q}{\partial q^2} \right)^{-1} \quad (1) \quad \epsilon_q \sim \hbar v_F q$$

$m^* \rightarrow \infty$

Use: $m^* = \hbar^2 k \left(\frac{\partial \epsilon_k}{\partial k} \right)^{-1} \quad (2)$

$$p = \hbar k = m^* v_g \quad (3)$$

$$v_g = \frac{1}{\hbar} \frac{\partial \epsilon_k}{\partial k} \quad (4)$$

Putting (4) in (3)

$$p = \frac{m^*}{\hbar} \frac{\partial \epsilon_k}{\partial k} \Rightarrow m^* = \hbar p \left(\frac{\partial \epsilon_k}{\partial k} \right)^{-1} = \hbar^2 k \left(\frac{\partial \epsilon_k}{\partial k} \right)^{-1}$$

So, what we have done so far is we have obtained the low energy dispersion for the electrons in graphene and once we get that now it will be easier for us to talk about quantum Hall effect because this q or the $\hbar$ cross q or whatever you want to call as a momentum this momentum will now get modified or renormalized by this vector potential by this p minus $e A$ and we will put it into this equation and sort of start discussing about Hall effect. There is one thing that one should mention from the dispersion is clear that it is not a dispersion which is like a. So, the q dot σ tells you that this is like a 2 by 2 Hamiltonian.

So, the Hamiltonian is 2 by 2. So, the equations will become 2 by 2 anyway because of these 2 atoms per unit cell or which denotes the sub lattice degree of freedom. Now, if

you want to talk about the valleys in addition then it becomes a 4 by 4 problem and if you want to include real spin of electrons then it will become 8 by 8 problem. We will at least forget about the real spin because in discussing quantum Hall effect there is no need for real spins to be involved which we have discussed at some point of time. However, it is important that we talk about at least a 4 by 4 Hamiltonian that is including the 2 valleys the K and the K prime valleys and including the intrinsic degree of freedom that comes along with.

This is just one word of caution that I want to talk about here. This sigma does not depend does not denote the real spin of the electrons. This that is why it is called as a pseudo spinor and it denotes sub lattice degree of freedom that is A and B. So, this really is a very important thing. So, the Hamiltonian is 2 by 2 not because of the properties of spin half, but because we are talking about 2 degrees of freedom coming from the sub lattices the 2 sub lattices A and B that is why it is called as a pseudo spinor is not a real spinor, but yes we may have to include real spin we will take care of that when we come to this. Thank you.