Topology and Condensed Matter Physics

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Lecture – 15

Electronic structure of Graphene

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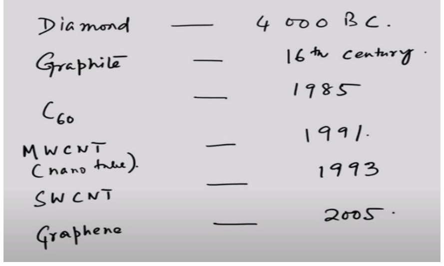

Diamond — 4000 BC.

Graphite — 16th century.

C_{60} — 1985

MWCNT (nano tube). — 1991.

SWCNT — 1993

Graphene — 2005.

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 was known for a very long time I mean 4000 BC. So, that is 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. So, it is a nanotube form was there in 1991 initially it was I think. So, 1991 was so this is a 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. So, this is how the history unfolded of carbon and its allotropes.

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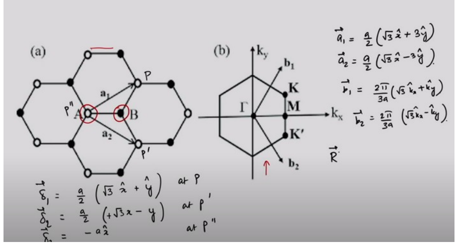

$$\vec{a}_1 = \frac{a}{2}(\sqrt{3}\hat{x} + 3\hat{y})$$
$$\vec{a}_2 = \frac{a}{2}(\sqrt{3}\hat{x} - 3\hat{y})$$
$$\vec{b}_1 = \frac{2\pi}{3a}(\sqrt{3}\hat{k}_x + \hat{k}_y)$$
$$\vec{b}_2 = \frac{2\pi}{3a}(\sqrt{3}\hat{k}_x - \hat{k}_y)$$
$$\vec{R}$$
$$\vec{\delta}_1 = \frac{a}{2}(\sqrt{3}\hat{x} + \hat{y}) \quad \text{at } P$$
$$\vec{\delta}_2 = \frac{a}{2}(+\sqrt{3}x - y) \quad \text{at } P'$$
$$\vec{\delta}_3 = -a\hat{x} \quad \text{at } P''$$

So, let us 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. 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.

$$\vec{a_1} = \frac{a}{2}(\sqrt{3}\hat{x} + 3\hat{y})$$
$$\vec{a_2} = \frac{a}{2}(\sqrt{3}\hat{x} - 3\hat{y})$$
$$\vec{b_1} = \frac{2\pi}{3a}(\sqrt{3}\hat{k_x} + \hat{k_y})$$
$$\vec{b_2} = \frac{2\pi}{3a}(\sqrt{3}\hat{k_x} - \hat{k_y})$$

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 A1 and A2 are called as the unit cell vectors or the primitive lattice vectors and B1and B2 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 A1 and A2 are the primitive lattice vectors or this unit cells are given by these A1 and A2. 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 delta1 which is A by 2 root over 3 x cap plus y cap. So, this is delta 1 which is this one which you see it here let us call it as some point say B and a P prime and a P double prime. So, a delta1 connects the B atom to P point and similarly one can write down the delta2 which is A by 2 it is a minus root 3 x and plus y. So, one can put actually a plus root 3 x and a minus y because it is below that and then the last one is actually a delta 3 which is equal to a minus Ax cap that is at the point.

$$\vec{\delta_1} = \frac{a}{2}(\sqrt{3}\hat{x} + \hat{y})$$
$$\vec{\delta_2} = \frac{a}{2}(\sqrt{3}\hat{x} - \hat{y})$$
$$\vec{\delta_3} = -a\hat{x}$$

So, at P at P prime and at P double prime and we can write down the A1 and A2 vectors as A1 equal to A by 2 root over 3 x cap plus 3y cap and A2 equal to A by 2 root 3 x cap minus 3y cap and similarly the B1 which are the reciprocal lattice vectors can be written as 2 pi over 3 a and root 3 k x cap plus ky cap and B2 would be 2 pi over 3a and root 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 A2 where n and m are integers and A1 A2 are shown here. So, n m are integers.

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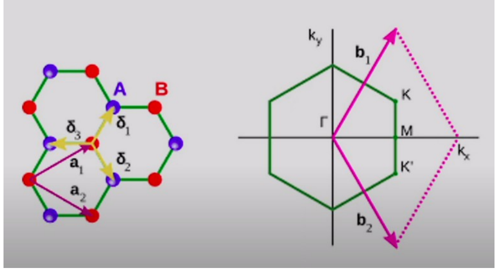

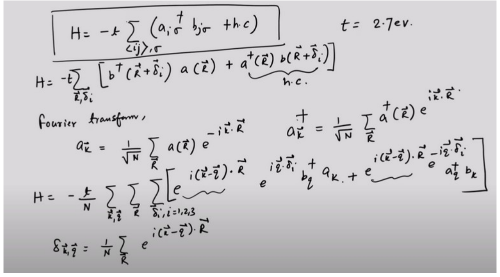

$$\boxed{H = -t \sum_{\langle ij \rangle, \sigma} (a_{i\sigma}^{\dagger} b_{j\sigma} + h.c)}$$

$t = 2.7ev.$

$$H = -t \sum_{\vec{R}, \vec{\delta}_i} \left[b^{\dagger}(\vec{R} + \vec{\delta}_i)\, a(\vec{R}) + \underbrace{a^{\dagger}(\vec{R})\, b(\vec{R} + \vec{\delta}_i)}_{h.c.} \right]$$

fourier transform,

$$a_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} a(\vec{R})\, e^{-i\vec{k}\cdot\vec{R}} \qquad a_{\vec{k}}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} a^{\dagger}(\vec{R})\, e^{i\vec{k}\cdot\vec{R}}$$

$$H = -\frac{t}{N} \sum_{\vec{k}, \vec{q}} \sum_{\vec{R}} \sum_{\vec{\delta}_i, i=1,2,3} \left[e^{i(\vec{k}-\vec{q})\cdot\vec{R}}\, e^{i\vec{q}\cdot\vec{\delta}_i}\, b_q^{\dagger} a_k + e^{i(\vec{k}-\vec{q})\cdot\vec{R}}\, e^{-i\vec{q}\cdot\vec{\delta}_i}\, a_q^{\dagger} b_k \right]$$

$$\delta_{\vec{k},\vec{q}} = \frac{1}{N} \sum_{\vec{R}} e^{i(\vec{k}-\vec{q})\cdot\vec{R}}$$

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. Alright, we will come to this discussion in just a while. 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.So, this is like a Ai sigma dagger Bj sigma plus a Hermitian conjugate of that and sigma. So, I am using the second quantized notation where Ai sigma creates an electron with spin sigma at the ith side which belongs to the A sub lattice and it destroys an electron with spin sigma at the jth side in B sub lattice and just to make sure that these i and j are nearest neighbors there is a angular bracket that is shown and this sigma actually denotes the spin of the electrons.

$$H = -t \sum_{<ij>,\sigma} (a_i\sigma^{\dagger} b_{j\sigma} + h.c.)$$

$$H = -t \sum_{\vec{R},\delta_i} [b^{\dagger}(\vec{R} + \vec{\delta_i}) a(\vec{R}) + a^{\dagger}(\vec{R}) b(\vec{R} + \vec{\delta_i})]$$

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 delta and this is like I am writing it slightly differently, but they mean the same thing delta i where delta 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 delta i's delta 1 delta 2 delta 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 b R plus delta i these are all vectors.

$$\vec{a_k} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} a\vec{R} e^{-\vec{k}.\vec{R}}$$

$$\vec{a_k^{\dagger}} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} a^{\dagger}(\vec{R}) e^{\vec{k}.\vec{R}}$$

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 delta 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 the b sub lattice and vice versa and there is a sum over all these delta 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 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 delta 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, ak dagger will come with a1 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 a1 b1 a2 b2 and so on because they are not simply just algebraic quantities they involve a column vector. So, the first term is that and then exponential i q dot delta i these and then b q dagger a k.

So, we can write it down here as plus exponential i k minus q dot R exponential minus i q dot delta i and a q dagger b 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 k q this is equal to 1 by n summation over R and it is a exponential k minus q dot R. So, you see that there is a sum over 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 k and q to be same and with that what one gets is a following.

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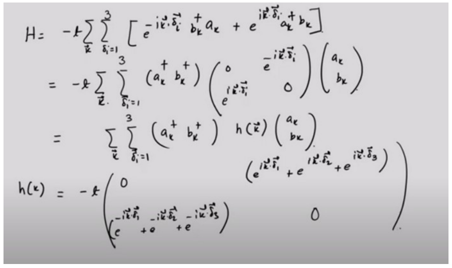

$$H = -t\sum_{\vec{k}}\sum_{\delta_i=1}^{3}\left[e^{-i\vec{k}\cdot\vec{\delta}_i}\, b_k^{+} a_k + e^{i\vec{k}\cdot\vec{\delta}_i}\, a_k^{+} b_k\right]$$

$$= -t\sum_{\vec{k}}\sum_{\vec{\delta}_i=1}^{3}\begin{pmatrix} a_k^{+} & b_k^{+}\end{pmatrix}\begin{pmatrix} 0 & e^{-i\vec{k}\cdot\vec{\delta}_i} \\ e^{i\vec{k}\cdot\vec{\delta}_i} & 0\end{pmatrix}\begin{pmatrix} a_k \\ b_k\end{pmatrix}$$

$$= \sum_{\vec{k}}\sum_{\vec{\delta}_i=1}^{3}\begin{pmatrix} a_k^{+} & b_k^{+}\end{pmatrix} h(\vec{k})\begin{pmatrix} a_k \\ b_k\end{pmatrix}$$

$$h(k) = -t\begin{pmatrix} 0 & \left(e^{i\vec{k}\cdot\vec{\delta}_1} + e^{i\vec{k}\cdot\vec{\delta}_2} + e^{i\vec{k}\cdot\vec{\delta}_3}\right) \\ \left(e^{-i\vec{k}\cdot\vec{\delta}_1} + e^{-i\vec{k}\cdot\vec{\delta}_2} + e^{-i\vec{k}\cdot\vec{\delta}_3}\right) & 0\end{pmatrix}$$

So, the Hamiltonian is written as minus t sum over k and then these delta i's will go from 1 to 3 which we have said and there is a minus k dot because k and q have become same. So, it is i k dot delta i b k dagger a k and a plus exponential i k dot delta i a k dagger a k dagger bk.

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 k and you again have this delta i equal to 1 2 3 and I can write it just like a matrix where a k dagger b k dagger. So, this is like a row vector and this is a 0 and exponential minus ik dot delta i exponential i k dot delta i and then 0 and then you have a a k and bk ok. Now you see that there is no term that contains a ak dagger ak 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. Similarly there is no term which is b k dagger b k that is why this matrix that you see at the middle sandwiched between the row vector and the column vector actually does not have any diagonal elements, but it only has off diagonal elements.

$$
\begin{aligned}
H &= -t\sum_{\vec{k}}\sum_{\delta_i=1}^{3}[e^{-i\vec{k}.\vec{\delta_i}}b_k^\dagger a_k + e^{-i\vec{k}.\vec{\delta_i}}a_k^\dagger b_k] \\
&= -t\sum_{\vec{k}}\sum_{\delta_i=1}^{3}(a_k^\dagger b_k^\dagger)\begin{pmatrix} 0 & e^{-i\vec{k}.\vec{\delta_i}} \\ e^{-i\vec{k}.\vec{\delta_i}} & 0 \end{pmatrix}\begin{pmatrix} a_k \\ b_k \end{pmatrix} \\
&= \sum_{\vec{k}}\sum_{\delta_i=1}^{3}(a_k^\dagger b_k^\dagger)h(\vec{k})\begin{pmatrix} a_k \\ b_k \end{pmatrix}
\end{aligned}
$$

So, this can be written as a sum over k and again a delta 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 ak bk that is your Hamiltonian and what is the form of h k? Now h k involves a sum of 3 terms with the delta 1 and delta 2 and delta 3 that we have mentioned earlier that is delta 1 delta 2 and delta 3 which are written here ok. So, once when you put that then hk becomes a sum of 3 terms let me also take this minus t here. So, that I do not write the minus t here.

$$
h(k) = -t\begin{pmatrix} 0 & (e^{-i\vec{k}.\vec{\delta_i}} + e^{-i\vec{k}.\vec{\delta_i}} + e^{i\vec{k}.\vec{\delta_1}} + e^{i\vec{k}.\vec{\delta_2}} + e^{i\vec{k}.\vec{\delta_3}}) \\ e^{-i\vec{k}.\vec{\delta_1}}e^{-i\vec{k}.\vec{\delta_2}}e^{-i\vec{k}.\vec{\delta_3}} & 0 \end{pmatrix}
$$

So, I take it with h k. So, that this becomes like a 0 exponential ik dot delta1 plus exponential i k dot delta 2 plus exponential i k dot delta 3 ok. 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 dot delta 1 plus exponential minus i k dot delta 2 plus exponential minus i k dot 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 ok. Now the difference between this delta 1 and delta 2 or delta 2 and delta 3 or delta 1 and delta 3 must give you a lattice vector which is r.

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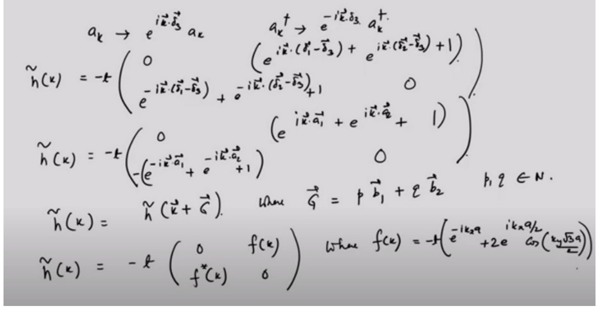

$$a_k \to e^{i\vec{k}\cdot\vec{\delta}_3} a_k \qquad a_k^{\dagger} \to e^{-i\vec{k}\cdot\delta_3} a_k^{\dagger}$$

$$\tilde{h}(k) = -t\begin{pmatrix} 0 & (e^{i\vec{k}\cdot(\vec{\delta}_1-\vec{\delta}_3)} + e^{i\vec{k}\cdot(\vec{\delta}_2-\vec{\delta}_3)} + 1) \\ e^{-i\vec{k}\cdot(\vec{\delta}_1-\vec{\delta}_3)} + e^{-i\vec{k}\cdot(\vec{\delta}_2-\vec{\delta}_3)} + 1 & 0 \end{pmatrix}$$

$$\tilde{h}(k) = -t\begin{pmatrix} 0 & (e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2} + 1) \\ -(e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2} + 1) & 0 \end{pmatrix}$$

$$\tilde{h}(k) = \tilde{h}(\vec{k}+\vec{G}) \quad \text{where} \quad \vec{G} = p\vec{b}_1 + q\vec{b}_2 \qquad p, q \in N.$$

$$\tilde{h}(k) = -t\begin{pmatrix} 0 & f(k) \\ f^{*}(k) & 0 \end{pmatrix} \quad \text{where} \quad f(k) = -t\left(e^{-ik_x a} + 2e^{ik_x a/2}\cos\left(\frac{k_y\sqrt{3}a}{2}\right)\right)$$

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 to the power i k dot delta 3 ak and ak dagger will be exponential minus i k dot delta 3 and a k dagger ok. 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 H tilde it is equal to minus t and 0 here and exponential i k delta 1 minus delta 3 plus exponential i k delta 2 minus delta 3 and plus 1 and then you have a.

$$\widetilde{h(k)} = -t\begin{pmatrix} 0 & (e^{i\vec{k}.(\vec{\delta_i}-\vec{\delta_3})} + e^{i\vec{k}.(\vec{\delta_i}-\vec{\delta_3})} + 1) \\ (e^{-i\vec{k}.(\vec{\delta_i}-\vec{\delta_3})} + e^{-i\vec{k}.(\vec{\delta_i}-\vec{\delta_3})} & 0 \end{pmatrix}$$

$$\widetilde{h(k)} = -t\begin{pmatrix} 0 & (e^{i\vec{k}.\vec{a_1}} + e^{i\vec{k}.\vec{a_2}} + 1) \\ (e^{-i\vec{k}.\vec{a_1}} + e^{-i\vec{k}.\vec{a_2}} + 1 & 0 \end{pmatrix}$$

So, this is a term there and then one can actually have exponential minus i k delta 1 minus delta 3 plus exponential minus i k delta 2 minus delta 3 plus 1 and there is a 0 here and that is becomes the matrix. If we use the definitions of delta1 and delta 2 so, you see now that one term has become equal to 1 just for the simplicity now we put delta 1 and delta 2 and delta 3 and then one gets this H of k to be rather H tilde of k to be minus t and it is a 0 exponential i k dot a 1 plus exponential i k dot a 2 i k dot a 2 and a plus 1 and there is a minus there is a minus sign minus i k dot a 1 plus exponential minus i k dot a 2 plus a 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 H tilde obeys this equal to H tilde k plus g where g is the proper reciprocal lattice vector which is defined as.

$$\widetilde{h}(k) = \widetilde{h}(\vec{K} + \vec{G})$$

$$\widetilde{h}(k) = -t \begin{pmatrix} 0 & f(k) \\ f^*(k) & 0 \end{pmatrix}$$

$$f(k) = -t(e^{-ik_x a} + 2e^{ik_x a/2} \cos(\frac{k_y \sqrt{3}a}{2}))$$

So, this is defined as p of b1 plus q of b2 and again p q alright. So, this is the form and then let us write a little more neatly where we write this as minus t 0 f of k and f star of k and 0 where f of k is equal to this is just the simplified form of this 2 by 2 matrix where this is equal to minus t exponential minus i kx a plus 2 exponential i kx a by 2 and a cosine of k y root 3 k y root 3 a by 2 ok. That is the form for f of k and we can now diagonalize this matrix H tilde of k and get the energy dispersion for the tight binding problem of for graphene.

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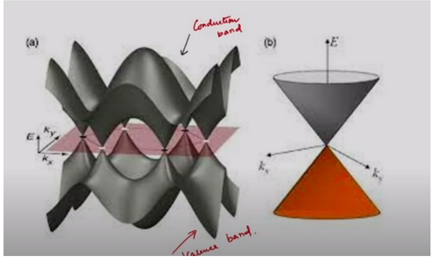

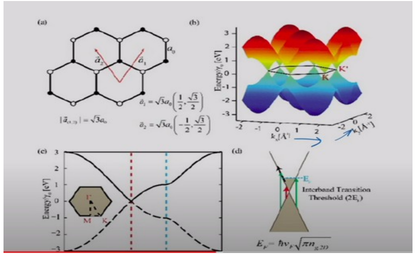

So, this is equal to plus minus t root over of f k mod square and this is equal to plus minus t and 3 plus 2 cosine root over 3 a k y plus 4 cos root 3 k y a by 2 and a cosine 3 a k x by 2. Ideally this should have been the end of the problem because we have found out there are 2 bands one correspond to plus sign and the other other correspond to minus sign and there are 2 bands because there are 2 atoms per unit cell.

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 pi to pi 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 epsilon 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 dot p plus beta m c square where alpha and beta are matrices and p is the momentum and m c square 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.

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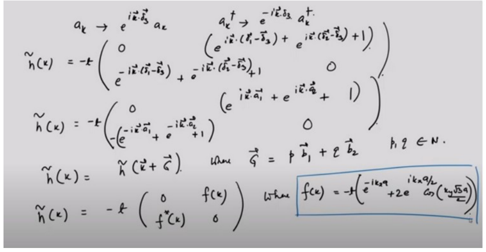

$$a_k \to e^{i\vec{k}\cdot\vec{\delta}_3} a_k \qquad a_k^\dagger \to e^{-i\vec{k}\cdot\delta_3} a_k^\dagger$$

$$\tilde{h}(k) = -t\begin{pmatrix} 0 & \left(e^{i\vec{k}\cdot(\vec{\delta}_1-\vec{\delta}_3)} + e^{i\vec{k}\cdot(\vec{\delta}_2-\vec{\delta}_3)} + 1\right) \\ e^{-i\vec{k}\cdot(\vec{\delta}_1-\vec{\delta}_3)} + e^{-i\vec{k}\cdot(\vec{\delta}_2-\vec{\delta}_3)} + 1 & 0 \end{pmatrix}$$

$$\tilde{h}(k) = -t\begin{pmatrix} 0 & \left(e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2} + 1\right) \\ \left(e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2} + 1\right) & 0 \end{pmatrix}$$

$$\tilde{h}(k) = \tilde{h}(\vec{k}+\vec{G}) \quad \text{where } \vec{G} = p\vec{b}_1 + q\vec{b}_2 \quad p, q \in N.$$

$$\tilde{h}(k) = -t\begin{pmatrix} 0 & f(k) \\ f^*(k) & 0 \end{pmatrix} \quad \text{where } \boxed{f(k) = -t\left(e^{-ik_x a} + 2e^{ik_x a/2}\cos\left(\frac{k_y\sqrt{3}a}{2}\right)\right)}$$

Now, we need to understand because condensed matter physics deals with low energy properties of systems we need to understand that what is the 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 kx and a ky and so on and then these red colored red and yellowish that corresponds to the conduction band and then blue and greenish tints 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 3 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 kx 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.

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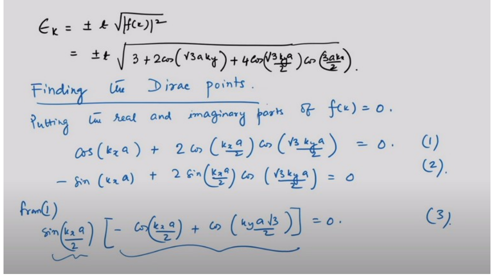

$$\epsilon_k = \pm t\sqrt{|f(k)|^2}$$

$$= \pm t\sqrt{3 + 2\cos(\sqrt{3}ak_y) + 4\cos\left(\frac{\sqrt{3}k_y a}{2}\right)\cos\left(\frac{3ak_x}{2}\right)}.$$

Finding the Dirac points.

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

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

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

from (1)

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

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 this equations as you can check them. So, it is a cos kx a by 2 cos root 3 k y a by 2 equal to 0 and minus sin k x a plus 2 sin k x a by 2 cos root 3 ky a by 2 equal to 0.

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

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

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 points these red circle points are what I am trying to determine and because the dispersion gives you 0 value.

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

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

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

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 by 2 and a minus cos kx a by 2 plus a cos ky a root 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 kx a by 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.

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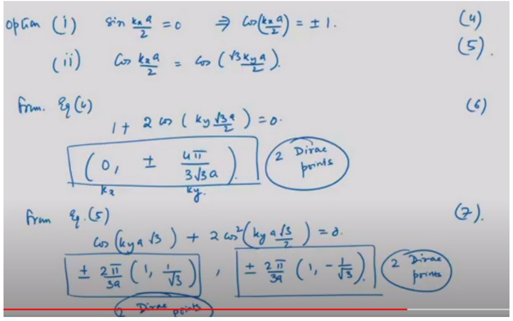

option (i) $\sin\frac{k_x a}{2} = 0 \Rightarrow \cos(\frac{k_x a}{2}) = \pm 1.$ (4)

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

From. Eq (4) (6)

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

$$\boxed{(\underset{k_x}{0}, \pm \underset{k_y}{\frac{4\pi}{3\sqrt{3}a}}).}$$

2 Dirac points

From Eq.(5) (7).

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

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

2 Dirac points

2 Dirac points

Option 1 its sin k x a by 2 equal to 0 which also means that cosine of k x a by 2 is either plus 1 or minus 1. So, sin 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 kx a by 2 equal to cosine ky a root 3 by 2. So, this is equal to a cosine kx a by 2 and equal to cosine root 3 ky a by 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 plus 2 cosine ky root 3 a 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 4 pi by 3 root 3 a. So, these are the so, this k x and these are k y. So, I get 2 points 0 and 4 pi by 3 root 3 a another is 0 minus 4 pi by 3 root 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 ky a root 3 which is plus a 2 cosine square ky a root 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 2 pi by 3 a 1 and a 1 by root 3 and plus minus 2 pi by 3 a 1 minus 1 by root 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. So, we have these 6 Dirac points.

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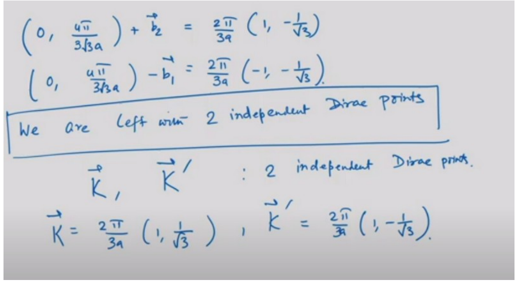

$$\left(0, \frac{4\pi}{3\sqrt{3}a}\right) + \vec{b}_2 = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right)$$

$$\left(0, \frac{4\pi}{3\sqrt{3}a}\right) - \vec{b}_1 = \frac{2\pi}{3a}\left(-1, -\frac{1}{\sqrt{3}}\right).$$

We are left with 2 independent Dirac points

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

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

However, it can actually be checked that the 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 root 3 a plus a b2 b2 has been defined earlier if you see that b 2 has been defined here b1 and b2. So, once you add b1 or b2 to this the first point you get a 1 other Dirac point which is 1 minus 1 by root 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 4 pi by 3 root 3 a plus or minus a b 1 that gives another 1 which is 2 pi by 3 a minus 1 minus 1 by root 3.

$$\sin\frac{k_x a}{2} = 0 \quad \Rightarrow \cos(\frac{k_x a}{2}) = \pm 1$$

$$\cos(\frac{k_x a}{2}) = \cos(\frac{\sqrt{3}k_y a}{2})$$

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 prime ok. They are also referred to as valleys. Now, whenever I write it a big k and a k prime 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 2 pi by 3 a 1 1 by root 3 and the k prime is equal to 2 pi by 3 a 1 minus 1 by root 3 ok.

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

$$k_y \to \pm\frac{2\pi}{3a}(1, 1/\sqrt{3})$$

$$k_y \to \pm\frac{2\pi}{3a}(1, -1/\sqrt{3})$$

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 ok. So, at these points one has massless Dirac kind of dispersion for the electrons of graphene ok. Now, since we have found these points the Dirac points we can expand the electronic dispersion about these points ok.

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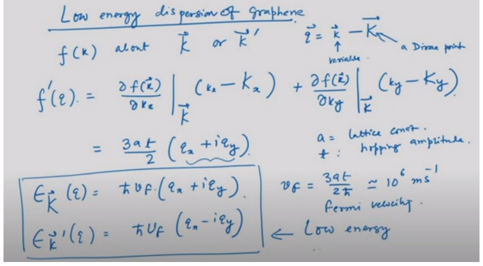

Low energy dispersion of graphene

$f(k)$ about $\vec{K}$ or $\vec{K}'$

$\vec{q} = \vec{k} - \vec{K}$ ← a Dirac point

$\uparrow$ variable

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

$$= \frac{3at}{2}(q_x + iq_y)$$

a = lattice const.

t : hopping amplitude.

$$\boxed{\begin{aligned} \epsilon_{\vec{K}}(q) &= \hbar v_F(q_x + iq_y) \\ \epsilon_{\vec{K}'}(q) &= \hbar v_F(q_x - iq_y) \end{aligned}}$$ ← Low energy

$v_F = \frac{3at}{2\hbar} \simeq 10^6\, ms^{-1}$

Fermi velocity.

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 ok.Now this is a momentum variable ok, 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.

$$
\begin{aligned}
f'(q) = \frac{\delta f(\vec{k})}{\delta k_x}|_{\vec{k}}(k_x - K_x) + \frac{\delta f(\vec{k})}{\delta k_y}|_{\vec{k}}(k_y - K_y) \\
= \frac{3at}{2}(q_x + iq_y) \\
\epsilon_{\vec{K}}(q) = \hbar\nu_F(q_x + iq_y) \\
\epsilon_{\vec{K}'}(q) = \hbar\nu_F(q_x - iq_y)
\end{aligned}
$$

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 a del fk del kx. So, this is like at the k point and this is like a k x minus a k x ok. This is the x component of the Dirac point in the Brillouin zone and this small k x is actually a variable plus a del f k del k y at the k point and k y minus k y ok. So, if you do that then this yields a spectrum which is 3 a t divided by 2 qx plus i q y ok, where a is 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 qx and qy i is of course, the imaginary number this dispersion at k the low energy dispersion is h cross V f where V f is the scale and this is equal to qx plus i qy. Now, if you repeat this for the other k point which is k prime at q this will give a h cross V f and a qx minus i qy where Vf is nothing, but 3 a t divided by 2 h 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 ok. These is very important this gives the low energy dispersion of graphene.

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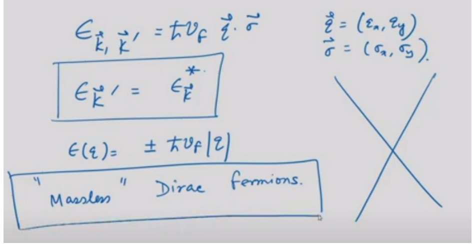

$\epsilon_{\vec{k},\vec{k}'} = \hbar v_F \vec{q}\cdot\vec{\sigma}$

$\vec{q} = (q_x, q_y)$

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

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

$\epsilon(q) = \pm \hbar v_F |q|$

"Massless" Dirac fermions.

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 a k prime just combined is equal to a h cross of Vf a q dot sigma where q is a 2 dimensional wave vector and this sigma is they denote the Pauli matrices.

$$\epsilon_{\vec{k},\vec{K'}} = \hbar \nu_F \vec{q}.\vec{\sigma}$$
$$\epsilon_{\vec{K'}} = \epsilon^*_{\vec{K}}$$

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 ok. 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 h cross V f and a q. So, that explains the dispersion like this which is what we have seen. So, because there is a mod 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 ok.

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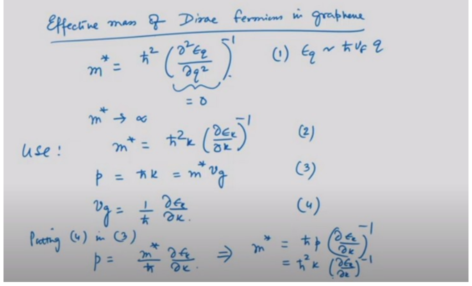

Effective mass of Dirac fermions in graphene

$$m^* = \hbar^2 \Big(\underbrace{\frac{\partial^2 \epsilon_q}{\partial q^2}}_{=0}\Big)^{-1} \qquad (1)\ \epsilon_q \sim \hbar v_F q$$

$$m^* \to \infty$$

Use:

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

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

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

Putting (4) in (3)

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

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 h cross square divided by del 2 epsilon say q del q square or you can write it with k, k is just a wave vector.

Now you see here the dispersion is linear. So, epsilon q is like h cross 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 star 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 ok.

$$\begin{aligned} m^* &= \hbar^2 (\frac{\delta^2 \epsilon_q}{\delta q^2})^{-1} \\ &= 0 \end{aligned} \qquad \text{(Equation 1)}$$

$$\mathrm{m}^* = \hbar^2 k (\tfrac{\delta \epsilon_k}{\delta k})^{-1} \qquad \text{(Equation 2)}$$

$$\mathrm{p} = \hbar k = m^* v_g \qquad \text{(Equation 3)}$$

$$\nu_g = \tfrac{1}{\hbar} \tfrac{\delta \epsilon_k}{\delta k} \qquad \text{(Equation 4)}$$

For that we have to use a formula m star is equal to h cross square k del E del 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 h cross k which is nothing, but the m star into Vg where Vg denotes the group velocity ok. So, this Vg has a form which is equal to like 1 by h cross del E del k that is the group 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 by h cross del E del k. So, if you put 4 in 3. So, your p becomes equal to m star by h del E del k and that gives you m star equal to h cross p del E del k inverse and if you put p equal to h cross k this becomes h cross square k del E del 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 del E del k here it is of course,q we have sort of been a little casual in talking about the wave vector, but this.

$$\begin{aligned} p &= \frac{m^*}{\hbar} \frac{\delta \epsilon_k}{\delta k} \\ \Rightarrow m^* = \hbar p (\frac{\delta \epsilon_k}{\delta k})^{-1} &= \hbar^2 k (\frac{\delta \epsilon_k}{\delta k})^{-1} \end{aligned}$$

So, this is a linear in q. So, we have we can save the definition it is some a 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. 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 h 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 it is clear that it is not a dispersion which is like a. So, the q dot sigma 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 this 2 atoms per unit cell or which is 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 a 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 spinner and it denotes sub lattice degree of freedom that is a and b ok. 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 spinner is not a real spinner, but yes we may have to include real spin we will take care of that when we come to this. Thank you.