

Topology and Condensed Matter Physics
Prof. Saurabh Basu

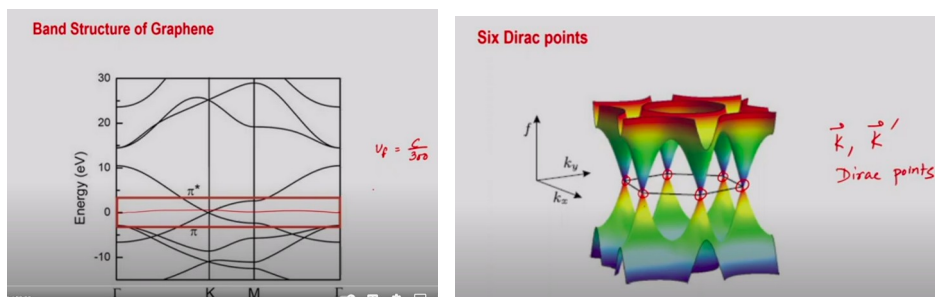
Department of Physics

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Lecture – 16

Symmetries and QHE in Graphene

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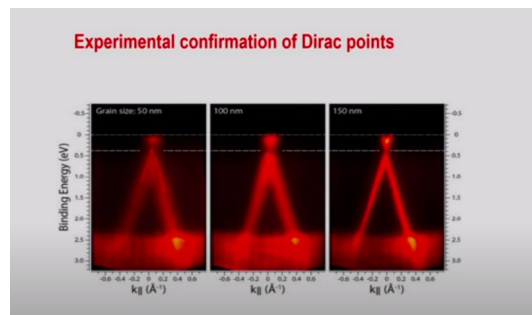


We have been talking about Graphene, the main thing is about the electronic structure of Graphene which is under consideration for this course. So we have derived the low energy dispersion of Graphene, the energy as a function of k this Γ K M Γ these are points in the Brillouin zone and the band structure is shown here this is a density functional theory band structure DFT band structure it is called and you see the π and the π^* which are the 2 bands which are closest to the Fermi level and the Fermi level is kind of boxed in red. In fact this is the Fermi energy at 0 and if you look at it carefully this π and π^* bands they cross linearly at these points these the Γ and the M points and this is what gives rise to the low energy linear dispersion which is why they are called as massless Dirac Fermions.

However they are not massless they have electronic mass and they are also the density of state is also linear in energy and so on even though they look like pseudo relativistic dispersion the velocity is still $c/300$ which is you know the 300 times smaller than the velocity of light so and that corresponds to the Fermi velocity of electrons in most metals so this falls in that category and you know look at the 6 Dirac points whose coordinates have been found and these are the 6 Dirac points that you see here what we have

discussed is that they are not all independent they depend on each other by the addition or subtraction of the reciprocal lattice vectors and only two of them being independent and the rest four can be generated by adding or subtracting the reciprocal lattice vectors and these points which are independent are called as the K and the K prime points and these are known as the Dirac points and the name came because the dispersion is Dirac like which is that of in this case it is a massless Dirac form and linear dispersion. So this is something that is slightly non-trivial in the context of condensed matter physics in condensed matter physics these relativistic dispersions are not common and in fact the K square dispersions are more common but in this particular case they are the low energy dispersion is linear and they correspond to massless Dirac fermions.

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So these are things that we have discussed now this is the experimental confirmation of the Dirac points these are the photo emission studies will not discuss where one actually calculates the binding energy and as a function of the planar wave vector so it is basically a photon is made to shine on the surface and these electrons are emitted and these electrons are captured which would tell us this binding energy and so on and this is plotted as a function of the planar wave vector the KXY wave vector and these are given as \vec{K} parallel and you see this Dirac like dispersion which are very apparent here linear dispersion at or near the Fermi level and this is taken from this paper there are many other confirmations of the Dirac spectrum.

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Dirac Hamiltonian

$$h(\vec{q}) = v_F (q_x \tau_x \sigma_x + q_y \sigma_y) \quad \hbar = 1$$

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

σ : Sublattice degree of freedom.
 τ : Valley degree of freedom.

$h(\vec{q}) = v_F \cdot (q_x \sigma_x + q_y \sigma_y)$: at \vec{K}
 $= v_F (-q_x \sigma_x + q_y \sigma_y)$: at \vec{K}'

$\vec{q} = \vec{k} - \vec{K}$
 $= \vec{k}' - \vec{K}'$

$\tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$: +1 : \vec{K} valley
-1 : \vec{K}' valley.

So we come back to the Hamiltonian for graphene and the Hamiltonian looks like this I have taken \hbar cross equal to 1 and v_F is you can write it a V capital F that corresponds to the Fermi velocity Q_X and Q_Y are small wave vectors where the K vectors which are I mean we usually represent the K vectors the wave vectors by the K so this K is so Q is equal to K minus K or K minus K prime. So you expand the wave vectors in the vicinity of the Dirac points which are K and K prime points and write the small wave vector as Q and this is what is written in terms of Q_X and Q_Y so this Q is nothing but Q_X Q_Y and v_F is the Fermi velocity σ_X and σ_Y they are Pauli matrices however they do not represent the spin degrees of freedom σ actually stands for the sub lattice degree of freedom and you see a γ_Z here which is so this is the the valley degree of freedom and here γ_Z is exactly same as the Z component of the Pauli matrix but they it's a 2 by 2 matrix where plus 1 denotes the K valley that is the K Dirac point and minus 1 that corresponds to the K prime value.

$$h(\vec{q}) = v_F(q_x \tau_z \sigma_x + q_y \sigma_y)$$

$$\vec{q} = (q_x, q_y), \quad \vec{q} = \vec{k} - \vec{K}$$

Okay so that so essentially what happens is that you have a H of Q which is equal to a v_F and there is a $Q_X \sigma_X$ plus a $Q_Y \sigma_Y$ this is the Hamiltonian at the K point one of the Dirac points and for the other one you have a minus sign here $Q_X \sigma_X$ minus $Q_Y \sigma_Y$ so this is at K prime. So in a compact notation we can write down at both the Dirac points we can write down the Hamiltonian like this one has to keep in mind that there is no spin in the problem however the Pauli spin matrices they denote the sub lattice degree of freedom and in addition to that the γ denotes the valley degree of freedom.

$$\tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

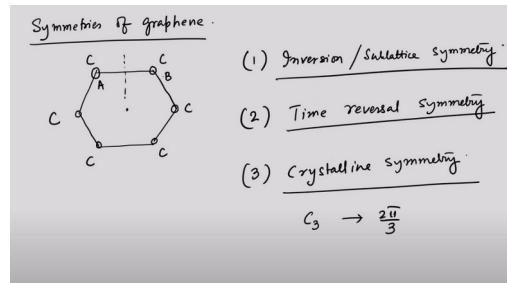
$$h(\vec{q}) = v_F(q_x \sigma_x + q_y \sigma_y)$$

$$= v_F(-q_x \sigma_x + q_y \sigma_y)$$

Okay now what is intended here is that to understand what are the symmetries of graphene and what do the symmetries do what will happen when we break these symmetries and one of the main things that happens is that these Dirac points are robust that is there is no gap that opens up in any of the six points the Dirac points that we had shown and out of

that we will only talk about the K and K prime so these are the symmetries of graphene actually protect these Dirac points. So this is what we have to understand and in that context we have to understand the symmetries of graphene.

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So the question is what are the symmetries of graphene just quick look at the unit cell okay and each of them are occupied by the carbon atoms okay and carbon atoms in this 1 is to 2 is to 2 p to configuration and so per carbon atom there are two electrons however one electrons forms a sigma bond which gives the stability of the structure and the pi electrons are only available for conduction as we have shown in the band structure.

Now the two symmetries that are quite important in this context is that we will talk about the inversion symmetry or this is also called as the sub lattice symmetry and this quite common or rather it is quite trivial to understand that if you draw an axis which is perpendicular to the bond connecting the two carbon atoms so this corresponds to A sub lattice and this corresponds to the B sub lattice then a changing A to B and B to A will not change the structure or will not do anything to the Hamiltonian and that is why this is the Hamiltonian that we have written in the last slide this is invariant under this transformation or these it has inversion and sub lattice symmetry okay. And the next thing that we will do we will show in details is a time reversal symmetry and in this particular case as we have seen earlier that there is no spin here so because there is no spin the time reversal operation is simply the complex conjugation or in some literature you will actually see that it is written with a unitary operator multiplied by the complex conjugation but they mean the same thing.

There is a third symmetry which is a crystalline symmetry and this is called as a C3 symmetry what it means is that it is a C3 rotational symmetry so if you take a point in the at the center of the hexagon and then you give a 2 pi by 3 rotation to the entire system then you know this carbon atom here will go here and this will go here and so on okay. So they will just move and the honeycomb or the hexagon will remain unchanged and this is the crystalline symmetry that we have. Now this we are not going to discuss one is that this of course forms the Dirac points but this has no role in preserving the Dirac points or making the Dirac points to be invariant or it does not sort of give anything or

rather impart anything to the topological considerations for graphene. So we will not talk about it in details but then one should know that this symmetry crystalline symmetry exists. So let me look at the inversion symmetry.

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(1) Inversion Symmetry

$$\sigma_z H(k) \sigma_z = -H(k)$$

$$H(k) = (\hbar v_F (\tau_x \sigma_x + \tau_y \sigma_y))$$

Terms

$$\sigma_z \sigma_x \sigma_z \rightarrow -\sigma_x$$

$$\sigma_z \sigma_y \sigma_z \rightarrow -\sigma_y$$

$$\sigma_z H(k) \sigma_z = \hbar v_F (-\tau_x \sigma_x \tau_z - \tau_y \sigma_y \tau_z)$$

$$= -\hbar v_F (\tau_x \sigma_x \tau_z + \tau_y \sigma_y \tau_z)$$

$$= -H(k)$$

Graphene has inversion/sublattice Symmetry

So this inversion symmetry can be tested by a sigma z operator and this sigma z h of q sigma z that has to be tested and this should come out to be minus h of q okay. So this denotes that graphene has inversion symmetry so it is not difficult to see that because you have this h of q simply has apart from that V_f it has a q_x sigma x plus a q_y sigma y and then we will have terms such as so sigma z sigma x sigma z that will give rise to minus sigma x and a sigma z sigma y sigma z will again give rise to a minus sigma y. So your sigma z h of q sigma z is equal to h cross V_f well we can drop h cross but or you can keep h cross it does not matter.

$$\sigma_z H(q) \sigma_z = -H(q)$$

$$H(q) = (q_x \sigma_x + q_y \sigma_y)$$

$$\sigma_z \sigma_x \sigma_z \rightarrow -\sigma_x$$

$$\sigma_z \sigma_y \sigma_z \rightarrow -\sigma_y$$

$$\sigma_z H(q) \sigma_z = \hbar v_F (-q_x \sigma_x \tau_z - q_y \sigma_y \tau_z)$$

$$= -\hbar v_F (q_x \sigma_x \tau_z + q_y \sigma_y \tau_z)$$

$$= -H(q)$$

This is equal to minus q_x sigma x gamma z which you know connects or rather denotes both k and k prime Hamiltonians and then there is a q_y sigma y okay and this can be easily taken out the minus sign and then we have a q_x sigma x gamma z plus a q_y sigma y which is nothing but equal to minus h of q okay. So graphene has inversion symmetry and as I said that you can also call it a sub lattice symmetry okay. So this is one of the important things about graphene that it is the Dirac points are protected by these

symmetries of course we will have to consider one more which is a time reversal symmetry.

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② Time Reversal Symmetry:
 K : Complex Conjugation operator. $H(k) = \hbar v_F (\sigma_x k_x + \sigma_y k_y)$ at K point.
 At K $K H(\vec{k}) K^\dagger = \hbar v_F (\sigma_x k_x - \sigma_y k_y) = -\hbar v_F (-\sigma_x k_x + \sigma_y k_y) \rightarrow$ Hamiltonian at the K' point.
 $K H(\vec{k}) K^\dagger = H^*(-\vec{k})$.
 $H^*(-\vec{k}) = \hbar v_F (-\sigma_x k_x + \sigma_y k_y)$.
 Graphene Hamiltonian remains invariant under both Inversion & Time reversal symmetry.

So this 2 okay and what we mean by time reversal symmetry is we just define k to be this complex conjugation operator. In fact if the real spin is included which may be done when the spin orbit coupling is there then alone these complex conjugation operator will not be sufficient we will have to also include the sigma y part okay. So this h of q this dagger this is equal to h cross v_f now I will write it at only at the k point so this is so I just take only one Hamiltonian this q . So I only write it at k point which is $q_x \sigma_x$ plus $q_y \sigma_y$ so this is at k point.

$$H(q) = \hbar v_F (q_x \sigma_x + q_y \sigma_y)$$

$$K H(\vec{q}) K^\dagger = \hbar v_F (\sigma_x q_x - \sigma_y q_y)$$

$$= -\hbar v_F (-\sigma_x q_x + \sigma_y q_y)$$

If you want to write it at the other Dirac point that is at the other valley these are called valleys these Dirac points are called valleys. The time reversal symmetry actually what it does is that it changes the Hamiltonian from one valley to another and so this is at k at the one of the Dirac points if you apply this time reversal operator then it gives you this which can be written as minus h cross v_f and I hope you understand why there is a minus sign the minus sign arises because sigma y is a complex matrix even though it is Hermitian it is like this okay. So that is why it changes sign when you do a complex conjugation it changes sign so this is equal to a minus sigma x q_x plus sigma y q_y and that is nothing but the Hamiltonian at the k prime point okay.

$$K H(\vec{q}) K^\dagger = H^*(-\vec{q})$$

$$H^*(\vec{q}) = \hbar v_F (-\sigma_x q_x + \sigma_y q_y)$$

So that tells you that we get this k h of q k inverse this is equal to a h star of minus k okay and you can just do h star of minus k or k or rather this is I should write it as q because q is a small wave vector this is q this is equal to h cross v_f minus $\sigma_x q_x$ plus $\sigma_y q_y$ and so on okay because we take a h star and then we also change so this term does not change sign because σ_y changes sign upon this doing a star of that which means taking a complex conjugate and q_y is also changed sign because there is a minus q there I should write it with a vector here but the first term that is $\sigma_x q_x$ σ_x does not change sign but q_x changes sign and that is why you get a minus sign and this is nothing but you know the Hamiltonian that corresponds to the k prime point. If you take the k point Hamiltonian to be the plus sign then this is a minus k or you could take it alternatively the k prime Hamiltonian to have a plus sign and then the k will have a minus sign so there is no nothing that's puts a restriction on which one you can take k or k prime one of them is k the other is k prime okay. So what it tells you is that the graphene Hamiltonian remains invariant under both inversion and time reversal.

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Combined both these symmetries:

$$(\sigma_z K) H^*(-\vec{q})(\sigma_z K)^\dagger = -H(\vec{q})$$

→ Particle-hole symmetry.

Can we make graphene Topological??

So this is one and this is another and it remains invariant under both and the product of them so combined both these symmetries $\sigma_z k$ this and then h star of minus k and $\sigma_z k$ dagger this is equal to minus h of well you can write it as k or q depending upon we will write as q okay. So this is called as the particle hole symmetry it is just a the some literature calls it as particle hole symmetry because it is a product of these two symmetries that are one of them is the inversion the other is a time reversal symmetry okay.

$$(\sigma_z K) H^*(-\vec{q})(\sigma_z K)^\dagger = -H(\vec{q})$$

So we go back to our earlier discussion that these symmetries are essential for giving rise to a topological invariant or giving rise to something that remains you know invariant and in this particular case of course the even if you sort of them as you sweep k or the q momentum vector the number of energy levels below the Fermi energy and number of energy levels above the Fermi energy they do not change and so the system remains

invariant under these symmetries and then what is the you know in other than that what remains invariant the Dirac points remain invariant in the sense that Dirac points can move in the Brillouin zone if you do something to the band structure but if you do not do any additional gap closing then the Dirac points will remain where they are or rather they will have zero band gap at the Dirac points okay. They may move in the Brillouin zone if you change the bands or rather you know deform the bands but the gap will not open okay.

One of the main things that is important in this particular case is that whether we can make graphene topological okay. Let me box this and why we are asking this question? We are asking this question based on a few hunches that we have or suspicion that we have and I will tell you what those suspicions are but can we make graphene like a quantum hall sample which had chiral edge states and so on that is the edge is behave completely differently than the bulk that is the bulk remains insulating and the edges conduct can we make graphene to have those kind of properties can it behave like a quantum hall sample which has sort of topological invariant as a Chern number and so on. So that question or rather this kind of hunches arise from the fact that the Berry phase in graphene is non-zero. So we have discussed Berry phase we know what Berry phase is just to remind you that okay.

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Berry Phase in graphene.

$$H(\lambda(t))$$

$$h(t) = \frac{1}{\sqrt{2}} e^{-iEt/\hbar} \begin{pmatrix} \cos \phi \\ \sin \phi \end{pmatrix} \quad (1)$$

$$\dot{h}(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} -\sin \phi \dot{\phi} \\ \cos \phi \dot{\phi} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i\dot{\phi} \\ i\dot{\phi} & 0 \end{pmatrix} h(t) \quad (2)$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} -\lambda & -i\dot{\phi} \\ i\dot{\phi} & -\lambda \end{pmatrix} h(t)$$

Eigenvalues are $\pm \frac{1}{2}$.

$e^{iE_F t/\hbar}$
 $e^{-iE_F t/\hbar}$

Just to remind you that if H the Hamiltonian of a system depends on some parameter λ and this λ depends on time and λ is a slow function of time say for example and then you change λ and you ask the question that after one complete oscillation in t that is t comes back to the same point after you know sort of full rotation whether the Hamiltonian comes back to the original configuration or rather it represents exactly the same system or there is a phase that it picks up and this phase is irreducible and this irreducibility actually is not the same as the dynamical phase that we are mostly familiar with that is exponential iEt/\hbar by H cross it is not that kind of a phase because that kind of a phase will not appear in observables because you will take a mod square and

exponential i e t by h cross and an exponential minus i e t by h cross will go away and will not have any phase information left and the time will also go away.

$$h(\vec{q}) = \vec{q} \cdot \vec{\sigma} \quad (\text{Equation 1})$$

$$\vec{q} = |\vec{q}| \begin{pmatrix} \cos \phi \\ \sin \phi \end{pmatrix} = q \begin{pmatrix} \cos \phi \\ \sin \phi \end{pmatrix} \quad (\text{Equation 2})$$

So is it like that or is there anything special about the Berry phase in graphene and it turns out that there is something that is interesting and which gives rise to the fact that we do have a reason to believe that graphene can become topological. So let us calculate the Berry phase in graphene. So let me take this Hamiltonian the low energy Hamiltonian to be h of Q which is let us call it a Q dot sigma I have taken sort of omitted the V f also it does not matter you can put it back if you are writing the full Hamiltonian with h cross V f and so on so forth. Because of this two dimensionality we can write Q in the polar coordinates so you can write this as a Q and then a cos phi and a sin phi. It is like Q x and Q y where Q x is equal to Q cos phi and Q sin phi and this is actually the magnitude of Q is let us just write it as simply as Q.

$$\begin{aligned} h(\vec{q}) &= q \begin{pmatrix} 0 & \cos \phi - i \sin \phi \\ \cos \phi + i \sin \phi & 0 \end{pmatrix} \\ &= q \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \\ &= q \begin{pmatrix} -\lambda & e^{-i\phi} \\ e^{i\phi} & -\lambda \end{pmatrix} \\ &E q^{\pm} = \pm q \end{aligned}$$

So this is the Q vector in this Hamiltonian that we have written let us call it equation number 1 and let us call it equation number 2 and phi is the polar angle that we consider in two dimension. So h of Q which is what we have written here is nothing but so now I will just add this Pauli matrices reminding you once again that they do not really express the spin degrees of freedom but rather they are the sub lattice degrees of freedom and this is like a cosine phi minus I sin phi coming from this one is coming from sigma x the first term and the second term is coming from sigma y. So cos phi plus I sin phi and a 0 and so this is the Hamiltonian it is a 2 by 2 Hamiltonian very easy to solve you can just solve it by putting the determinant equal to 0 and find out the eigenvalues and the eigenfunctions.

You can make further simplification in which you can write it as a Q 0 exponential $i\phi$ minus $i\phi$ exponential $i\phi$ and 0 and you can diagonalize it by just simply you know minus λ exponential minus $i\phi$ exponential $i\phi$ and a minus λ this will give you a Q and a minus λ etc. I mean so then you take the determinant equal to 0 and when you take the determinant equal to 0 this gives you the eigenvalues are plus minus Q . So let us call it a EQ plus minus is equal to plus minus Q . So this is the eigenvalues of this 2 by 2 matrix how about the eigenvectors the eigenvectors can also be found they are pretty simple I just write down the results but I am sure that you can do this.

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$$|\psi_{-}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-i\phi} \\ 1 \end{pmatrix}$$

$$|\psi_{+}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi} \\ 1 \end{pmatrix}$$

Berry Connection

$$\vec{A} = i \langle \psi_{-} | \frac{d}{d\phi} | \psi_{-} \rangle$$

(Taking Contribution from the filled band).

$$\frac{d}{d\phi} \begin{pmatrix} -e^{-i\phi} \\ 1 \end{pmatrix} = \begin{pmatrix} i e^{-i\phi} \\ 0 \end{pmatrix}$$

$$\vec{A} = \frac{i}{2} \begin{pmatrix} -e^{-i\phi} & 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} i e^{-i\phi} \\ 0 \end{pmatrix} = -\frac{i}{2} \begin{pmatrix} e^{-i\phi} & 1 \end{pmatrix} \begin{pmatrix} e^{i\phi} \\ 0 \end{pmatrix}$$

$$\vec{A} = -\frac{i}{2} \begin{pmatrix} 1 & e^{-i\phi} \end{pmatrix}$$

So the two eigenvectors corresponding to the plus and minus remember that there is there plus and minus signs. So let us call it a 3 so correspond to the plus sign and the minus sign the wave functions are written as like 1 by root 2 these are normalized and minus exponential minus $i\phi$ and 1 and ψ_{-} is equal to 1 by root 2 exponential $i\phi$ and 1 sorry this plus. So this corresponds to ψ_{-} and ψ_{+} they correspond to the wave function corresponding to the minus and the plus signs of the eigenvalues.

$$|\psi_{-}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix}$$

$$|\psi_{+}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi} \\ 1 \end{pmatrix}$$

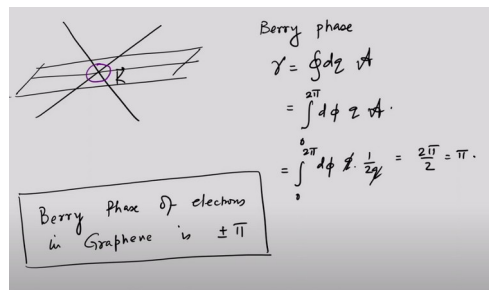
Let us now calculate the Berry connection and how is Berry connection defined we have defined this let us write it like this this is equal to i and a ψ_{-} and there is a Q and then there is a ψ_{-} and why minus because just to remind you that the Berry connection is calculated by taking the contribution only from the filled band. Let me write this alright so the filled band is the negative sign and which corresponds to the valence band so filled means the valence band ok. So the band which is lower here we are talking about the ones that are below the Fermi energy ok. So that is a filled band and

we are just talking about the filled band ok. So we can calculate the Berry connection now one has to remember that this has to be taken as a gradient with respect to the Q it is we are taken as cylindrical coordinate so it is a Q phi kind of space.

$$\begin{aligned}\vec{A} &= i \langle \psi_- | \vec{\nabla}_q | \psi_- \rangle \\ \vec{V}_q &= \left(\frac{\delta}{\delta q} \hat{q} + \frac{1}{q} \frac{\delta}{\delta \phi} \hat{\phi} \right) \\ \vec{A} &= \frac{i}{2} \begin{pmatrix} e^{-i\phi} & 1 \end{pmatrix} \frac{1}{q} \frac{\delta}{\delta \phi} \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix} = \frac{-i^2}{2} \begin{pmatrix} e^{-i\phi} & 1 \end{pmatrix} \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix} \\ \vec{A} &= \frac{1}{2a} \hat{\phi}\end{aligned}$$

So this is denoted by ∇_Q of Q cap plus 1 by Q ∇_ϕ of ϕ cap ok. Remember that in that sense this is actually a vector quantity and we should write it with a vector so ∇_Q is also a vector operator. Now you see that these ψ_- or ψ_+ we are essentially interested in ψ_- it does not depend upon Q it only depends upon ϕ thus this term will not be there the only term that will be present is 1 by Q ∇_ϕ of ϕ cap. So then this is equal to it is a i over 2, 2 coming from the normalization this 1 over root 2 here that will give rise to a factor of 2 here and then a minus exponential $i\phi$ I am taking the conjugate wave vector that is the bra of ψ_- and i and 1 by Q ∇_ϕ of exponential minus $i\phi$ and 1. So now I will have to take this so ∇_ϕ of exponential $i\phi$ you will get a minus i out and this the next one will be 0 so this is equal to i square divided by 2 so there is a exponential minus $i\phi$ 1 and this will be exponential $i\phi$ and 0 and this will give rise to I think I missed out a minus sign here and this will give rise to a 1 by 2 Q ϕ cap.

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Berry phase

$$\begin{aligned}\gamma &= \oint \vec{A} \cdot d\vec{r} \\ &= \int_0^{2\pi} d\phi \, 2 \cdot \frac{1}{2q} \\ &= \int_0^{2\pi} d\phi \, \frac{1}{2q} = \frac{2\pi}{2} = \pi.\end{aligned}$$

Berry phase of electrons in Graphene is $\pm \pi$

So this is the Berry connection for graphene and we are eventually interested in the Berry phase which is obtained from the Berry connection by taking a line integral of this Berry connection in the vicinity of the k point that is so suppose you have this as the one

of the k points say there is a k point and now so this is the Fermi energy ok. So now in this so this is like a 2D plane I am just drawing a plane and so the electron encircles this k point and whether it picks up a phase that is unusual or there is a finite Berry phase and that is what we want to find out and so the Berry phase that is γ this is equal to dQ because we are in the Q space we are in the low energy limit of the Hamiltonian. Now make sure that this calculation that we have done for the low energy Hamiltonian also holds for the full tight binding Hamiltonian which we have derived.

So we have initially derived the tight binding Hamiltonian and from there we have expanded the wave vectors in the vicinity of the Dirac points to get a low energy Hamiltonian but all these symmetry considerations or even calculation of the Berry phase or other things they all hold for the entire tight binding model. You might wonder that so the linearity is only in the vicinity of the Dirac point and but you know as we move away from the Dirac point the linearity sort of goes away this because of these cosine terms and so on and cosine and sine terms so it is not there. Now the analytic calculations are very easy in the low for the low energy Hamiltonian and that is why we are doing it for the low energy Hamiltonian nevertheless as I said that it also holds if you want to show the time reversal symmetry or the sub lattice symmetry inversion symmetry that is you can still show it with the full tight binding Hamiltonian.

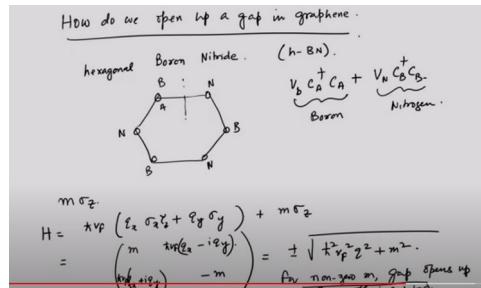
So we calculate the Berry phase here by taking a closed curve in the Q space in near the K point if you have noticed it we have taken this Hamiltonian in the vicinity of the K point so this is like because there is a sign that we have ignored here because there would have been a sign with the σ_x term that we have ignored and so this is at K point. If you do it at the K' point you would get results which is slightly different with some minus signs etcetera and that will also be discussed just in a moment.

So we calculate the Berry phase by taking the line integral of the Berry connection over a closed contour in the you know the Fermi plane about the Dirac point. So we are right now talking about the K Dirac point and this one is nothing but it is 0 to 2π and $d\phi$ and q a so just to remind you that dq is nothing but $q d\phi$ that is the polar angle converting into the polar angle so that the angular variables get integrated over 0 to 2π and so this is equal to 0 to 2π and $d\phi$ and q and a is nothing but $1/2q$ from the last so this $1/2q$ in the ϕ direction and so this will sort of go away and you get a 2π over 2 this is equal to π .

So the Berry phase of electrons in graphene is π but then if you would have done the same calculation at the K' point you would have got a minus π . So this is really a plus and minus π and this is another reason for suspecting that one can actually make graphene topological and that would have to be seen. So what we mean by topological is that we will have to open up a gap at the Dirac points but nevertheless there will be chiral edge modes so there will be modes energy modes or energy states that will traverse

across the Fermi surface and will give rise to conductivity. So if you take a strip of graphene it will look different in the bulk of the sample that is it will look insulating or rather it will have insulating properties but it will have only conducting properties at the edges. So the gap will open up so the bulk will have a gap but there will be conduction that is electronic states will be able to conduct through the edge modes and this is exactly the picture that we have presented earlier in the context of quantum Hall samples.

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So this is the Berry phase comes out as you know sort of plus minus pi because of this of course the Berry curvature which is usually defined by something like this is equal to curl of A which is equal to 0 because A is like 1 over 2q phi cap direction so if you take this curl in the polar coordinates you will see that this is equal to 0 and the Chern number automatically vanishes for graphene and because Chern number is actually this F into the D2k over the surface and this is equal to 0 because the Berry curvature vanishes. Now Chern number is equal to 0 is not a surprising result because you need to have broken time reversal symmetry in order to have a finite Chern number however we have shown that of course that is not the case we have time reversal symmetry for graphene and that is why the Chern number becomes equal to 0.

Now the question is the if you look at this Hamiltonian let us look at this Hamiltonian you see these the diagonal terms that are 0 and this is one of the reasons that there is 0 gap at the band gap at the Dirac points if you put a term there that is if you put a non-zero term there that is if there is a sigma z as well then the gap will open up. So the question is that is there only one way of opening up that gap we have two symmetries remember that which protect the Dirac points which we have said one of them is the inversion of the sub lattice symmetry and another one is the time reversal symmetry. So we can actually put a little bit of so let us go back to that picture that we have drawn here and both are carbon atoms but say for some reason we give a small bit of potential here and give a slightly different potential at this sides in which case these carbon atoms are not equivalent and one of the examples that we have is called as the hexagonal boron nitride.

Let me put a title here so how do we open up a gap in graphene. So let us talk about the hexagonal boron nitride and it is written with a symbol HbN in which case it has exactly the same structure excepting that these are not carbon atoms but one of them is boron nitrogen boron nitrogen boron nitrogen and so on it is a hexagonal structure nevertheless and now this sub lattice symmetry is gone which means that there are different potentials so onsite energies are different and if we want to write down a Hamiltonian will have terms such as say for example some potential corresponding to the boron site and let us call it as A sub lattice so it is like so I will write this boron with a small b because A and B will otherwise will have difficulty in understanding so it is a Ca dagger Ca and VN CB dagger CB.

$$H = \hbar v_F (q_x \sigma_x \tau_z + q_y \sigma_y) + m \sigma_z$$

$$= \begin{pmatrix} m & \hbar v_F (q_x - i q_y) \\ \hbar v_F (q_x + i q_y) & -m \end{pmatrix} = \pm \sqrt{\hbar^2 v_F^2 q^2 + m^2}$$

So this is the boron energy onsite energy and this is the nitrogen energy. What we really mean is that we can introduce a M sigma Z in the Hamiltonian what is M sigma Z the M sigma Z is in addition to your term which is like h cross VF qx sigma x plus a qy sigma y you can put a gamma Z here just to make sure that we write down the Hamiltonian in the most compact form for both K and K prime. So now we add a M sigma Z where M is a mass okay I mean which comes from the onsite potential and it has just for our convenience that it has a positive sign at A sub lattice and a negative sign at the B sub lattice.

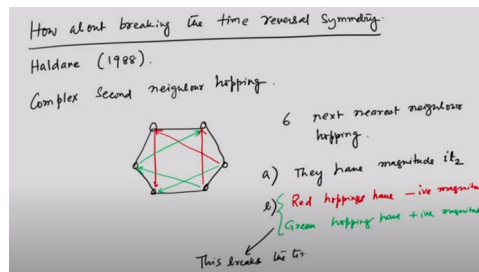
Now if we solve this Hamiltonian it is again a 2 by 2 Hamiltonian there is no problem in solving it now you will have a form which is h cross VF and then you have a term which is like a M and now we have a qx and so this is equal to a qx minus i qy and a qx plus i qy and a minus M and that Hamiltonian if you wish to solve of course this h cross VF let us put that equal to 1 at this moment because otherwise you know you will have to write h cross VF here that is also okay and h cross VF here so let us write that h cross VF and then there are M and minus M. If you solve this Hamiltonian you get eigenvalues that are given by plus minus h cross square VF square q square plus a M square okay. Now at q equal to 0 where the Dirac points exist now there is a gap that opens up and gap opening up really does not mean anything in the sense that as M increases the magnitude of the gap goes up at q equal to 0 that is at the Dirac points both at k and k prime you will have a gap that opens up.

Now opening up of this gap can be shown that it does not correspond to any topological insulator in fact it has a name called as a Semenov insulator. So for non-zero M gap

opens up and this is called a Semenov insulator okay which means that this insulator does not have any topological property and it acts like a band insulator.

Band insulator means just a normal insulator which is gapped and there are no counter propagating edge modes or there are no modes that are at the edges which behave differently than the bulk and this is a Semenov insulator. Now we have one more card in our hand we have tried breaking the sub lattice symmetry and we fail to get a topological insulator but then we also have a time reversal symmetry. If we break that can the system become a topological insulator okay.

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So let us ask this question how about breaking the time reversal symmetry? Well there are probably other ways of breaking the time reversal symmetry such as using a magnetic field which we have seen the magnetic field automatically breaks the time reversal symmetry. However Duncan Holden in a paper in 1988 it is a physical review letters paper in which he talked about a complex second neighbour hopping.

What is a complex second neighbour hopping? So he considered this graphene unit cell once again and so these are the carbon atoms and by the way this paper was written month before graphene was discovered. So it was honeycomb lattice which was taken as a model for breaking the time reversal symmetry and he wanted to say that if you break the time reversal symmetry there will be Hall effect quantized Hall effect not the one that you get in presence of a magnetic field. So this is called as the anomalous quantum Hall effect okay. So let me sort of show what kind of second neighbour hopping. There comes special kind of hopping so these ones that I am it is a second neighbour it is not a first neighbour the first neighbours are belonging to the other sub lattice.

So this is a neighbour which is a distant neighbour and it corresponds to hopping from A sub lattice to A sub lattice. Now you understand that when we write down the Hamiltonian in the sub lattice basis this will be in the diagonal term. So even though breaking the sub lattice symmetry or the inversion symmetry by putting a m term in the diagonal elements it did not do anything significant but these ones also will sit on the

diagonal element of the 2 by 2 Dirac Hamiltonian and let us see what it does it is not a priori clear what will happen but so this is okay. So these are 3 next nearest neighbour hopping I will draw the other 3 by another colour and there is a particular reason that I am doing it.

So this is 1 this is 1 and this is 1. So there are 6 next nearest neighbour hopping which have 2 characteristics one of them is that they have magnitude complex magnitude let us call this as $i t_2$, 2 for second neighbour and the i is a complex number root over minus 1 okay and B the red ones red one red hopping which are say anti-clockwise red hoppings have hoppings have negative magnitude that is minus $i t_2$ and green, green hoppings have positive magnitude or vice versa it does not matter but this is we can follow these convention and what happens is that this breaks the time reversal symmetry okay.

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The image shows handwritten mathematical expressions. At the top left, the vector current density is given as $\vec{j}(\vec{r}) = \frac{-ie\hbar}{2m} [\psi^* \nabla \psi - \psi \nabla \psi^*]$. To its right, the finite difference approximation of the derivative is shown: $\frac{df}{dx} \approx \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$. Below these, the discrete lattice current is expressed as $\frac{df}{dx} = \frac{f_{m+1} - f_{m-1}}{2a}$ and $\vec{j} = it_2 \sum_{\eta} (c_{i+\eta}^\dagger c_i - c_i^\dagger c_{i+\eta})$. Underneath the summation index η , arrows point to labels: 'next' for $\eta = a$, 'nearest' for $\eta = \pm a/2$, 'next-nearest' for $\eta = \pm a$, and 'next-nearest-nearest' for $\eta = \pm 3a/2$.

Let me just show very briefly why it does and how it does so if you remember that current is written as current is of course a vector which is written as minus $i e \hbar$ cross by $2 m$ or you can write it $e \hbar$ cross by $2 m i$ is the electronic charge and it is a ψ star del ψ minus ψ del ψ star okay that is the definition of current in quantum mechanical current and we have seen this in the context of equation of continuity where you know the divergence of j and this the time evolution of the probability density are related and they are related by the Schrodinger equation.

$$\vec{j}(\vec{r}) = \frac{-ie\hbar}{2m} [\psi^* \nabla \psi - \psi \nabla \psi^*]$$

$$\frac{\delta f}{\delta x} = \frac{f_{m+1} - f_{m-1}}{2a}$$

$$\vec{j} = it_2 \sum_{\eta} (c_{i+\eta}^\dagger c_i - c_i^\dagger c_{i+\eta})$$

And now this is like taking a gradient as you see that these are taking the gradient and gradient means that we talk about in a 1D sense these gradients can be replaced by these derivatives which can be written as you know $\frac{df}{dx}$ so say f is a function of x is like $f(m+1)$ I am writing it in discrete on a lattice so this is equal to $f(m-1)$ divided by $2a$ where a is the lattice spacing this is like a derivative which is written in a discrete notation so if you are making a particle hop from one to another then say m denote the site indices and so the particle will have to hop from $m+1$ to $m-1$ and then the derivative is actually divided by $2a$ there is of course a limit this comes from this $\frac{df}{dx}$ or $\frac{df}{dx} = \frac{f(x+h) - f(x-h)}{2h}$ limit $h \rightarrow 0$ okay.

So, these are we discretize derivatives and I am just written instead of this formula I have written a 2 point formula that is hopping from $m+1$ to $m-1$ and so on. So, if you apply that then the current operator in on a lattice is written as $\frac{it}{2} (c_{i+1}^\dagger c_i - c_i^\dagger c_{i+1})$ and so on okay. So, because of this negative sign there the time reversal symmetry is broken and so deliberately Holden assumed that there is a chiral hopping to the next neighbors chiral means that there is a direction dependent hopping the green ones and the red ones have different signs which means that the clockwise hopping have one sign and the anti-clockwise hopping of another sign at that breaks the time reversal symmetry of the Hamiltonian and these η are nothing, but the next nearest neighbors.

So, let me stop here for now and we will show that how these time reversals symmetry breaking second neighbor complex second neighbor chiral hoppings give rise to a new topological state in graphene and that is known as the Holden model okay and one will have the hall effect because the time reversal symmetry is broken and the Chern number will be non-zero however, there will be no Landau levels. In fact, the paper of Holden in 1988 it clearly says that there will be it is I mean hall effect without Landau levels okay and we will call it as an anomalous quantum Hall effect stop here and we carry on with the discussion of Holden model. Thank you.