Quantum Hall Effect
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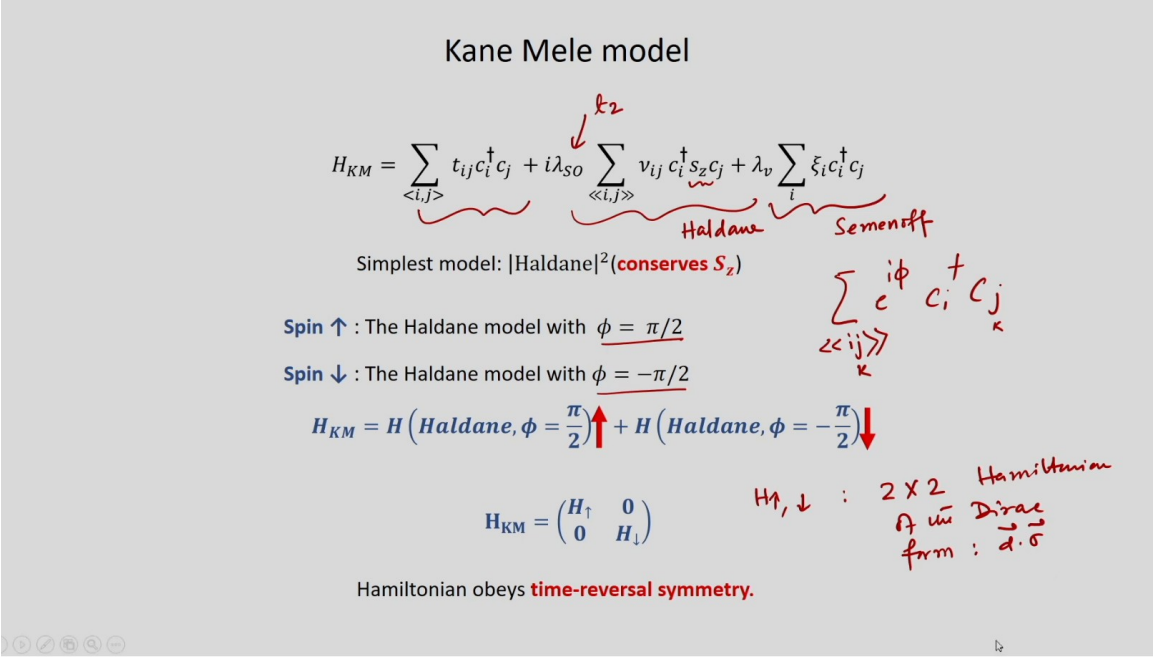
Week-08
Lec 18: Kane-Mele Model

So, in the last class we have talked about the Kane-Mele model, but I have gone a little fast there in order to you know finish up the calculation of the Z2 invariant which we have done it quite extensively. So, right now we will rerun some of the discussions that we already had and talk about the model a little more and show some of the results that we can get from the model okay. So, we start with this again with the Kane-Mele Hamiltonian, I have already told that there are certain features that are distinct from the Holden model and will again come to that in just a while. So, the first term is the first term is the tight binding term which is there in graphene, this is the really the Holden term and I have said this that you can use either a t2 or a lambda SO there mostly in literature it is used as lambda SO. So, I have written it as lambda SO and this is the Semenov term which opens up a gap of trivial nature at the Dirac points okay. So, it is a simple model which is two copies of the Holden model and that is why it is written as Holden square and it conserves the S z component or z component of the spin angular momentum and I have written it with a capital S z, but sometimes in literature it is written with a small sz.

So, here S z denotes the z component of the true spin or the actual electronic spin. So, this has been told that the spin up the up spin particles which correspond to a Holden model with a flux phi equal to pi by 2. You remember the flux comes from these the second neighbor hopping which is exponential i phi and then of course, one has a c i dagger c j. Now this is a second neighbor.

So, we write it with a i j or you can write it just in case you are not comfortable with i j because that is used for the nearest neighbor as we have done it for the first term you can use a i k also. So, instead of a j one can use a k just to make sure that that is the next nearest neighbor and not the nearest neighbor. We have shown this picture many times and similarly for the spin down electrons it is another Holden model and with us this flux equal to minus pi by 2. So, there is a flux pi by 2 for the up spin and minus pi by 2 for the down spin and there is exactly what is written here and it takes a block diagonal term where the upper block on the left is for the up spin and for the lower block down spin each one of them each of H up and H down like a 2 by 2 Hamiltonian of the Dirac form.

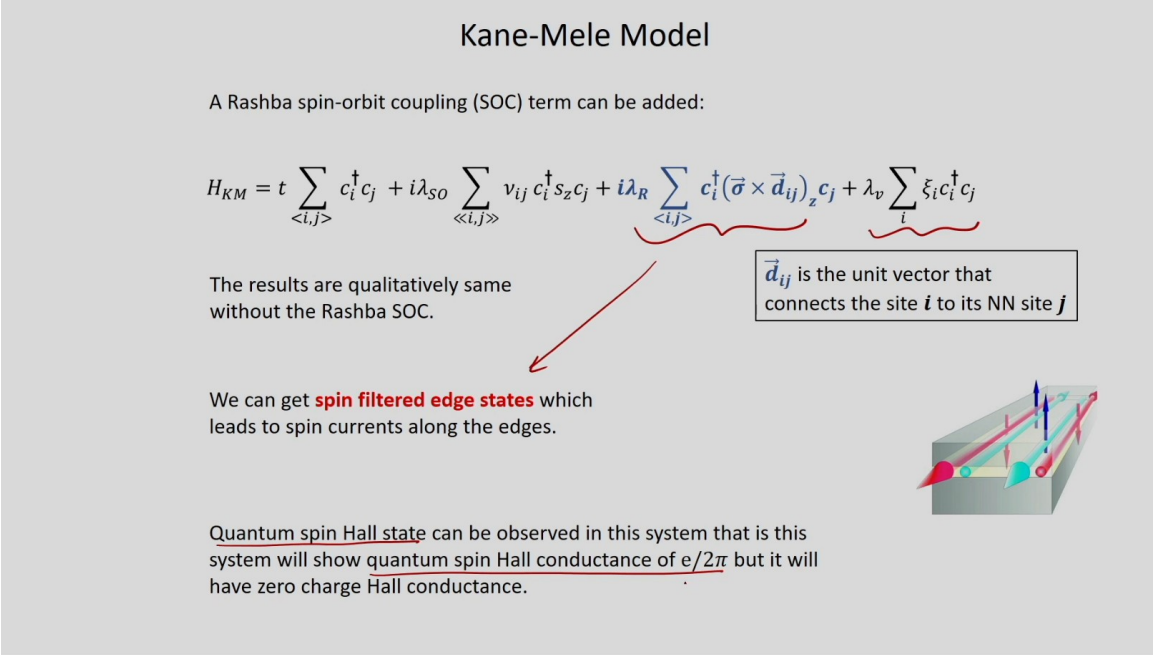
What I mean by Dirac form is that it can be written as d dot sigma and the Hamiltonian has time reversal symmetry now which we have discussed elaborately.



Now, there is another term that is added which is called as a Rashba spin orbit coupling we will do a little discussion on that in just a while and the term is written as i lambda r and there is a c i dagger and these sigma cross d i j will tell you what d i j is d i j is actually a unit vector that connects to the site from site i to a nearest neighbor site j and of course, the rest of the things are all same. Now, this creates one complication additional complication which is what we have seen here the Hamiltonian no longer remains as block diagonal as you can see here. There are off diagonal elements in this 4 by 4 Hamiltonian that arise and it does not have this you know block structure that you see here okay. Now, how do I get this term and you know how this thing comes into picture is what we will see and so, some of the results are same with and without the Rashba spin orbit coupling though they are quantitatively different and we will have large application in terms of spintronics if we apply or rather include this term and as I said earlier this term is quite possible in a 2 dimensional perfectly 2 dimensional system which our graphene is because there is an inversion symmetry breaking happening there which will give rise to an electric field and this the spin will couple to the electric field and so on okay. We will just come to that in just a while.

And we get spin filtered 8 states because of this term that we see here and there are the spin current that will be there and one gets a quantum spin Hall phase which is observed

in the system and there is a quantized Hall conductance in the spin sector which we call it as quantum spin Hall conductance as opposed to the charge Hall conductance which is equal to 0 here. It is 0 because the system has time reversal symmetry and we have shown that how the system has time reversal symmetry earlier. So, the spin Hall conductance is quantized at a value which is E over 2 pi. Let me try to derive this term that you see here the lambda r term and this is like how this sigma cross d i j and the z component of that come is what is important. I mean you have to take a note of this z component because we are writing a Hamiltonian whose eigenvalues will give energies.



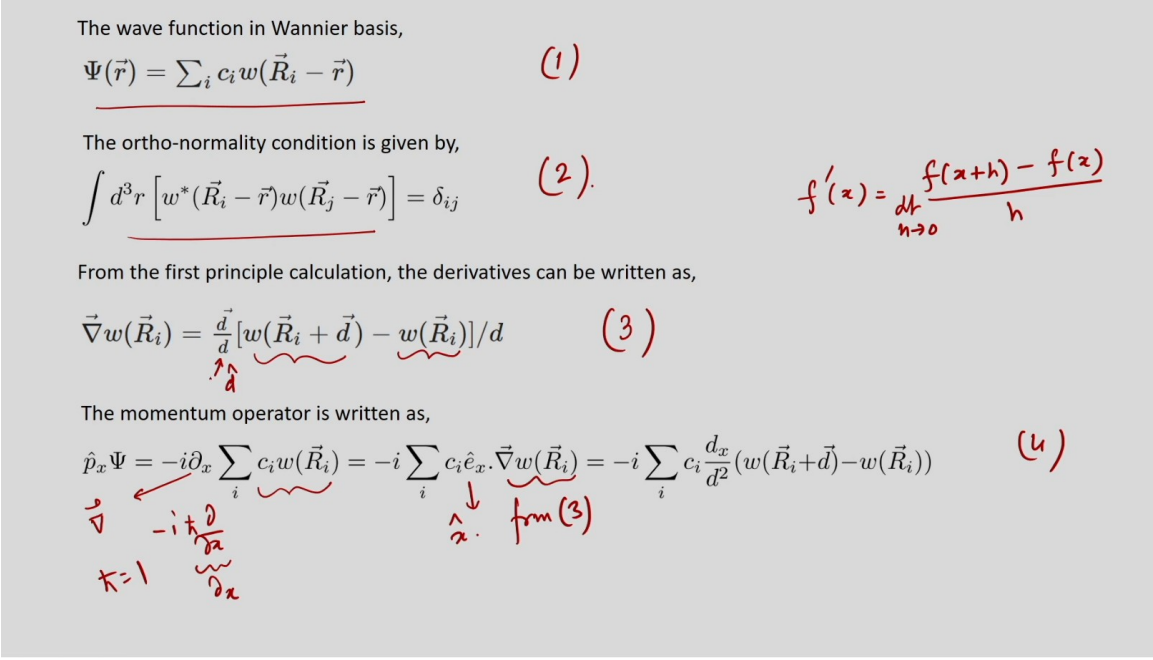
So, it cannot be just a vector. So, it will have a scalar and that z component makes it a scalar. So, we write down the wave function in the Wannier basis and the wave function is of this form where these c i s are the operators and these w s are the Wannier wave functions and the Wannier functions are localized at some sites which are given by this r i. These obey the orthonormality condition which is given by this equation. Let us call this as equation 1 and this as equation 2.

So, it is clear that it is w star which is a Wannier function r i minus r and the r j minus r where i and j are different sites will be equal to 0 and if i and j are same then that will lead to the normalization of the Wannier functions. Now, this is well known that when you want to write derivatives on a lattice one does it like this that. So, it is a f prime of x is equal to f of x plus h minus f of x divided by h and limit h tends to 0 that is the definition that we have learned probably in school. So, there is these Wannier functions

which are written at r i plus d site where d is the nearest neighbor site and taken a subtracted the Wannier function at the ith site and then because it is a gradient. So, it should have a direction.

So, this is that a d cap direction that is shown and divided by the d which is the length of the nearest neighbor vector or the distance nearest neighbor distance. So, because gradient is a vector so, thus this d cap which is in the direction connecting the two sites r i and r i plus d that is shown here. So, this is the definition of momentum or a gradient of a scalar function. Now, why is that required that is required because we need to write down the momentum the operation of the momentum on the wave function and this momentum is written as minus i h cross del del x. So, for del del x there is a shorthand notation which is del of x and we have taken h cross equal to 1 without any loss of generality and this is equal to a c i and w r i where c i is a is an operator at the site i and that is the Wannier function.

So, this can be written as minus i and then now you apply the gradient operator just from this equation 3 let us call that as equation 4. So, we apply the same thing. So, del del x is nothing, but say something like a gradient vector and this gradient is written as x cap dot you know the gradient of w at r i. Now this we already know from 3 and that can be expanded now since we have a x cap here you can write it as x cap as well. So, this is equal to dx by d square and so on okay.



So, that is exactly what we have done now this is no longer a vector this quantity because you have dotted with a x cap direction and this x cap comes because we have taken a p x it will be p y will get a y cap here. So, what we land up with is an operator and then this dx over d square and these the Wannier functions at the or the difference between the Wannier functions at the consecutive or the nearest neighbor sites. So, we are ultimately you know interested in a quantity like this which is psi dagger p x psi and that is because that would you know be there in this kind of a term. So, we are sort of trying to get that here. Now ultimately this will be related to the to the form that we just got and then we write down if you look at it carefully it is pretty easy.

So, this is that c i dagger c j coming from the dagger is coming from psi dagger and c j is coming from psi and then the p x operator is written here exactly in the same way that we have done it in equation 4 let us call this as equation 5. So, now because of the orthonormality condition that is this and this will only survive you know provided D connects to the nearest neighbor and this with this will give you a 0 because that is the orthonormality coming if i is not equal to j and of course, i is not equal to j. So, this left hand side that we have in equation 5 has a form which is nothing, but this 6 where this W star r i and W r j plus D will give you 1 because of the normalization where D connects to the neighboring sites and so on. So, this is a c i dagger c j and then the d x by d square and the volume integral over r goes on to make up for the orthonormality condition. And similarly for p y 1 gets this exactly the same let us write it as 7 and then we have a d x over d square and a d y over d square and so, this is p x and p y that one gets here.

Therefore,

$$\int d^3r \left[\Psi^\dagger(\vec{r})\hat{p}_x\Psi(\vec{r})\right] = -i\sum_{i,j} c_i^\dagger c_j \int d^3r \frac{d_x}{d^2}\left[w^*(\vec{R}_i)\{w(\vec{R}_j+\vec{d}) - w(\vec{R}_j)\}\right] \quad (5)$$

Because of the ortho-normality condition, only the contribution comes from $\overrightarrow{R_j} = \overrightarrow{R_i} + \vec{d}$.
The summation is reduced to the summation over i only along with its nearest neighbour.

Therefore we get,

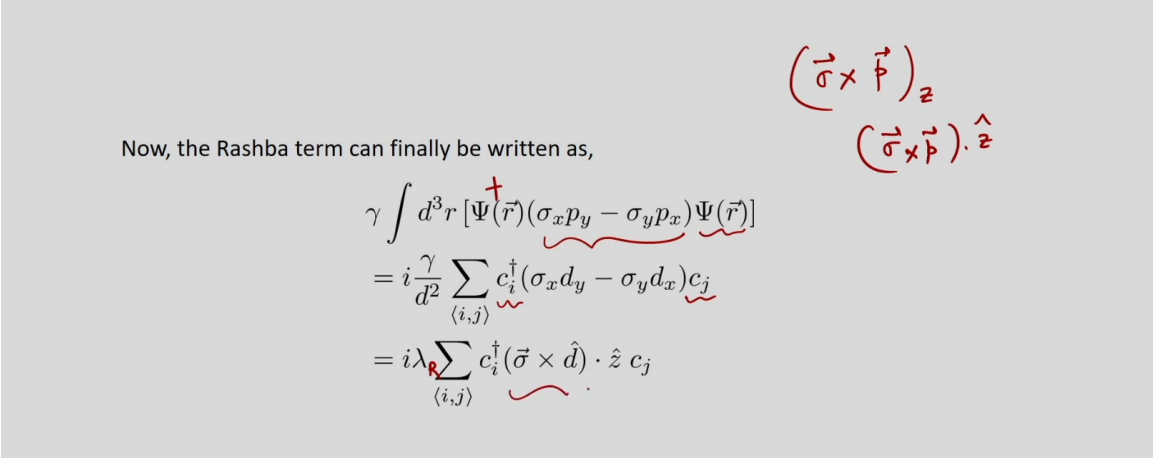
$$\int d^3r \left[\Psi^\dagger(\vec{r})\hat{p}_x\Psi(\vec{r})\right] = -i\sum_{\langle i,j\rangle} c_i^\dagger c_j \frac{d_x}{d^2} \quad (6)$$

Similarly for $\hat{p}_y$, one can get

$$\int d^3r \left[\Psi^\dagger(\vec{r})\hat{p}_y\Psi(\vec{r})\right] = -i\sum_{\langle i,j\rangle} c_i^\dagger c_j \frac{d_y}{d^2} \quad (7)$$

And of course, you do not see any p x and p y here, but then we will show that this is really coming out from a term like that okay. So, this is 6 and 7 make up for the 2 equations that we need for these the expectation values of p x and p y. Now, this you know that the Rasbha term is written as sigma x p y minus sigma y p x okay. This is basically the sigma cross p and the z component of that or you dotted with the with the z okay. And the z is nothing, but we will tell you in a moment that it is nothing, but the electric field direction of the electric field which occurs or other which arises because of there is a gradient of the crystal potential okay.

So, now, with all these things we have a there is a dagger that is missed here. So, psi dagger and so on this sigma x p y minus sigma y p x which is nothing, but sigma cross p the z component of that and a psi r. So, we get a c i dagger and a c j coming out from this and then a sigma x d y minus a sigma y d x exactly coming out from this and there is of course, a d square that comes out okay. And there is a i factor there and this gamma is simply nothing, but either you call it a lambda r or something, but lambda r we are going to get it here. So, we sort of wrote a constant a coefficient of this Rasbha term and this is nothing, but what we want okay.



So, the Rasbha term indeed has a form. So, this one is what you start with and then you end up with a term that is like this and this is exactly what is written here okay. This one needed a little bit of hand holding in order to derive this form, but I sort of wanted not to you know break the flow in calculation of the Z 2 invariant which is why I skipped it there, but now you have it here okay. And this has already been shown that the in the momentum space the Hamiltonian is written as this. Now we of course, do not have a block form this is a block here, this is a block here, but the blocks are being mixed by these off diagonal forms which are written in terms of rho k and the rho k if you look at it here it is purely coming out from the Rasbha term okay and this is a little lengthy derivation, but one should be able to do it without much problem because one just needs to Fourier transform each one of the terms that we have written in the Hamiltonian that we have written here okay.

So, this Hamiltonian so, this is the most important equation and let us call it as a capital 1 okay. And so, this is by Fourier transforming in that capital 1 okay. And the various other things which are there written here which is a xi k or some this is that thing that is coming out here that is here and the gamma k is also there which are part of the this is that nothing, but the T 2 the Holden term. So, it is a spin full Holden term here and the kinetic energy term which is there in graphene is the tight binding kinetic energy that is given by the xi k gamma k and rho k and this is the 4 by 4 Hamiltonian. You remember the Holden model was 2 by 2 because the spin was not taken into account it was only the sub lattice degrees of freedom and here of course, we have taken into account spin and that is why the size of the Hamiltonian now have gone up and it has become 4 by 4.

Kane-Mele Model

The momentum space Hamiltonian is given by,

By fourier transforming Eq. I.

$$H(\mathbf{k}) = \begin{pmatrix} \gamma(\mathbf{k}) + \lambda_v & \zeta(\mathbf{k}) & 0 & \rho(\mathbf{k}) \\ \zeta^*(\mathbf{k}) & -\gamma(\mathbf{k}) - \lambda_v & -\rho(-\mathbf{k}) & 0 \\ 0 & -\rho^*(-\mathbf{k}) & -\gamma(\mathbf{k}) + \lambda_v & \zeta(\mathbf{k}) \\ \rho^*(\mathbf{k}) & 0 & \zeta^*(\mathbf{k}) & \gamma(\mathbf{k}) - \lambda_v \end{pmatrix}$$

Where,

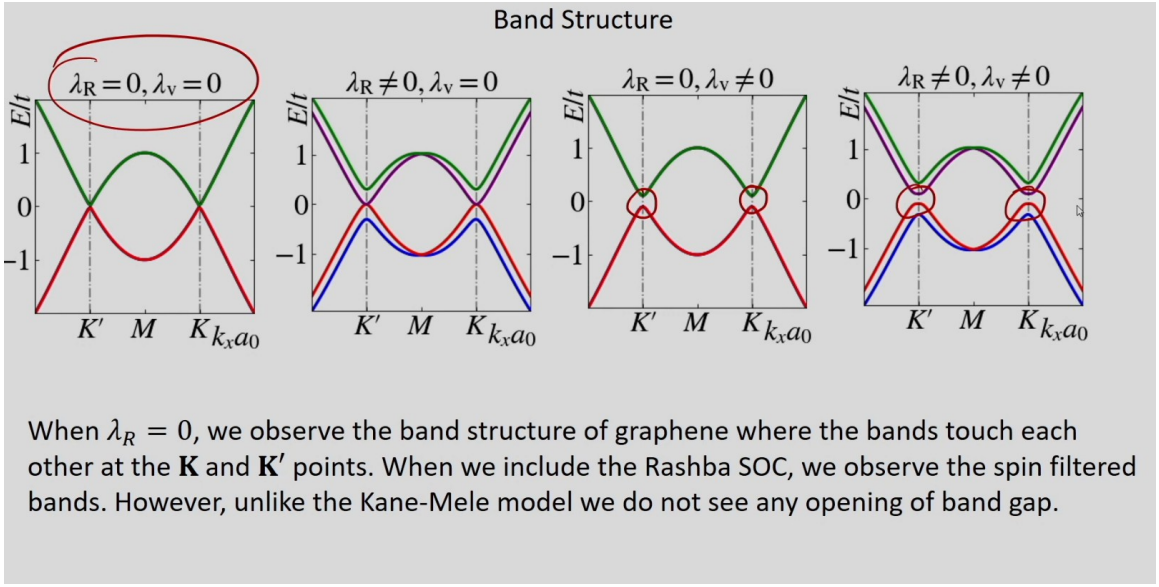
$$\zeta(\mathbf{k}) = te^{-ik_y a} + 2te^{\frac{ik_y a}{2}} \cos\frac{\sqrt{3}k_x a}{2},$$

$$\gamma(\mathbf{k}) = 2\lambda_{SO}\left[2\sin\frac{\sqrt{3}k_x a}{2}\cos\frac{3k_y a}{2} - \sin\sqrt{3}k_x a\right],$$

and

$$\rho(\mathbf{k}) = i\lambda_R\left[e^{-ik_y a} + e^{\frac{ik_y a}{2}} 2\cos\left(\frac{\sqrt{3}k_x a}{2} + \frac{\pi}{3}\right)\right]$$

And these are some of the band structure plots of these so, once when some diagonalizes this Hamiltonian which can be done in a computer and then one get for various parameters. Now, you see that we have shown it explicitly for a few parameters which are given by lambda r equal to 0 lambda v equal to 0 which means it is only the graphene thing and there is no lambda r or lambda v and then one has sort of touching direct points here and once when one switches on a lambda r then there is the band still touch, but the conduction band and the valence band they become spin resolved. So, the ones that you are seeing in blue and red are spin resolved valence bands and these pink or something magenta and the green they correspond to the conduction bands spin resolved conduction bands when you put lambda v equal to 0, but lambda r not equal to 0 a trivial gap opens up at the direct points which is a known result. Now, if you have both not equal to 0 that is the Rashba term as well as the Semenov term not equal to 0 there is a gap as well as the spin split bands can be seen okay. This is exactly what is written there. So, these are numerical calculations that are emerging out from this dispersion or this Hamiltonian that comes out here okay.



When $\lambda_R = 0$, we observe the band structure of graphene where the bands touch each other at the **K** and **K′** points. When we include the Rashba SOC, we observe the spin filtered bands. However, unlike the Kane-Mele model we do not see any opening of band gap.

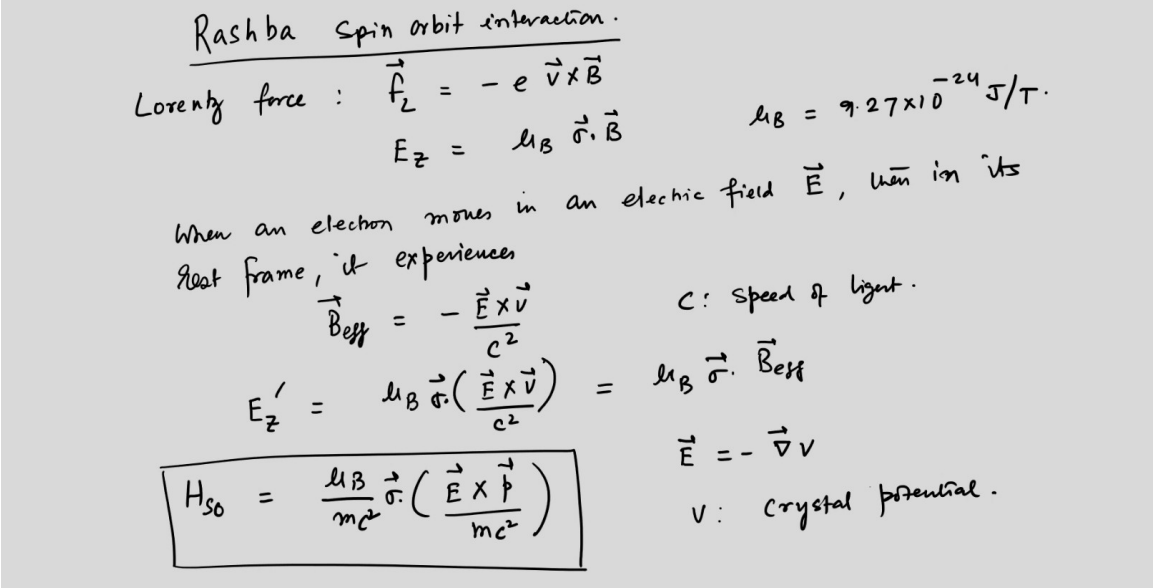
Let me do a little discussion on the Rashba term okay. A brief discussion has already been done this is little more to supplement that and so on. So, when you have a charged particle with a velocity v moving the velocity v in a magnetic in a region where there is a magnetic field B there is a low range force on the charged particle. So, the low range force is given by f L and which is equal to a minus V e V cross B.

So, V is the velocity and B is the magnetic field and because it also has spin which is now we have to necessarily include spin in our discussion there is also a Zeeman energy which is given by let us call it a e z and which is equal to a mu B sigma dot B okay. There is of course, one is force the other is energy. So, this is what we are writing and then mu B is called as a Bohr magneton which has a value 9.27 into 10 to the power minus 24 joule per Tesla okay. So, now when the electron is subjected to an electric field then in the rest frame of the electric of the electron it experiences a magnetic field.

So, let me write that in its rest frame it experiences an effective magnetic field a B effective which is given by minus e cross v divided by c square where c is the speed of light. This is electrodynamics you can check Griffith's book. So, that is the effective magnetic field that it experiences and this gives you an a net you know a Zeeman energy which is given by a mu B e cross v divided by c square dot sigma. So, its B dot sigma or sigma dot B does not matter I mean you can write it. So, this is the so, its sigma dot B which is nothing, but so, this is like mu B sigma dot B effective and B effective appears just on the step above.

So, this e z prime is nothing, but the spin orbit coupling term and we can write down if

we write it down in terms of operators then this spin orbit term is written as a mu B over m c square e cross. Now I make this v as p divided by m and this is written as m c square and there is a sigma dot there okay. So, this is the spin orbit coupling term that we are interested in and you will see that the Rashba term looks very similar to that and what is the origin of e in crystal lattice. So, e is originated by the crystal potential which is given by minus e equal to minus gradient of v where v is the crystal potential which is present due to the presence of ionic crystals or ionic sites and so on. Now what happens is that if you have a purely two dimensional sample which are graphene is then your e becomes in the direction of z cap okay.



So, its in the direction of z cap this yields a form for the HSO as say we write it with the alpha r by h cross and then there is a z cap across p dot sigma I have changed the order of this e and which I have been you know doing it. So, sigma dot this term or this term dot sigma it really does not matter. So, this is a z cap cross p dot sigma and then all these other things like mc square etcetera they are being absorbed here. So, alpha r by h is you know it replaces this mu b e z divided by mc square which are scalar quantities okay. So, the spin orbit coupling takes this form which is z cap is the direction unit vector in the z direction which is perpendicular to the 2D plane and this is crossed with the momentum and dotted with the electronic spin.

So, here make no mistake that we are really talking about spin by sigma usually when we write the graphene Hamiltonian we denote sigma to represent the sub lattice degrees of freedom, but this is a real spin okay. You know so, there are this alpha r is actually measurable and can also be enhanced by using gate voltage and various kinds of other

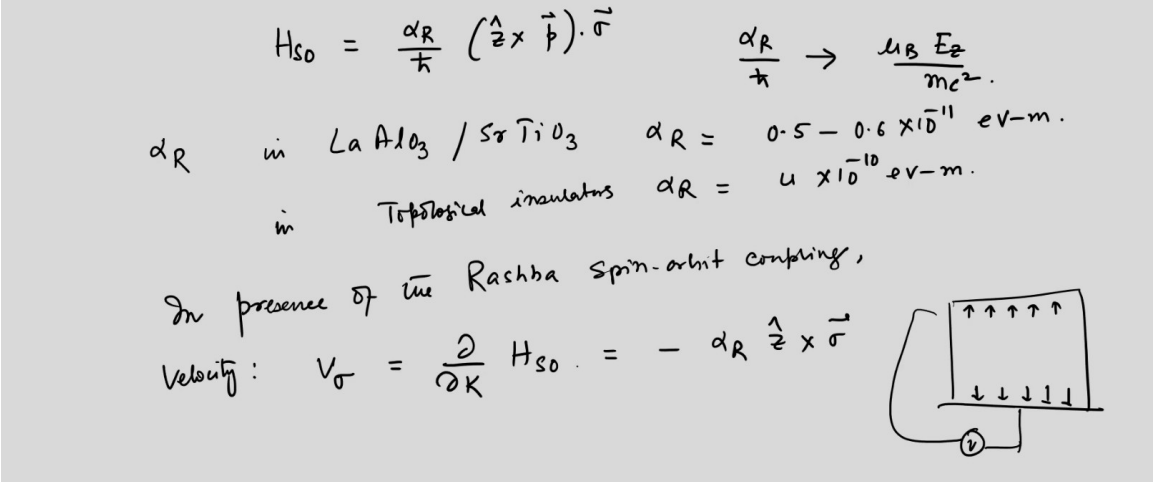
things such as heavy adder terms like gold etcetera in a graphene matrix, but I will not go into details of that. So, typical values of alpha r in these LaAlO 3 these are interface of this hetero structures SrTiO 3 etcetera this has a value it is about 0.5 to 0.6 into 10 to the power minus 11 eV m whereas, for some of the topological insulators alpha is typically 1 or 2 orders of magnitude large and it can have a value which is 10 to the power minus 10 eV meter and this can be further enhanced by using external means will not go into that, but how is this relevant for us why we are talking about it why we want to include an additional term as I said that this additional term obeys the time reversal symmetry or rather all the symmetries that graphene has.

So, if we add a term which does not violate any of the parent symmetries of graphene then it might as well be there okay. It unfortunately turns out that the magnitude of the spin orbit coupling or that alpha r or the strength of the spin orbit coupling in graphene is quite small it is of the order of a few m eV. However, it is still has a fundamental importance in this study of quantum spin Hall insulators and the study of spintronics which could be you know next generation devices for with replacing the electronic devices. For a number of reasons which I do not want to elaborate here, but one of them is that the spins do not undergo joule heating it is not scattered by impurities and so on and hence they could be you know potential candidates for doing a device making okay spintronic device making. So, what happens is that in presence of the spin Rashba term the velocity of the electrons becomes spin dependent at they are given by so this velocity and I write it with a subscript sigma because now it means that it is a spin dependent velocity which means that the up spin electrons will have a different velocity than the down spin electron.

This was not the case earlier where the Hamiltonian etcetera everything was spin independent as if we are talking about spin polarized that is spin does not enter into the discussion. Now that is not the case. So, this is equal to it is proportional to say a del del k of this Rashba term let us write it okay. We are writing it with a SO. So, let me write it with a SO and this is nothing, but this is equal to some alpha r z cap cross sigma and now you see that why I wrote it with v sigma because there is a sigma there and so on and this will give you different velocities to different spin components that is up spin and down spin component.

So, it is pretty much like you know the Magnus force that one sees in a classical spinning object where there is an effective force on that on there is a and that in this particular case would make these ups and down spin electron separate their ways in terms of you know when they move in a system they will sort of go in different directions and that will create a spin current or spin polarized current which depends on spin. So, there will be up spin and down spin will be segregated and also will give rise to a spin sort of voltage and this called as a spin Hall voltage because it is not in the

direction of the current of the electric field is perpendicular to that and one has what I am trying to say is that. So, here you will have up spin say for example and you will have down spin there and so there is a spin Hall voltage. So, if you calculate a voltage between this and so on. So, this there will be a spin Hall voltage and this spin Hall voltage can be if it is the magnitude is considerable it can contribute to spintronics okay.

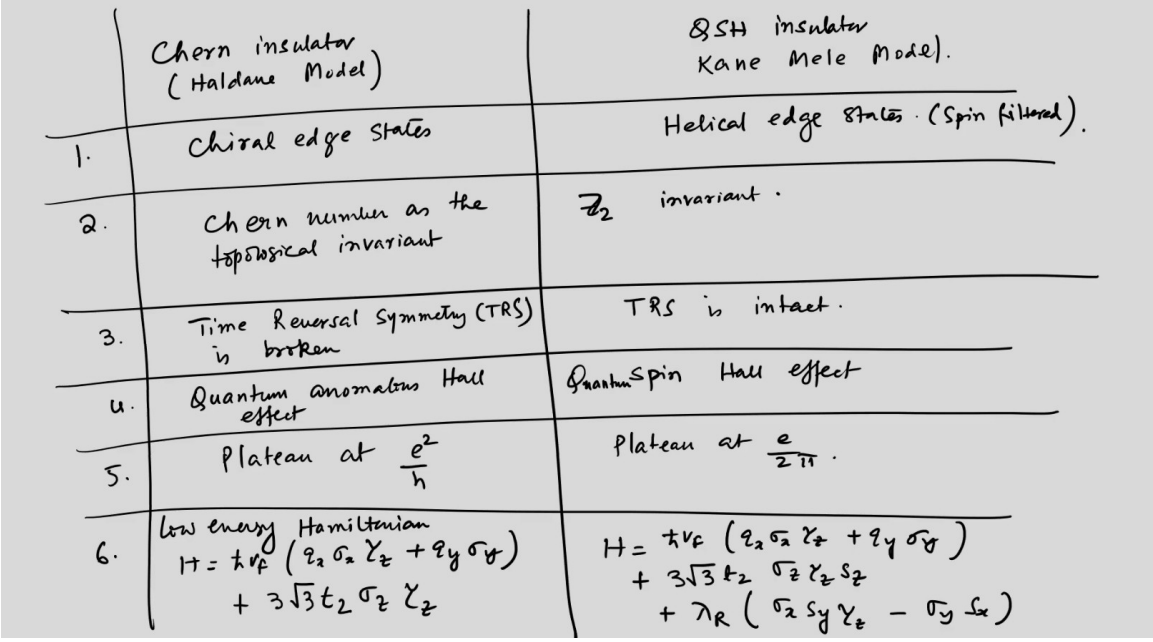


So, let me do a comparison between the Holden model or we what we call as a Chern insulator and this quantum spin Hall insulator. So, we will call a Chern insulator or same as Holden model and quantum spin Hall insulator QSH insulator and or a same as Kane-Mele model okay. So, let me make a comparison between the two in terms of a number of things that we have learned so far. It is like a summary of what we have learned.

So, we have in no particular order. So, there are chiral edge states that is electrons move in different directions in opposite sides of the sample and there are helical edge states where they are spin filtered. So, this is one so this spin filtered second is this is called as a Chern number as the topological invariant and that is why they are called as Chern insulator Z 2 invariant okay. Number 3 time reversal symmetry is broken let us call it as TRS is broken, TRS is intact. So, we have told about the implications of time reversal symmetry. So, it shows a quantum anomalous Hall effect shows spin hall effect will show you the spin conductivity or spin hall conductance spin hall effect quantum spin hall effect.

Quantum spin hall effect and one sees a plateau in the spin Hall conductivity at e square over h plateau at e over 2 pi last, but not the least of course we have a low energy Hamiltonian H equal to h cross V f q x sigma x tau z plus a q y sigma y plus 3 root 3 T 2 which you can call it either a lambda S O also sigma z tau z and similarly a low energy Hamiltonian is h cross V f q x sigma x tau z plus a q y sigma y and a plus this 3 root 3 T

2 sigma z tau z S z that is the spin and plus a lambda R and sigma x S y tau z minus sigma y S x. Compared to the last slide we had to change these notations a little because now sigma denotes the sub lattice degrees of freedom while S denotes the actual spin degrees of freedom okay. So, these are a summary of these two type of insulator and both are very important in their own right okay. So, here we just show that the graphene only with the Rashba term there is no Haldane term and so on. So, you see that this is just the tight binding graphene and this is the Rashba term.

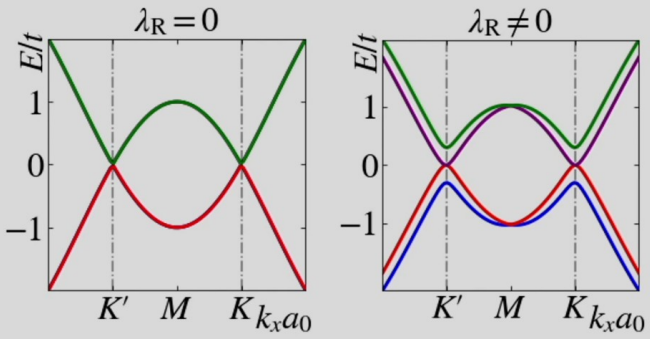


So, you see that there are this semi Dirac or semi metallic nature not semi Dirac semi metallic nature at the K and the K prime points which also that there is a band touching because without a sigma V or the Haldane term there will be no lifting of gap, but now you see the spin resolved bands okay. So, it is a gapless scenario there is no gap there even with lambda R not equal to 0 and you have. So, we have just done a Fourier transform of this and then have plotted this or rather solve this model and plotted this dispersion okay. So, finally, the spin Hall conductivity which is obtained using. So, this is the spin Hall conductivity with you can call it a S also, but it is written with a Z because you are talking about the Z component of the velocity.

Graphene with only Rashba term

Hamiltonian

$$H_{KM} = t\sum_{\langle i,j\rangle} c_i^{\dagger}c_j + i\lambda_R \sum_{\langle i,j\rangle} c_i^{\dagger}(\vec{\sigma}\times\vec{d}_{ij})_z c_j$$

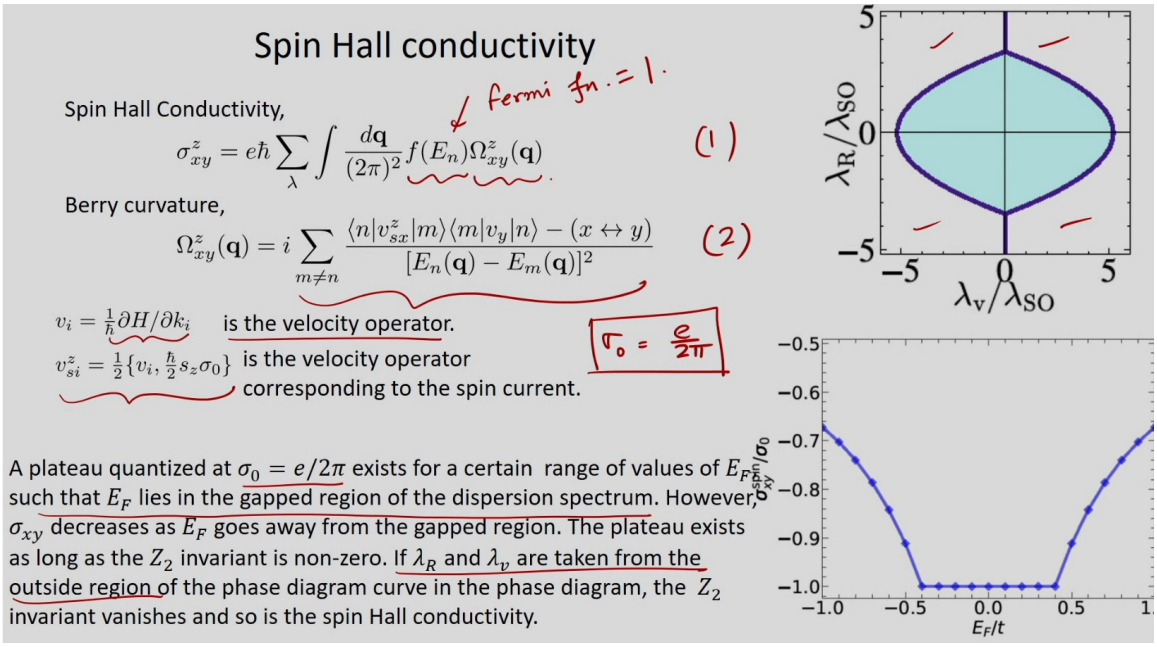


When $\lambda_R = 0$, we observe the band structure of graphene where the bands touch each other at the **K** and **K′** points. When we include the Rashba SOC, we observe the spin filtered bands. However, unlike the Kane-Mele model we do not see any opening of band gap.

So, this is really the spin Hall not the charge Hall conductivity which is equal to 0 anyway. So, this is equal to this is a Fermi function which is not important because if you are talking about 0 temperature then this is equal to 1 and this is the Berry curvature and the Berry curvature can be calculated using this formula which is a very similar to what you have seen for the Kubo formula and the velocities are calculated from this gradient of the Hamiltonian with respect to K x and K y or you differentiate. So, for V x you take a del K x and for V y take a del K y the only thing that is important is that now these were is the velocity operator, but that is not what is used here you use a V s i and the Z component which requires one to calculate the anti-commutation relation of these quantities. So, it is a if you want V s x Z then you take a V x and then h cross by 2 S Z sigma 0 sigma 0 is simply e over 2 pi this is just the scale of the conductance okay. So, one does this calculation and of the Berry curvature and then put it into the expression for spin Hall conductivity let us call it as 1 and 2.

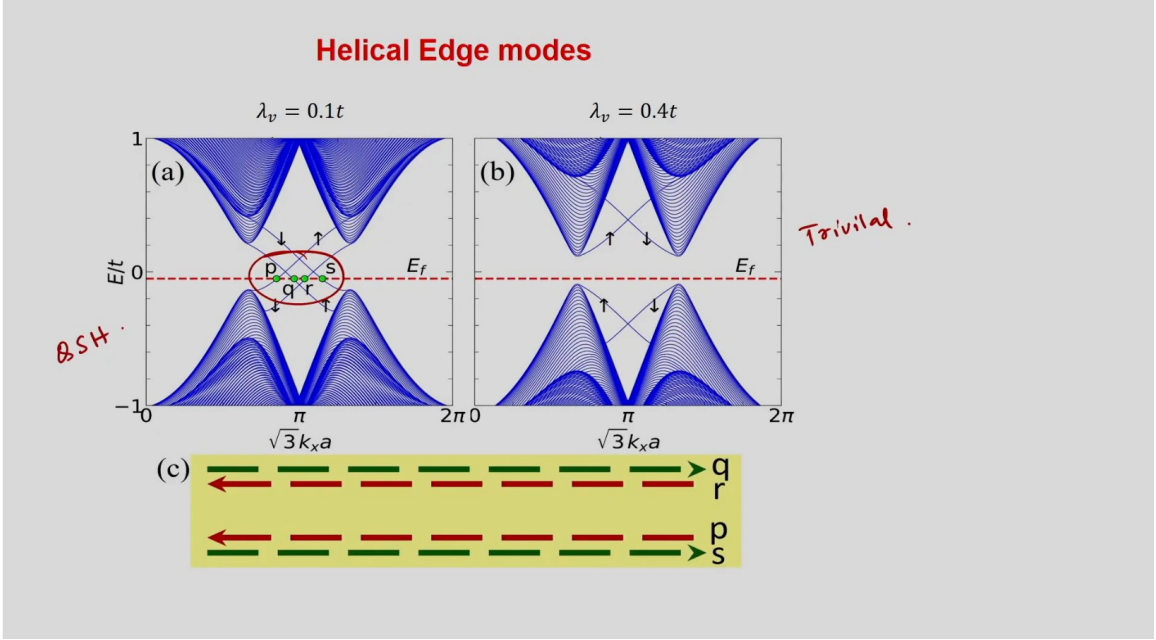
So, a 1 calculates 2 and then put it into 1 put Fermi function equal to 1 at t equal to 0 and then you calculate this spin Hall conductance and the spin Hall conductance comes out to be a very nice you know a form which is it is 0 in the vicinity of the Fermi energy. So, this is the bias voltage. So, you are biasing the system and this bias voltage changes the Fermi energy because the electron occupancy is altered as you bias it and you see that there is a very broad plateau in the vicinity of E F equal to 0 or 0 bias and it is it is very symmetric and so on. So, this is e over 2 pi that exists for certain range of values of the E F or the bias voltage and when E F lies in the gapped region of the dispersion

spectrum. So, when E F lies here which is what we have shown earlier if E F say for example, where both are non-zero.



So, when the E F lies in this gap and not inside the band then this is a it gives you a plateau and then as it the plateau sort of goes away and the spin Hall conductance becomes dispersive or it sort of rises when the Fermi energy such that it falls within one of the conduction or the valence band is exactly the feature that we have seen earlier okay. And so, in this so, if lambda r and lambda v are taken from the region outside that is this white region here or here or here or here then of course, the Z 2 invariant vanishes and the plateau structure vanishes as well okay. So, this is by and large what one gets from the Kane-Mele model and the explicit calculations of all the quantities that are of importance are presented here okay. So, these are the helical edge modes that we have shown earlier what is presented once again.

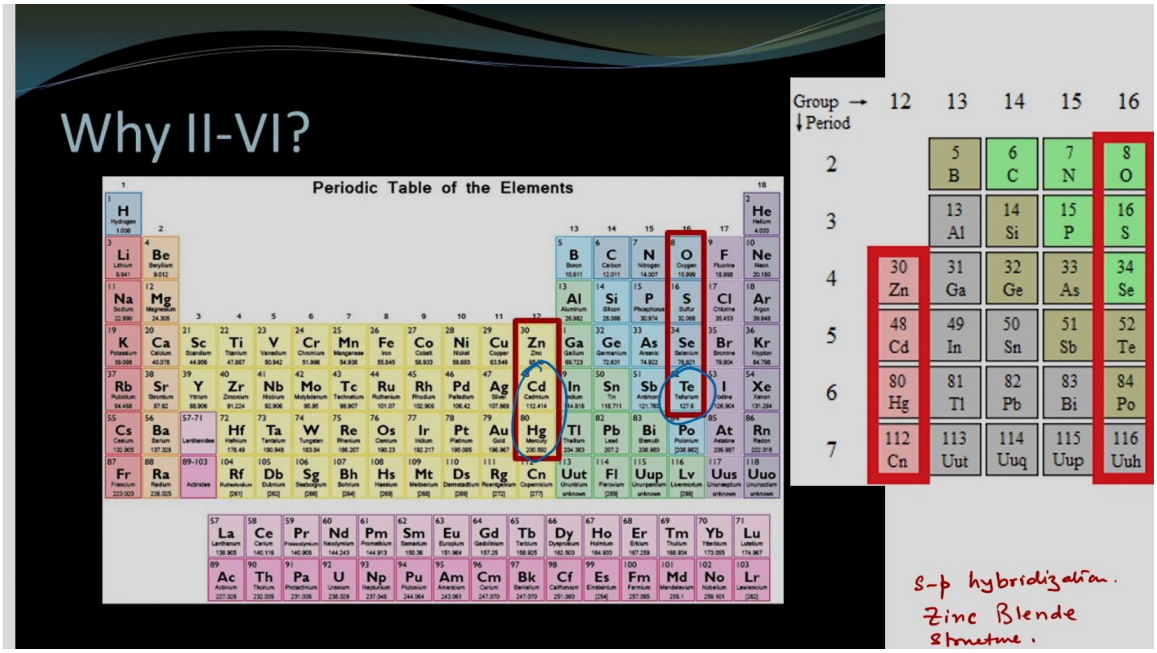
So, this p q r and s are these things here. So, this is a topological insulator that is a quantum spin Hall insulator. So, let me write it as QSH insulator and this is trivial insulator with no edge modes. So, here you are inside the blue region here the light blue region that is sky blue region inside and for the right panel you are outside okay. This is what completes the discussion on the Kane-Mele model.



Let me sort of do a sort of summary slide for the quantum spin Hall phase the mercury telluride and the cadmium telluride quantum wells and the Kane-Mele model just setting up a connection between them. These are some of the people who have contributed immensely on this topic of quantum spin Hall insulators and once when the Kane-Mele had proposed this model there somebody has done an experiment and the person who did that experiment is Molenkamp and the theory had been almost immediately proposed by Zhang. So, Molenkamp this is Taylor Hughes and this is Bernevig. So, these people and later on many other people have contributed immensely to the development of the field. So, what happens is that so there are these 2, 6 materials 2, 6 materials which are the semiconductors rather. So, there are these 2, 6 semiconductors which are important because these semiconductors have sp hybridization and along with these are these have a zinc blend structure okay.

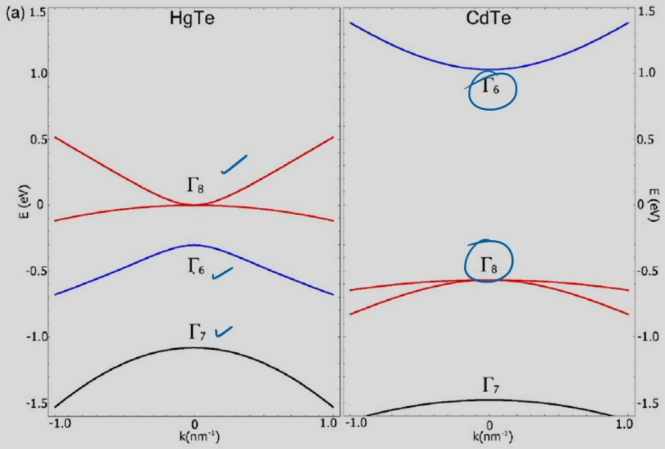
And so they actually belong to the this 12 and 16 columns of these periodic table and you see that there are zinc and cadmium and mercury this is what one of the things that are important I mean these 2 are important in this particular context. This cadmium and mercury and this either selenium or palladium this is important and so on and then this is what exactly we want to the hetero structures to form on the quantum well to form with this. So, this is that thing a little blown up there are these so cadmium and mercury and then there is a this thing that are important and so on. As I said that this sp hybridization so as opposed to the other the transition metal dichalcogenides Bi2 Se3 etcetera where only one orbital is near the Fermi level there are 2 orbitals involved in the you know in making up the energy levels close to the Fermi level. And even though this has been discussed I mean in the sense that this is this gamma is actually the high symmetry point

in the Brillouin zone and these gamma is subscripted with these 6, 7 and 8 you see that there is a 6 here there is a 7 here and there is a 8 here.



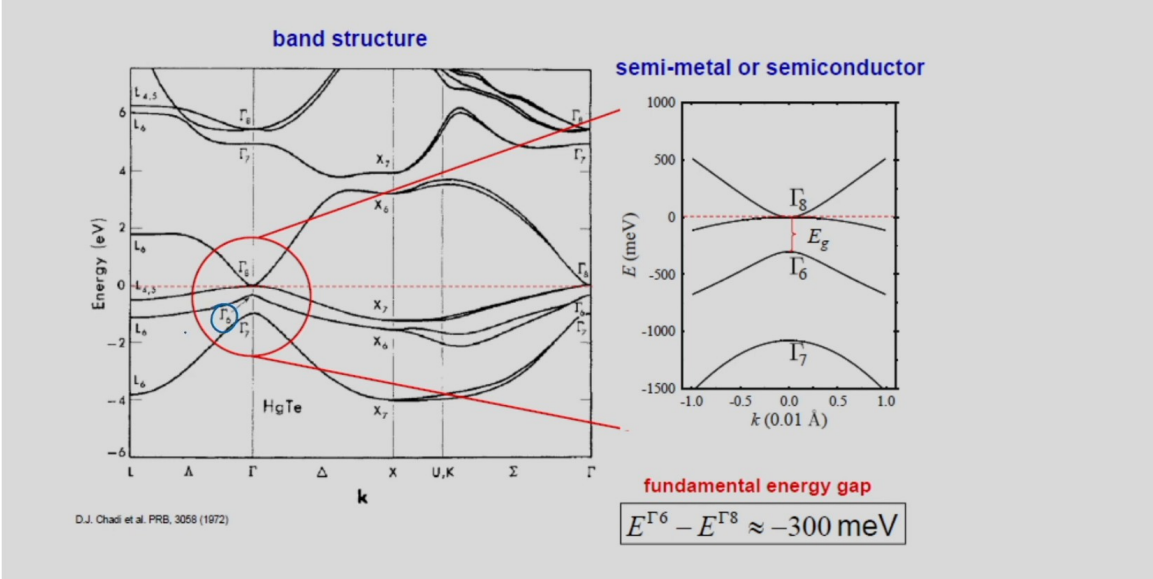
So, this 7 and 8 are split by the spin orbit coupling which is present in this material. In general this gamma 6 is in the conduction band and gamma 8 is in the valence band which is what you see. So, this is the conduction band in CdTe this is the conduction band and this is the valence band and which is the conduction band is of course above the valence band and these gamma 7 even though they are spin split but they are this gamma 7 is not under consideration because it is far away from the Fermi energy.

Γ is a high-symmetry point in the BZ. The high symmetry point Γ is subscripted with the 6,7 and 8. In normal insulator Γ_6 is in the conduction band and originates from the *s*-type band and Γ_8 is the valence band from the *p*-type band. The situation is exactly the opposite in the case of HgTe (Band inversion).

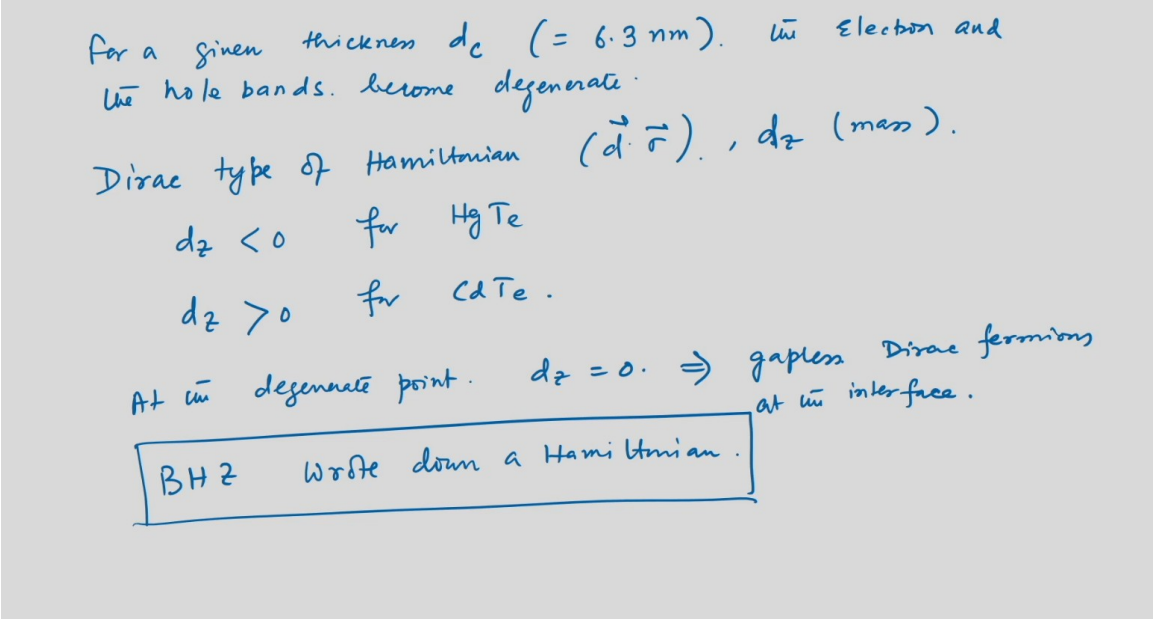


Very interestingly the mercury telluride HgTe has an inverted structure which is what has been told and here of course the gamma 6 comes below the gamma 8 and this is what creates all the interesting thing which is what these people who I had shown in the earlier slide they have understood and this is a closer picture and so on and you see that there is a gamma 6 in the this is HgTe and a gamma 8 is up there. So, the and the red line is actually the Fermi energy and you see that this gamma 6 and gamma 8 have an energy which is minus 0.3 electron volt or about 300 milli electron volt. So this is interesting and when you make a structure out of it when you make a you know a sort of sandwich the mercury telluride in between two cadmium telluride slabs when the mercury telluride start starts you know dominating the phase diagram or dominating the physics that's when there is a interesting thing happens and this interesting thing is shown here in the lower panel for D less than DC you see that there are these blue is the conduction band and this is a valence band and so on and this is HgTe is inside and there are these CdTes outside. So, the electron and the whole bands are shown by a blue and red colors and so on and when the width of the well it is increased. So, this way you increase the width of the well and when it happens then D greater than DC one has an inversion of the so the electronic level comes below the hole and that's where so this is a trivial insulator and this is a topological insulator or so topological and in particular if we talk about it is a QSH phase that emerges. Now there are a few inputs that one can get from this so for a given thickness D DC which is equal to I believe this is a value so what happens is that the electron and the whole bands they become degenerate. So, this one so E1 and H1 they merge so this basically is shown one electron band and whole band that the cartoon picture is it's good enough to only show one and they merge and then they switch order

and when they merge that's called as the degenerate point and this can be exploited in the following sense.



So, at this thickness the E1 and the H1 will merge it's less than DC if it is less than DC then E1 will be higher than H1 and if D is greater than DC then E1 will lie lower than H1. So, that tells you that if you think in terms of a Dirac type of Hamiltonian this is like a D dot sigma then the DZ which is the mass term. So, this DZ is you know is less than 0 for a Hg Te which means it's negative that's why the inverted band structure comes and DZ greater than 0 for C D Te. So, at the degenerate point DZ is equal to 0.



So where one sees the gapless Dirac fermions at the interface. So, based on this BHZ wrote down a Hamiltonian and this is what we have seen that 4 by 4 Hamiltonian and which of course, has a block diagonal nature comprising of the gamma 6 and the gamma 8 levels which are connected by time reversal symmetry because this has time reversal symmetry. So, they are basically the Kramer's pairs and the spin split Kramer's pairs. And so, in the same spirit the Kane-Mele Hamiltonian is also block diagonal without the Rashba term and that gives rise to a spin Hall quantum spin Hall phase. So, there is a connection between this and the Kane-Mele Hamiltonian which also is block diagonal in the in the spin space and one can calculate and that is what we have shown here. Thank you.