

**Topology and Condensed Matter Physics**  
**Prof. Saurabh Basu**

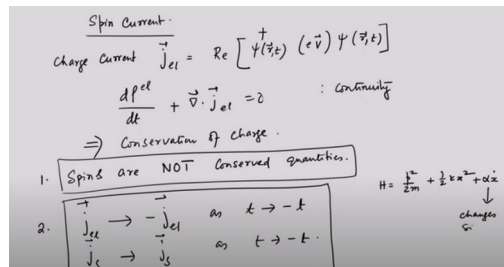
**Department of Physics**

**Indian Institute of Technology Guwahati**

**Lecture – 20**

**Spin current, quantum spin Hall effect**

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We have been talking about spin hall effect which arises because of the passage of charge current. So, there is a charge current which causes the spins to segregate at the you know the transverse edges of the sample which will constitute a spin current and this happens not in the presence of an external magnetic field rather there is a requirement of spin orbit coupling and we have discussed spin orbit coupling and in particular it in two dimensional material or rather low dimensional material because of the lack of inversion symmetry a kind of particular kind of spin orbit coupling is important which is called as a RASPA spin orbit coupling we have discussed that as well. So, let us discuss the spin current which is at the heart of these spintronic devices and this if the spin current is large at least that is what the attempt is in terms of experiments so that fabrication of devices can be made. So, the spin current is actually different than the charge current it has different properties than the charge current and because it is you know central to the study of spin hall effect we need to understand what these properties are and how different they are from the charge the usual current that we refer to which is the charge current.

So, just to remind you that the charge current has a form well known in quantum mechanics it is  $J$  let us write it with an electron because it is the charge degree of freedom

this is equal to the real part of  $\psi^* \nabla \psi$  and  $e \mathbf{v}$  where  $e$  is the electronic charge and  $\mathbf{v}$  is the velocity and this is  $\psi^* \nabla \psi$  where  $\psi$  is the wave function if you remember that it has a form which is  $\psi^* \nabla \psi$  I mean  $\psi^* \nabla \psi - \psi \nabla \psi^*$  this can be written in a simplified form like this. And this current the charge current obeys the continuity equation which is given by  $\frac{d\rho}{dt} + \nabla \cdot \mathbf{J} = 0$  I am just putting this electron just to talk about the charge and this plus a divergence of  $\mathbf{J}$  electron this is equal to 0 and this is called as a continuity equation.

$$\vec{j}_{el} = \text{Re}[\psi^\dagger(\vec{r}, t)(e\vec{V})[\psi(\vec{r}, t)]]$$

$$\frac{d\rho^{el}}{dt} + \nabla \cdot \vec{j}_{el} = 0$$

And the continuity equation confirms that there is a conservation of charge or invariance of charge. So, this is conservation of charge as opposed to that spins are not conserved quantities ok. And this is an important statement and this happens because in most of these materials that we are talking about at least now they have spin orbit coupling and in presence of spin orbit coupling the components of  $\mathbf{s}$  are no longer good quantum numbers which is what we have seen. For example, if you have  $\mathbf{L} \cdot \mathbf{s}$  and this spins are not good quantum numbers and not only that there is another property which is distinct as compared to the for the spin current which is different than the charge current is that the charge current changes sign under time reversal that is as time is reversed.

$$\vec{j}_{el} \rightarrow -\vec{j}_{el} \text{ as } t \rightarrow -t$$

$$\vec{j}_s \rightarrow \vec{j}_s \text{ as } t \rightarrow -t$$

So,  $\mathbf{J}$  goes to minus  $\mathbf{J}$  as  $T$  goes to minus  $T$  and the reason is that because  $\mathbf{J}$  is equal to say  $E$  into  $\mathbf{V}$  velocity, velocity changes sign under the time reversal operation. So, this is for the electron. However,  $\mathbf{J}_s$  does not change sign as a  $T$  tends to minus  $T$  ok. So, this is a very important thing and this is related to the fact that this spin current they can actually propagate without any dissipation. And if you want to understand it in a simple language that how a time reversal invariance breaking term gives rise to dissipation then you can understand it if you write down the Hamiltonian for say harmonic oscillators a  $p^2$  square by  $2m$  plus half  $k x^2$  square.

So, this is the oscillator that we all know this has a time reversal invariance as T changes to minus T and none of these terms changes sign. However, if say for example a dissipative term which I write it as alpha into velocity which is x dot and now this changes sign as T tends to minus T ok. So, that tells you that dissipative term or a term which changes sign as T tends to minus T actually is dissipative. So, that is why the charge current is dissipative because it is odd under time reversal whereas, the spin current is non-dissipative because of the time reversal invariance that it maintains ok. So, how do I write the spin current.

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Spin Current  

$$\vec{j}_s = \text{Re} [\psi^\dagger(r,t) (\vec{v} \cdot \vec{s}) \psi(r,t)]$$

$$= \text{Re} [\psi^\dagger v_\alpha s_\beta \psi] = \text{Re} [\psi^\dagger s_\alpha v_\beta \psi]$$

$$\vec{I}_s = \int dA \hat{n} \cdot \vec{j}_s(r,t) = \int dA [\psi^\dagger(r,t) \frac{1}{2} (\vec{v} \cdot \vec{\sigma} + \vec{\sigma} \cdot \vec{v}) \psi(r,t)]$$

$$\vec{s} = \frac{\hbar}{2} \vec{\sigma}$$

$$\vec{j}_s = \frac{\hbar}{4} \{ \sigma_\alpha, v_\beta \}$$

$$\{ \sigma_\alpha, \sigma_\beta \} = \sigma_\alpha \sigma_\beta + \sigma_\beta \sigma_\alpha = 2\delta_{\alpha\beta}$$

So, the spin current is written as I said that we write it with a Js and this is written with a real part a pretty similar fashion as earlier it is a RT and this is equal to a V dot s ok and psi of RT. In fact, this is one of the ways that you can understand that this term is invariant under time reversal because both V and s would change their signs and so, the product would not change signs and that is how it is invariant under time reversal. So, this is a form of the spin current and one can you know write it as components of this real part can be written as the inside the real part we can write it as a psi dagger I am not writing this RNT dependence which in general it would depend upon this RNT and this is equal to a V alpha and s beta and psi this is equal to real part of psi dagger s alpha V beta psi ok. So, you can write it as V alpha s beta which is same as s alpha that is alpha components. So, alpha and beta are the components x y and z ok. So, these are just components and so on.

$$\vec{j}_s = \text{Re}[\psi^\dagger(r,t)(\vec{V} \cdot \vec{s})\psi(r,t)]$$

$$= \text{Re}[\psi^\dagger v_\alpha s_\beta \psi] = \text{Re}[\psi^\dagger s_\alpha v_\beta \psi]$$

So, this is the current density. So, this is the spin current density is written as this and one can write down the spin current which is equal to say da where a some area over which this current is being considered and this is like so, some component and then Js Rt.

So,  $J_s$  also function of  $R$  and  $T$  which we can write it as a da and then a psi dagger  $R T$  and so, we can write as half of  $V \cdot s$  plus  $s \cdot V$  and this comes from the step above where this is equal to this. So, we write the  $V \cdot s$  terms as half of  $V \cdot s$  plus  $s \cdot V$  and then psi of  $R T$ . Now that brings in an anti commutator and this can be written as so, this  $J_s$  alpha beta can be written as this half of  $V \cdot s$  plus  $s \cdot V$ .

$$I_s = \int dA \hat{\alpha} \cdot \vec{j}_s(r, t) = \int dA [\psi^\dagger(r, t) \frac{1}{2} (\vec{r} \cdot \vec{s} + \vec{s} \cdot \vec{r}) \psi(r, t)]$$

$$j_s^{\alpha\beta} = \frac{1}{2} (\vec{v} \cdot \vec{s} + \vec{s} \cdot \vec{v})$$

$$\vec{s} = \frac{\hbar}{2} \vec{\sigma}$$

So, this is the current operator and if you use this  $s$  equal to  $\hbar$  cross over 2 sigma where sigma denotes the Pauli matrices in that case we can write this as the  $J_s$  alpha beta is equal to 1 over 4 I have taken  $\hbar$  cross equal to 1 and this is a sigma alpha and a phi beta come anti commutator. So, this is an anti commutator. So, you know what an anti commutator is it is basically given by say you have a  $AB$  and anti commutator of that is equal to  $AB$  plus  $BA$  a commutator will have a minus sign here. Alright so, this is the form and where we have taken  $\hbar$  cross equal to 1. So, this is the form of the spin current and its components and so on.

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Example

$$\alpha = z, \beta = y$$

$$v_y = \frac{\partial H}{\partial p_y}$$

$$H = \frac{p^2}{2m} - \lambda_R \vec{\sigma} \cdot (\hat{z} \times \vec{p}) \quad (\hbar=1)$$

Rashba SOC.

$$v_y = \frac{p_y}{m} + \lambda_R \sigma_x$$

$$j_s^{yz} = \frac{1}{2m} \sigma_z p_y$$

Just like an electric current induces a magnetic field,  
a spin current induces an electric field.

And let us take a particular example this is a example say for example where we take alpha equal to  $Z$  and beta equal to  $Y$  is just some examples that we want to give in which your  $VY$  which is obtained from the Hamilton's equation as  $\text{del } H \text{ del } PY$  that is your  $VY$  and if you consider a Hamiltonian which is equal to  $P$  square over  $2m$  minus lambda. So, this is that Rashba we just put a  $R$  here just to make sure that it is a Rashba spin orbit coupling. So, it is sigma dot  $Z$  cap cross  $P$  and where we have taken again  $\hbar$  cross equal

to 1 without any loss of generality we can one can put it back. So, suppose this is the Hamiltonian this is the kinetic energy just free electron kinetic energy and this is the Rashba spin orbit coupling okay. And in that case I can calculate this  $\frac{\delta H}{\delta P_Y}$  in order to get the  $V_Y$  the Y component of the velocity.

$$\alpha = z, \quad \beta = y$$

$$v_y = \frac{\delta H}{\delta p_y}$$

$$H = \frac{p^2}{2m} - \lambda_R \vec{\sigma} \cdot (\vec{z} \times \vec{p})$$

So,  $V_Y$  becomes equal to  $P_Y$  over  $m$  plus  $\lambda_R \sigma_X$  okay because this is equal to  $\sigma_X P_Y$  minus  $\sigma_Y P_X$  and the other term will give you 0 when you take a derivative with respect to  $P_Y$  and that tells you that the spin current has this form which is  $YZ$  that is equal to it is equal to  $1$  over  $2m$  and a  $\sigma_Z P_Y$  okay. This is quite an important step in the sense that this is written the spin current is written in terms of the Pauli matrix and the  $P_Y$  the Y component of the momentum. And suppose you want to put it in the Kubo formula in order to calculate the Hall conductance or the longitudinal conductance these are the quantities that are going to be you know used and they have to be taken the expectation values of these terms have to be taken within the states of the Hamiltonian and the Hamiltonian appears here okay.

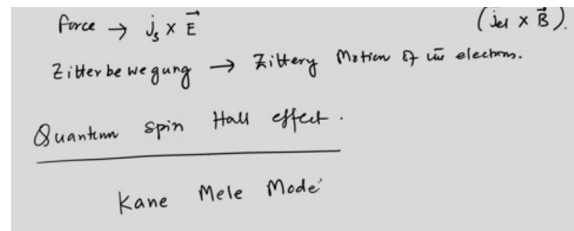
$$v_y = \frac{p_y}{m} + \lambda_R \sigma_z$$

$$j_S^{yz} = \frac{1}{2m} \sigma_z p_y$$

So, once you solve the Hamiltonian you get the eigenstates and these  $J$ 's have to be the expectation values of  $J_X$  and  $J_Y$  etcetera etcetera will have to be taken between these states and then one can calculate the Hall conductivity or the longitudinal conductivity basically the conductance formula using the Kubo formula. So, just like an electric current it produces a magnetic field a pure spin current also induces or an electric field okay and this is quite an important thing.

So, a spin current actually creates or produces an electric field and basically the spin current actually experiences a force because of this electric field just like a magnetic field or rather than electric current induces a magnetic field a spin current induces an electric field okay.

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So, this tells you that if there is a spin current in an electric field induced by itself it experiences a force and the force is given by is  $J_s$  cross  $E$  just like we know that the this electric field experiences a force which is  $J$  cross  $B$ . So, this is because of the magnetic field and these force even though it is small it produces observable effects in a system in terms of course the renormalizing the spin current etcetera and also it produces a sort of effect called at the zitter bugung zitter BWE which is called as the jittery motion of the electrons okay.

So, it has observable effects and so on okay and over the last decade or decade and a half there are have been studies on these finding out the spin current and its magnitude and how to actually enhance this in order to have or rather realize devices which are called as a spintronic devices and the advantage of this spintronic devices are that they have infinite lifetime that is the spin currents have infinite lifetime they do not dissipate and which we have already talked about they do not dissipate and then it can be used or rather the spin current can be used for you know propagation of information which will not have any dissipation in terms of the joule heating or in terms of you know scattering from the impurities or disorder. So, this will be a very robust and dissipation less transport which would be very important and is definitely an improvement over the conventional electronic devices okay.

And as we have said that this dissipation less transport is fundamentally because of the fact that the spin current is invariant under time reversal okay alright. So, this is about the spin current now we have to talk about another important topic which is called as a quantum spin hall effect and of course we have talked about spin hall effect but what is a quantum spin hall effect and we will show you some cartoons on that but this was around 2005-6 if they were you know first proposed as a model which would give rise to this spin hall effect and will not have any charge hall effect which means that the system is

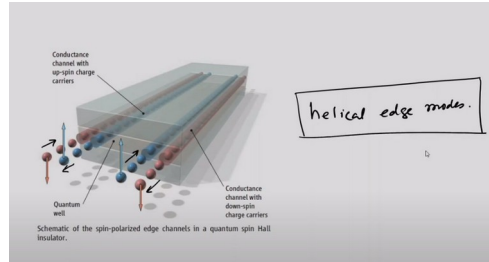
not subjected to an external magnetic field but it has spin orbit coupling. So, the usual charge hall effect vanishes and the Chern number of the system is 0 but however another invariant stays which or rather another invariant comes up which is nonzero and that will give rise to the quantum spin hall effect. In fact after these 80-81 when this quantum hall insulators are discovered 25 years nearly 2 and a half decades later another type of topological insulator which was discovered are these the quantum spin hall materials of quantum spin hall devices.

So, initially it came as a theoreticians you know proposal that this can be done in fact one of the things that we do not discuss here is called as a Koehn-Miele model where Koehn and Miele Charlie Koehn and F Miele they had realized that if you take 2 copies of the Holden model where this Holden model is actually the second neighbour hopping complex second neighbour hopping in a honeycomb lattice or in graphene if you take 2 copies of that one having flux to be say  $\pi/2$  and another having a flux to be another spin I mean one spin has a flux of  $\pi/2$  and another spin has a flux of minus  $\pi/2$  and if you superpose them then you actually regain back the time reversal symmetry that's broken in this Holden model and that's called as a Koehn-Miele model.

And in this system if you put in a Rashba-Orbit coupling you will see that the bands actually split band dispersion or the electronic dispersion the band split and there are edge modes that propagate across the Fermi level from the valence to the conduction band and instead of one pair of edge modes that propagate one finds actually two pairs of edge mode one pair for each spin. So, one pair for up spin edge mode and one pair for the down spin edge mode and these are called as a quantum spin hall insulators and they very importantly denote another type of or another class of topological insulators one of them being the quantum hall insulators which we have been talking about. So, in addition to this application oriented side of it or face of it these fundamentally they are also important because this is one additional class of topological insulator that could be realized. And soon after this proposal there the people led by Molenkamp etcetera they actually realize this in physical systems which is what we are going to discuss. And they realize it in quantum well super lattice structures formed by the CDT the cadmium telluride and the mercury telluride systems okay.

So, it is basically a mercury telluride which is sandwiched between the cadmium tellurides and beyond a certain width of this structure quantum well structure for the mercury telluride one has a quantum spin hall phase. We will do not very detailed calculation one can look at these the papers by Bernabe, Hughes and Zhang and also Molenkamp et al in order to get more insights into it particularly the experimental aspects I will not go into details that much but we will talk about the material.

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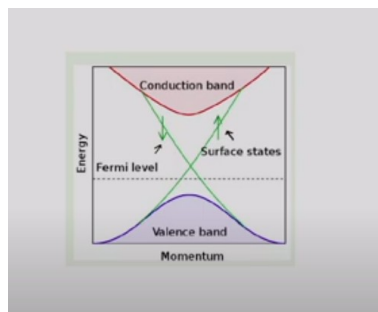


So, let me show you a cartoon of this quantum spin hall insulator. So, you see that this shaded region is a sample and so this formed by as it says some quantum well and conductance channel for the down spin charge carriers is shown by the red. You see that the red denotes down spin and the blue denotes an up spin.

So, at each of the transverse edges of the sample that is these two edges which are say respectively right and left there are instead of one edge mode there are two edge modes at each edge and one corresponds to up spin and the other corresponds to the down spin and so on okay. And so these are shown by this red dots and the blue dots and the spin directions are also shown and these are called as a helical edge modes. So, it's in the quantum hall samples we have seen that there are only one edge modes which are chiral that is they're propagating in different direction. Here at each edge we have two modes corresponding to two spins which are pointing in the different I mean they're opposite directions. So, it's like you know a sort of a set of two highways where the red are say the cars moving in one direction and blue the cars moving in the other direction and similarly the other lane of the highway has exactly the same things.

Now of course this blue moves in the opposite direction. So, if the blue moves in this direction that is up spin move in this direction on the left edge of the sample then this would move in this direction in the right direction on the other edge of the sample and similarly this would move the down spin would move say in this right and they would move in the left. So, it's a strange kind of arrangement and they are called as a helical edge modes as opposed to chiral edge modes of quantum hall systems okay. This is just a cartoon showing a quantum spin hall phase okay.

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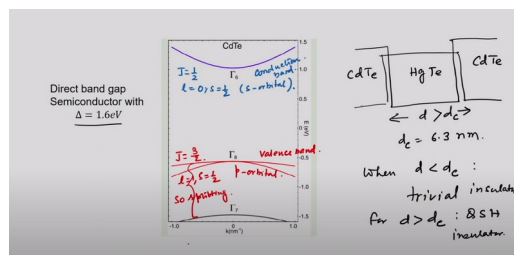




So, let me show another cartoon of these are of course you see that only one pair because I mean it is not exactly it is just a cartoon picture, but if you calculate the band dispersion for the ken milli model without a Rajbhatam they look similar and you see the conduction band and the valence band these green lines that traverse these are the edge modes one of them a corresponds to the down spin and the other corresponds to the up spin.

So, these will give rise to these edge states or edge modes that are present in the system. So, this energy versus momentum and the conduction band is shown in red and the valence band is shown in blue and this is a function of the momentum you could ask this question that this momentum is actually a vector suppose in two dimension it should be a two component quantity that is a two component vector, but of course these calculations are done on a nano ribbon which is what I have shown you earlier and in the nano ribbon there is just one k that is a good quantum number the other k is not a good quantum number because there is no transnational periodicity or there is transnational invariance in the other direction. So, this corresponds to the momentum which has a periodicity or which has you know a periodic boundary conditions and they can be defined as a good quantum number. So, that momentum is being talked about not the other. So, if you have a ribbon along the x direction that this is actually  $k_x$  the x component is missing here, but it means that x component of the momentum ok.

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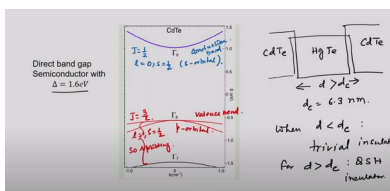


So, let me talk about the experiment and before I come to the band structure let me show you So, these are you know sort of super lattice structure where there is a HGTE inside CDTE cadmium telluride here. So, this is the structure and there is something very interesting about HGTE which is what will be talked about. However CDTE is a well behaved semiconductor. Now this kind of structure when this thing D crosses some DC that is of the HGTE well this quantum well has a width which is greater than some DC where DC is equal to 6.3 nanometer ok. And when it crosses then HGTE that is mercury telluride band structure becomes important and this mercury telluride has got a strange

band structure and this is what makes it interesting and the system undergoes a band inversion and this band inversion is responsible for the quantum spin Hall phase. So, let me show the first non-interesting one that is the CDTE cadmium telluride it is a direct band gap semiconductor with  $\Delta = 1.6$  eV which is fairly large. So, let me show you this. So, this one is less than that so when  $D$  is less than  $D_C$  it is a trivial or band or trivial insulator for  $D$  greater than  $D_C$ ,  $D_C$  is some critical width which has a value in this particular case as 6.3 nanometer and when  $D$  is greater than  $D_C$  then one has a quantum spin Hall we will write it as QSH insulator ok. So, to carry on with the band structure of CDT one can see that so there are these blue band which is denoted by  $\gamma_6$  here and so this actually is the conduction band. So, this is conduction band and this  $\gamma_6$  band for the CDT has a  $J$  equal to half and it corresponds to  $L$  equal to 0 ok. So,  $L$  equal to 0 and  $S$  equal to half that makes it this has a property which is like a  $S$  is like a  $S$  band or  $S$  orbital ok. Now  $\gamma_8$  corresponds to so this is a valence band and this is for  $J$  equal to 3 half now this is  $L$  equal to 1 and  $S$  equal to half ok.

So, this is a  $P$  orbital ok and this  $\gamma_7$  that you see is separated from this is basically this is the spin orbit splitting. So, it actually has the same symmetry but this is this correspond to  $J$  equal to 3 half and this correspond to  $J$  equal to half and it is not important for the discussion the only things that are important in this quantum well structure are these  $\gamma_6$  band and the  $\gamma_8$  band and so on ok. So, this is a sort of well behaved semiconducting system its conduction band is above the Fermi level and the valence band is below the Fermi level and so on ok.

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This is the most important thing you see that this is like a 0 band gap semiconductor because the  $\gamma_8$  level is almost I mean it is touching the Fermi level. So, it is a 0 band gap semiconductor and not only that there are interesting consequences here so these are valence band ok.

And again it is  $S$  orbital so it is a  $S$  type and so on and this is again that  $J$  equal to 3 half. So, this is  $J$  equal to 3 half and it is a  $P$  orbital ok. Now what happens is that these are the spin orbit coupled or rather split bands ok and the part of the conduction band so this is the conduction band. So, the part of the conduction band is below the valence band and so this is called as a inverted structure and this inverted structure actually is important

and so gamma 7 and gamma 8 are SO split band and the whole dispersion is shown near this point which is called as the gamma point.

So, this is the center of the BZ ok. So, this one again this corresponds to so S type which means this is equal to J equal to half and so on. So, this of course is J equal to half because these are spin orbit coupled band and this has an inverted structure and this AGT when it becomes important a dominant player in this quantum well it happens when the thickness or width of the quantum well exceeds certain value then the AGT or the mercury telluride band dispersion becomes more prominent or more important and that's when it becomes a quantum spin hall insulator ok. So and these are really these super lattices is formed by a molecular beam epitaxy or even probably by a sputtering methods and so on.

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Bernawig Hughes and Zhang (BHZ)

4x4 Hamiltonian:

$$H_{eff}(\vec{k}) = \begin{pmatrix} H^+(\vec{k}) & 0 \\ 0 & H^-(\vec{k}) \end{pmatrix} \begin{pmatrix} |l_0, +\rangle |l_0, -\rangle \\ |l_1, +\rangle |l_1, -\rangle \end{pmatrix}$$

where  $H^+(\vec{k}) = \begin{pmatrix} H^+(\vec{k}) & 0 \\ 0 & H^+(\vec{k}) \end{pmatrix}$  and  $H^-(\vec{k}) = \begin{pmatrix} H^-(\vec{k}) & 0 \\ 0 & H^-(\vec{k}) \end{pmatrix}$ .

The eigenvalues are  $\langle l_0, + | H^+ | l_0, + \rangle$ ,  $\langle l_0, - | H^+ | l_0, - \rangle$ ,  $\langle l_1, + | H^- | l_1, + \rangle$ , and  $\langle l_1, - | H^- | l_1, - \rangle$ .

So this had given idea to people called as a Bernawig Hughes and Zhang and to write down a Hamiltonian and solve it and that's why it's called as a BHZ model ok. So, they wrote down a Hamiltonian and they sort of solved it in order to get the band structure and so on. So, what they did is that they wrote down a 4 by 4 Hamiltonian comprising of so this gamma 6 J equal to so these MJ values which are plus minus half and gamma 8 bands plus minus half. So, we talk about this by gamma 6 and gamma 8 we talk about the symmetries of the band this is a S orbital so it's even and this is a P orbital so even means L equal to 0 and this is P so this is odd because it's equal to L equal to 1 just to remind you that even an odd is said in terms of so what happens to a particular orbital when it is inverted which means that when you change theta to theta plus pi and phi to phi minus pi. So the YLM function the spherical harmonics it picks up a minus 1 whole to the power L.

So when L equal to 0 it doesn't pick up a sign and when L equal to 1 it picks up a sign that will define that they are whether they're even or odd and that's how they are written and these half etcetera I mean this is the MJ the magnetic quantum number of the full the total J quantum number because they're spin orbit coupling. So we can't talk about individually about L and S so one talks about J and J is a good quantum number even

though the near the this gamma point K parallel equal to 0 the parallel component of the momentum equal to 0. So these BHZ wrote down a 4 by 4 Hamiltonian we have seen such 4 by 4 Hamiltonians earlier and in this basis so the basis is a gamma 6 up and a gamma 8 up gamma 8 up and gamma 6 down and a gamma 8 down and so this is the basis for that 4 by 4 and so there is a gamma 6 up and gamma 8 up well I'm not writing anything one should actually write like this on and gamma 6 down and gamma 8 down and so on.

So one gets a Hamiltonian so it's actually a block Hamiltonian with no components mixing the spins so this is equal to H of K and so 0 and 0 H star of minus K and that gives you an effective Hamiltonian written in this basis. So we are just simply modeling the HGT, CDT the quantum well super lattice structure and taken the bands that are closest to the Fermi level and their respective symmetries and the spins. Spins are important now this are not pseudo spinners these are real spins in graphene if you remember that we have talked about Pauli matrices but they do not really denote the spin degrees of freedom but here they do.

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$$H(\vec{k}) = \epsilon(\vec{k}) \mathbb{1}_{3 \times 3} + \vec{d}(\vec{k}) \cdot \vec{\sigma} \quad (1)$$

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

$$d_x + id_y = A (k_x + ik_y)$$

$$d_z = M - B (k_x^2 + k_y^2)$$

$$\epsilon(\vec{k}) = C - D (k_x^2 + k_y^2)$$

$$\vec{k} = (k_x, k_y), \quad A, B, C, D \text{ are material dependent constants.}$$

$$B: \text{classical mass}$$

$$M: \text{Dirac mass}$$

$$\text{If } B=0, \text{ the Hamiltonian is a Dirac Hamiltonian.}$$

$$\text{In } (2.1) \text{ denominator:}$$

So we can write down this as so I will not go into details but let me write down the Hamiltonian and the Hamiltonian is like a epsilon K and I, I is basically a 2 by 2 matrix so this is that and then a Dirac Hamiltonian form which we have seen earlier for graphene.

So these sigma they denote the Pauli matrices so sigma X, sigma Y and sigma Z and this D vectors can be written as DX plus IDY equal to some constant A into KX plus I KY. So this is just a low energy Hamiltonian near the gamma point where this Hamiltonian is linearized. So you see that at the K equal to 0 that is a gamma point in the vicinity of the Fermi energy it is approximated by a linear dispersion okay. So that is why it is a KX plus I KY I will take care of the from it will come from the sigma Y and so this D dot sigma is called as a Dirac Hamiltonian so it has a Dirac form plus this 2 by 2 and the DZ where D is of course a function of K where K actually varies from a minus pi to plus pi for both KX and KY these are the it is basically a 2 dimensional momentum and this is

equal to  $KX^2 + KY^2$  okay. Where all these things will just say in a moment that all these things are constants  $C$  minus  $D(KX^2 + KY^2)$ .

$$H(\vec{k}) = \epsilon(\vec{k})1_{2 \times 2} + \vec{d}(\vec{k}) \cdot \vec{\sigma} \quad (\text{Equation 1})$$

So if you put in everything into this equation 1 so let us call this as equation 2 so if you put 1 in 2 it will have a form which is a 4 by 4 and that can be solved even if you have difficulty in solving it by hand it can always be solved in a using a software such as you know either you use python or MATLAB, Mathematica etcetera.  $K$  is nothing but a 2 dimensional momentum  $KX$  and  $KY$  and  $A$   $M$   $B$   $C$   $D$  are material dependent constants okay alright. So they can remain as constants if you see it you know  $DZ$  that goes with  $\sigma_z$  and  $\sigma_z$  has a diagonal structure which is  $1 \ 0 \ 0$  minus  $1$  and so  $M$  and  $B$  both appear with  $\sigma_z$  and because of this dot product  $DZ \sigma_z$ . So these are called mass terms the ones that appear at the diagonal are called mass terms. So  $B$  is the classical mass because that goes with the  $K$  squared dispersion and  $M$  is actually a Dirac mass okay.

$$\begin{aligned} dx + idy &= A(k_x + ik_y) \\ d_z &= M - B(k_x^2 + k_y^2) \\ \epsilon(\vec{k}) &= C - D(k_x^2 + k_y^2) \end{aligned} \quad (\text{Equation 2})$$

So in the absence of  $B$  it will give rise to 2 copies of the Dirac Hamiltonian in 2 plus 1  $D$ . If  $B$  equal to 0 the Hamiltonian so the the squared term vanishes and the second term of equation 1 is truly like a Dirac equation. So Hamiltonian denotes a Dirac Hamiltonian in 2 plus 1 dimension okay. And in fact will be fine if we only consider the edge of the sample so one can deal with the edge Hamiltonian and which will give the edge states which are of importance to us because this edge states will quantify or tell us about the quantum spin hall phase.

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Handwritten mathematical derivation showing the Dirac equation  $H\Psi = E\Psi$ , the form of  $\Psi$ , and the resulting equations for the components of  $\Psi$ .

Equation (3):  $\epsilon(k_x) = 0 \Rightarrow C - D k_x^2 = 0$

Equation (4):  $\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ ,  $\Psi_{\uparrow, \downarrow}$  have 2 components.

Equation (5):  $\psi_1 = \begin{pmatrix} \chi \\ 0 \end{pmatrix}$ ,  $\psi_2 = \begin{pmatrix} 0 \\ \chi \end{pmatrix}$ . Ansatz  $\chi = \psi e^{i\lambda x}$ .

Putting (4) in (3):  $\begin{bmatrix} (M + B\lambda^2)\sigma_z & -iA\lambda\sigma_x \\ & \end{bmatrix} \psi e^{i\lambda x} = 0$

Commutator relations:  $[\sigma_x, \sigma_z] = 2i\sigma_y$ ,  $\{\sigma_x, \sigma_z\} = 0$ ,  $\sigma_z\sigma_x - \sigma_x\sigma_z = 2i\sigma_y$ ,  $\sigma_z\sigma_x + \sigma_x\sigma_z = 0$ ,  $\sigma_x\sigma_x = \sigma_y\sigma_y = 1$ ,  $\sigma_x\sigma_x = i\sigma_y$ .

And if you do that subject to certain conditions and these conditions are simple in the sense that there are further conditions that can be imposed such as  $\epsilon$  of  $KX$  equal to 0 where which tells you that  $C - DKX^2$  equal to 0 in this condition let us write down the Schrodinger equation which is  $H\psi = E\psi$  with  $H$  as this Hamiltonian this Hamiltonian that you see or  $H$  effective so to say this is that effective Hamiltonian all right.

$$H\psi = E\psi \quad (\text{Equation 3})$$

So, where  $\psi$  is of course a 2 component spinner which is  $\psi_{\uparrow}$  and  $\psi_{\downarrow}$  and both you know  $\psi_{\uparrow}$  and  $\psi_{\downarrow}$  have 2 by 2 structure I mean it is a 2 component spinner each one of them okay. So, this  $\psi_{\uparrow}$  is equal to some  $\chi$  into 0 and  $\psi_{\downarrow}$  this up and this down this is equal to a 0  $\chi$  okay.

$$\psi = \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix} \quad (\text{Equation 4})$$

$$\psi_{\uparrow} = \begin{pmatrix} \chi \\ 0 \end{pmatrix} \quad \psi_{\downarrow} = \begin{pmatrix} 0 \\ \chi \end{pmatrix}$$

And let us make an ansatz to solve this ansatz says that so  $\chi$  is equal to some  $\psi_0 e^{-\lambda x}$  which is some amplitude and exponential  $\lambda x$ . So, you put that into this equation Schrodinger equation let us call it as equation 3 and let us call this as 4. So, putting 4 in 3 and along with this condition which we have said this condition this is simplifies things and so this becomes equal to  $M + B\lambda^2 \sigma_z - iA\lambda \sigma_x$  this is  $I A \lambda \sigma_x$  and  $\psi_0 e^{-\lambda x}$  is equal to 0 of course a  $\psi_0 e^{-\lambda x}$  is not equal to 0.

$$\chi = \psi_0 e^{-\lambda x} \quad (\text{Equation 5})$$

$$[(M + B\lambda^2)\sigma_z - iA\lambda\sigma_x]\psi_0 e^{-\lambda x} = 0 \quad (\text{Equation 6})$$

So, this has to vanish so this is equal to 0 in order to have a non trivial solution of the problem and so that can be done. So, this can be solved if you multiply it by sigma X because of the reason that I told you this earlier that so a sigma Z sigma X will be equal to so the anti commutation relation and the commutation relations if you combine then this is equal to some sigma Y so that is why you multiply it by sigma Y.

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Multiplying by  $\sigma_y$

$$(M + B\lambda^2)\sigma_y\psi_0 - A\lambda\psi_0 = 0.$$

$$\lambda_{\pm} = \frac{1}{2B} \left\{ A \pm \sqrt{A^2 - 4BM} \right\}.$$

So, let me just write down just to help you in getting the steps we have written this earlier that sigma I sigma J so sigma Z sigma X so this is equal to 2I sigma Y that is the commutation relation and what is the anti commutation relation the anti commutation relation says that sigma Z sigma X is equal to 0 okay so that is the anti commutation relations. So sigma Z sigma X is minus sigma X sigma Z equal to 2I sigma Y and sigma Z sigma X plus sigma X sigma Z equal to 0 so if we add both of them we have a 2 sigma Z sigma X equal to 2I sigma Y so this 2 will cancel so sigma Z sigma X becomes I sigma Y and that is why we multiply these let us call it as 5 by sigma X so that I get a sigma Y and sigma X square is equal to 1 so this will be independent of that Pauli matrix and this one the first term will have a sigma Y. So multiplying by sigma Y one gets M plus B lambda square sigma Y and a psi 0 and minus A lambda psi 0 equal to 0 now you see this becomes simple because this now psi 0 is an eigenfunction of sigma Y which is known okay sigma Y can be solved sigma Y as eigenvalues plus minus 1.

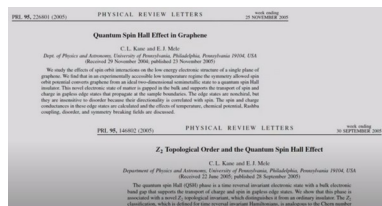
$$(M + B\lambda^2)\sigma_y\psi_0 - A\lambda\psi_0 = 0$$

$$\lambda = \frac{1}{2B} \{A \pm \sqrt{A^2 - 4BM}\}$$

So if you solve for lambda, lambda comes out as  $1 \pm \sqrt{2B/A + \sqrt{A^2 - 4BM}}$  and so if we you know plot it as a function of K near K equal to 0 etcetera and so on and then this should give rise to the similar band dispersion as we have seen for the HGT, CDT and the quantum well structures and will of course the nature of the edge modes will depend upon the specifics of the boundary condition. So one can actually solve it numerically in order to get the different you know the dispersion of the BHZ model for various choices of A, B, M etcetera and it can be plotted in the Brillouin zone to get this dispersion and this for you know choices of the parameters there will be the edge modes will occur in the system and for other choices of parameters there will be no edge modes. So the edge modes the ones the corresponding the parameters that have edge modes will be called as a topological system or a quantum spin hall insulator whereas the ones which do not have edge modes and simply there is a gap there is an energy gap in the bulk of the spectrum that represents a band insulator. So this is another study that we have done in the family of hall effects other than the hall effect that we have done quite rigorously and this hall effect is called as spin hall effect and we have talked several times that it has significant applications in the spintronic devices.

So if a material has strong spin orbit coupling then one can actually get these band inversion properties and this band inversion is key to getting this quantum spin hall insulators of this quantum spin hall phases and here it turns out for a thickness of the mercury telluride slab to be larger than certain thickness which is 6.3 nanometer one has a dominance of the mercury telluride in the in the overall band structure which is when the band inversion occurs and hence that gives rise to a quantum spin hall insulator. And Bernawieck, Hughes and Zhang have written down Hamiltonian considering all the symmetries and the low energy properties they wrote down a Hamiltonian which can be solved and nature of the eigenvalues and the eigen functions can be discussed.

**(Refer Slide Time:50.04)**



We shall come back to the BHZ model after we look at a theoretical model proposed by Ken and Millie in 2005 which also describes a quantum spin hall insulator. We shall further establish a connection between the Ken Millie model and the BHZ model that we have looked at. Thank you.