

Topology and Condensed Matter Physics
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Lecture – 22

Kane Mele model with Rashba spin-orbit coupling, spin Hall conductivity

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Kane Mele model

$$H_{KM} = \sum_{i,j} t_{ij} c_i^\dagger c_j + i\lambda_{so} \sum_{i,j} v_{ij} c_i^\dagger s_z c_j + \lambda_v \sum_i \xi_i c_i^\dagger c_i$$

Simplest model: $|Haldane|^2$ (conserves S_z)

Spin \uparrow : The Haldane model with $\phi = \pi/2$

Spin \downarrow : The Haldane model with $\phi = -\pi/2$

$$H_{KM} = H(Haldane, \phi = \frac{\pi}{2}) + H(Haldane, \phi = -\frac{\pi}{2})$$

$$H_{K\downarrow} = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix}$$

$H_{K\downarrow}$: 2x2 Hamiltonian in Dirac basis

Hamiltonian obeys time-reversal symmetry

So, in the last class we have talked about the Ken Milley model, but I have gone a little fast there in order to finish up the calculation of the Z_2 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 ok. So, we start with this again with the Ken Milley Hamiltonian, I have already told that there are certain features that are distinct from the Holden model and we 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 T_2 or a λ SO there mostly in literature it is used as λ SO. So, I have written it as λ SO and this is the Semenoff term which opens up a gap of trivial nature at the Dirac points ok. So, it is a simple model which is 2 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 s_z .

$$H_{KM} = \sum_{\langle i,j \rangle} t_{ij} C_i^\dagger c_j + i\lambda_{so} \sum_{\langle\langle i,j \rangle\rangle} v_{ij} c_i^\dagger s_z c_j + \lambda_v \sum_i \xi_i c_i^\dagger c_j$$

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 Halden model with a flux ϕ equal to π by 2. You remember the flux comes from these the second neighbor hopping which is exponential $i\phi$ and then of course, so one has a $c_i^\dagger c_j$ now this is second neighbor. So, we write it with the 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.

$$H_{KM} = \begin{pmatrix} H_\uparrow & 0 \\ 0 & H_\downarrow \end{pmatrix}$$

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 Halden model and with us this flux equal to minus π by 2. So, there is a flux π by 2 for the up spin and minus π by 2 for the down spin and this 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_\uparrow and H_\downarrow like a 2 by 2 Hamiltonian of the Dirac form. What I mean by Dirac form is that it can be written as $d \cdot \sigma$ and the Hamiltonian has time reversal symmetry now which we have discussed elaborately.

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Kane-Mele Model

A Rashba spin-orbit coupling (SOC) term can be added:


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

The results are qualitatively same without the Rashba SOC.

We can get **spin filtered edge states** which leads to spin currents along the edges.

\vec{d}_{ij} is the unit vector that connects the site i to its NN site j

Quantum spin Hall state can be observed in this system that is this system will show quantum spin Hall conductance of $e/2\pi$ but it will have zero charge Hall conductance.



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 $i\lambda_R \sum_{\langle i,j \rangle} c_i^\dagger (\vec{\sigma} \times \vec{d}_{ij})_z c_j$ and there is a c_i^\dagger and these $\sigma \times d_{ij}$ will tell you what d_{ij} is, d_{ij} 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 block structure that you see here. So, now how do I get this term and how this thing comes into picture is what we will see.

$$H_{KM} = t \sum_{\langle ij \rangle} c_i^\dagger c_j + i\lambda_{so} \sum_{\langle \langle i,j \rangle \rangle} v_{ij} c_i^\dagger s_z c_j + i\lambda_R \sum_{\langle i,j \rangle} c_i^\dagger (\vec{\sigma} \times \vec{d}_{ij}) c_j + \lambda_v \sum_i \xi_i c_i^\dagger c_j$$

And so, some of the results are same with and without the Rashba spin orbit coupling though they are quantitatively different and 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 now 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. Ok 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 2π . Let me try to derive this term that you see here the λ_R term and this is like how this $\sigma \times d_{ij}$ 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.

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The wave function in Wannier basis,

$$\Psi(\vec{r}) = \sum_i c_i w(\vec{R}_i - \vec{r}) \quad (1)$$

The ortho-normality condition is given by,

$$\int d^3r [w^*(\vec{R}_i - \vec{r}) w(\vec{R}_j - \vec{r})] = \delta_{ij} \quad (2)$$

From the first principle calculation, the derivatives can be written as,

$$\vec{\nabla} w(\vec{R}_i) = \frac{d}{d} [w(\vec{R}_i + \vec{d}) - w(\vec{R}_i)]/d \quad (3)$$

The momentum operator is written as,

$$\hat{p}_z \Psi = -i\hbar \sum_i c_i \vec{\nabla} w(\vec{R}_i) = -i \sum_i c_i \hat{e}_z \cdot \vec{\nabla} w(\vec{R}_i) = -i \sum_i c_i \frac{d}{dz} (w(\vec{R}_i + \vec{d}) - w(\vec{R}_i)) \quad (4)$$

Handwritten notes include: $\frac{f'(x)}{dx} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$ and $\vec{\nabla} = -i\hbar \frac{\partial}{\partial \vec{r}}$.

Ok so we write down the wave function in the Vanier basis ok and the wave function is of this form where these c_i s are the operators and these w_s are the the Vanier wave functions and the Vanier 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^* which is a Vanier 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 Vanier functions. Ok now this is well known that when you want to write derivatives on a lattice one does it like this that.

$$\psi(\vec{r}) = \sum_i c_i \omega(\vec{R}_i - \vec{r}) \quad (\text{Equation 1})$$

$$\int d^3r [\omega^*(\vec{R}_i - \vec{r}) \omega(\vec{R}_j - \vec{r})] = \delta_{ij} \quad (\text{Equation 2})$$

So, it is a f' 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 a definition that we have learned probably in school. So, there is these Vanier functions which are written at r_i plus d site where d is the nearest neighbor site and taken a subtracted the Vanier function at the i th 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 $i\hbar$ cross ∇ of x . So, for ∇ of x there is a shorthand notation which is ∇ of x and we have taken \hbar 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 an operator at the site i and that is the Vanier 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.

$$\vec{\nabla} \omega(\vec{R}_i) = \frac{\vec{d}}{d} [\omega(\vec{R}_i + \vec{d}) - \omega(\vec{R}_i)] / d \quad (\text{Equation 3})$$

$$\begin{aligned}
 \dot{p}_x &= -i\delta_x \sum_i c_i \omega(\vec{R}_i) = -i \sum_i c_i \hat{e}_x \cdot \vec{\nabla} \omega(\vec{R}_i) \\
 &= -i \sum_i c_i \frac{dx}{d^2} (\omega(\vec{R}_i + \vec{d}) - \omega(\vec{R}_i))
 \end{aligned}
 \tag{Equation 4}$$

So, del del x is nothing, but say something like a gradient vector and this gradient is written as x cap dot 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 d x by d square and so on ok. 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 d x over d square and these the Vanier functions at the or the difference between the Vanier functions at the consecutive or the nearest neighbor sites.

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Therefore,

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

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

Therefore we get,

$$\int d^3r [\Psi^\dagger(\vec{r}) \hat{p}_x \Psi(\vec{r})] = -i \sum_{(i,j)} c_i^\dagger c_j \frac{dx}{d^2} \tag{6}$$

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

$$\int d^3r [\Psi^\dagger(\vec{r}) \hat{p}_y \Psi(\vec{r})] = -i \sum_{(i,j)} c_i^\dagger c_j \frac{dy}{d^2} \tag{7}$$

So, we are ultimately interested in a quantity like this which is psi dagger p x psi and that is because that would be there in this kind of a term. So, we are 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.

$$\int d^3r [\psi^\dagger(\vec{r}) \hat{p}_x \psi(\vec{r})] = -i \sum_{i,j} c_i^\dagger c_j \int d^3r \frac{dx}{d^2} [\omega^*(\vec{R}_i) \{\omega(\vec{R}_j + \vec{d}) - \omega(\vec{R}_j)\}] \tag{Equation 5}$$

$$\int d^3r [\psi^\dagger(\vec{r}) \hat{p}_x \psi(\vec{r})] = -i \sum_{i,j} c_i^\dagger c_j \frac{dx}{d^2} \tag{Equation 6}$$

So, this is that $c_i^\dagger c_j$ coming from the dagger is coming from ψ^\dagger and c_j is coming from ψ 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 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 .

$$\int d^3r [\psi^\dagger(\vec{r}) \hat{p}_y \psi(\vec{r})] = -i \sum_{i,j} c_i^\dagger c_j \frac{d_y}{d^2} \quad (\text{Equation 7})$$

So, this left hand side that we have in equation 5 has a form which is nothing, but this 6 where this W_{ri} and W_{rj} 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^2 and the volume integral over r goes on to make up for the orthonormality condition. And similarly for p_y let us write it as 7 and then we have a d_x over d^2 and a d_y over d^2 and so, this is p_x and p_y that one gets here. 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 ok. 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 .

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Now, the Rashba term can finally be written as,

$$\begin{aligned} & \gamma \int d^3r [\Psi^\dagger(\vec{r}) (\sigma_x p_y - \sigma_y p_x) \Psi(\vec{r})] \\ &= i \frac{\gamma}{d^2} \sum_{(i,j)} c_i^\dagger (\sigma_x d_y - \sigma_y d_x) c_j \\ &= i \lambda \sum_{(i,j)} c_i^\dagger (\vec{\sigma} \times \hat{d}) \cdot \hat{z} c_j \end{aligned}$$

$(\vec{\sigma} \times \hat{d})_z$
 $(\vec{\sigma} \times \hat{d}) \cdot \hat{z}$

Now, this that the Rashba term is written as $\sigma_x p_y$ minus $\sigma_y p_x$ ok. This is basically the σ cross p and the z component of that or you dotted with the z ok. 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 ok. 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.

$$\begin{aligned} & \gamma \int d^3r [\psi(\vec{r})(\sigma_x p_y - \sigma_y p_x)\psi(\vec{r})] \\ &= i \frac{\gamma}{d^2} \sum_{i,j} c_i^\dagger (\sigma_x d_y - \sigma_y d_x) c_j \\ &= i \lambda \sum_{i,j} c_i^\dagger (\vec{\sigma} \times \vec{d}) \cdot \hat{z} c_j \end{aligned}$$

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 ok. 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 wrote a constant a coefficient of this Rajbha term and this is nothing, but what we want ok. So, the Rajbha 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 ok.

This one needed a little bit of hand holding in order to derive this form, but I wanted not to break the flow in calculation of the Z 2 invariant which is why I skipped it there, but now you have it here ok.

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Kane-Mele Model

The momentum space Hamiltonian is given by, *By Fourier transforming Eq. I.*

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

Where,

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

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

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 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

Rajbha term ok 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 hereok. So, this Hamiltonian so, this is the most important equation and let us call it as a capital 1 ok. And so, this is by Fourier transforming that capital 1 ok.

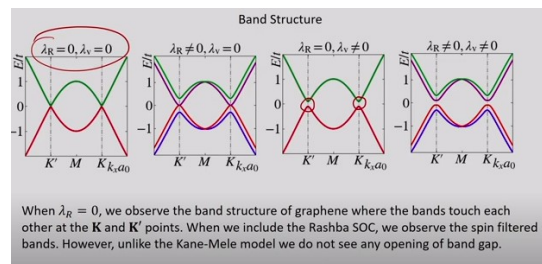
$$\zeta(k) = te^{-ik_y a} + 2te^{\frac{ik_y a}{2}} \cos \frac{\sqrt{3}k_x a}{2}$$

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

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

And 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 winding 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. 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.

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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 λ_r or λ_v and then one has a touching Dirac points here and once when one switches on a λ_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 λ_v equal to 0, but λ_r not equal to 0 a trivial gap opens up at the Dirac 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. 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.

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Rashba spin orbit interaction.

Lorentz force : $\vec{F}_L = -e \vec{v} \times \vec{B}$ $\mu_B = 9.27 \times 10^{-24} \text{ J/T}$

$E_z = \mu_B \vec{\sigma} \cdot \vec{B}$

When an electron moves in an electric field \vec{E} , then in its rest frame, it experiences

$\vec{B}_{\text{eff}} = -\frac{\vec{E} \times \vec{v}}{c^2}$ c : speed of light.

$E_z' = \mu_B \vec{\sigma} \cdot \left(\frac{\vec{E} \times \vec{v}}{c^2} \right) = \mu_B \vec{\sigma} \cdot \vec{B}_{\text{eff}}$

$H_{so} = \frac{\mu_B}{mc^2} \vec{\sigma} \cdot \left(\frac{\vec{E} \times \vec{p}}{mc} \right)$ $\vec{E} = -\vec{\nabla} V$
 $v: c$

Let me do a little discussion on the Rashba term. 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 Lorentz force on the charged particle. So, the Lorentz force is given by \vec{F}_L and which is equal to a minus $e \vec{v} \times \vec{B}$. 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 E_z and which is equal to a $\mu_B \vec{\sigma} \cdot \vec{B}$. There is of course one is force the other is energy.

$$\vec{F}_L = -e \vec{v} \times \vec{B}$$

$$E_z = \mu_B \vec{\sigma} \cdot \vec{B}$$

So, this is what we are writing and then μ_B is called as a Bohr magneton which has a value 9.27×10^{-24} joule per Tesla. So, now when the electron is subjected to an electric field then in the rest frame of the electron it experiences a magnetic field. So, let me write that in its rest frame it experiences an effective magnetic field $B_{\text{effective}}$ which is given by $-\frac{e}{c} \mathbf{v} \times \mathbf{E}$ where c is the speed of light. This is electrodynamics you can check Griffiths book.

So, that is the effective magnetic field that it experiences and this gives you an effective Zeeman energy which is given by $\mu_B \mathbf{B}_{\text{effective}} \cdot \mathbf{\sigma}$. So, it is $\mathbf{B} \cdot \mathbf{\sigma}$ or $\mathbf{\sigma} \cdot \mathbf{B}$ does not matter I mean you can write it. So, this is the so it is $\mathbf{\sigma} \cdot \mathbf{B}$ which is nothing but so this is like $\mu_B \mathbf{\sigma} \cdot \mathbf{B}_{\text{effective}}$ and $B_{\text{effective}}$ appears just on the step above. So, this $\mathbf{v} \times \mathbf{E}$ 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 $\frac{\mu_B}{mc^2} \mathbf{L} \cdot \mathbf{\sigma}$ now I make this \mathbf{v} as \mathbf{p}/m and this is written as $\frac{\mu_B}{mc^2} \mathbf{L} \cdot \mathbf{\sigma}$ and there is a $\mathbf{\sigma}$ dot there ok. 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 \mathbf{E} in crystal lattice.

$$B_{\text{eff}} = \mu_B \mathbf{\sigma} \cdot \left(\frac{\mathbf{E} \times \mathbf{p}}{c^2} \right)$$

$$H_{SO} = \mu_B / mc^2 \mathbf{\sigma} \cdot \left(\frac{\mathbf{E} \times \mathbf{p}}{mc^2} \right)$$

So, \mathbf{E} is originated by the crystal potential which is given by $-\nabla V$ 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 \mathbf{E} becomes in the direction of \hat{z} cap ok.

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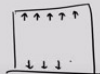
$$H_{SO} = \frac{\alpha_R}{\hbar} (\hat{z} \times \mathbf{p}) \cdot \mathbf{\sigma} \quad \frac{\alpha_R}{\hbar} \rightarrow \frac{\mu_B E_z}{mc^2}$$

α_R in $\text{LaAlO}_3 / \text{SrTiO}_3$ $\alpha_R = 0.5 - 0.6 \times 10^{-11} \text{ eV-m}$

in Topological insulators $\alpha_R = 4 \times 10^{-10} \text{ eV-m}$

In presence of the Rashba spin-orbit coupling,

Velocity: $V_{\sigma} = \frac{\partial H_{SO}}{\partial \mathbf{p}} = -\alpha_R \hat{z} \times \mathbf{\sigma}$



So, it is in the direction of \hat{z} this yields a form for the HSO as say we write it with the α_R by \hbar cross and then there is a \hat{z} cap across \vec{p} dot $\vec{\sigma}$ I have changed the order of this \vec{e} and which I have been doing it. So, $\vec{\sigma}$ dot this term or this term dot $\vec{\sigma}$ it really does not matter. So, this is a \hat{z} cap cross \vec{p} dot $\vec{\sigma}$ and then all these other things like mc^2 etcetera they are being absorbed here.

$$H_{SO} = \frac{\alpha_R}{\hbar} (\hat{z} \times \vec{p}) \cdot \vec{\sigma}$$

$$V_\sigma = \frac{\delta}{\delta k} H_{so} = -\alpha_R \hat{z} \times \vec{\sigma}$$

So, α_R by \hbar is it replaces this $\mu_B \hat{z}$ divided by mc^2 which are scalar quantities ok. So, the spin orbit coupling takes this form which is \hat{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 $\vec{\sigma}$ usually when we write the graphene Hamiltonian we denote σ to represent the sub lattice degrees of freedom, but this is a real spin ok.

so, there are this α_R is actually measurable and can also be enhanced by using gate voltage and various kinds of other things such as heavy adlayer terms like gold etcetera in a graphene matrix, but I will not go into details of that. So, typical values of α_R in these La AlO₃ these are interface of this hetero structures SRTIO₃ etcetera this has a value it is about 0.5 to 0.6 into 10^{-11} eV m whereas, for some of the topological insulators α is typically 1 or 2 orders of magnitude large and it can have a value which is 10^{-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 ok. It unfortunately turns out that the magnitude of the spin orbit coupling or that α_R or the strength of the spin orbit coupling in graphene is quite small it is of the order of a few meV. However, it is still has a fundamental importance in this study of quantum spin hall insulators and the study of spintronics which could be 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 potential candidates for doing a device making ok 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 ok.

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 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 when they move in a system they will 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 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 ok.

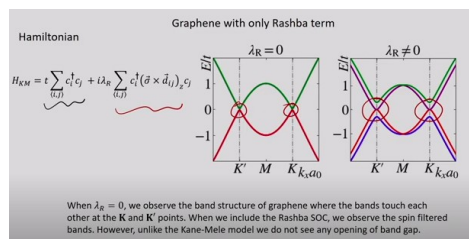
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	Chern insulator (Haldane Model)	QSH insulator (Kane Mele Model)
1.	Chiral edge states	Helical edge states (Spin filtered)
2.	Chern number as the topological invariant	\mathbb{Z}_2 invariant
3.	Time Reversal Symmetry (TRS) is broken	TRS is intact
4.	Quantum anomalous Hall effect	Spin Spin Hall effect
5.	Plateau at $\frac{e^2}{h}$	Plateau at $\frac{e}{2\pi}$
6.	Low energy Hamiltonian $H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \frac{1}{2} \sum_i \sigma_i^x$	$H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \frac{1}{2} \sum_i \sigma_i^x$

So, let me do a comparison between the Holden model or we what we call as a churn insulator and this quantum spin hall insulator. So, we will call a churn insulator or same as Holden model and quantum spin hall insulator QSH insulator and or a same as Kenmele model ok. 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 churn number as the topological invariant and that is why they are called as churn insulator Z_2 invariant ok. 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^2/h last, but not the least of course, we have a low energy Hamiltonian $h = \hbar v_F q_x \sigma_x + \hbar v_F q_y \sigma_y + \frac{3}{2} \sqrt{3} \tau_z$ which you can call it either a λ SO also $\sigma_z \tau_z$ and similarly a low energy Hamiltonian is $h = \hbar v_F q_x \sigma_x + \hbar v_F q_y \sigma_y + \frac{3}{2} \sqrt{3} \tau_z \sigma_z$ that is the spin and plus a λ 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 σ denotes the sub lattice degrees of freedom while S denotes the actual spin degrees of freedom ok. So, these are a summary of these two type of insulator and both are very important in their own right ok.

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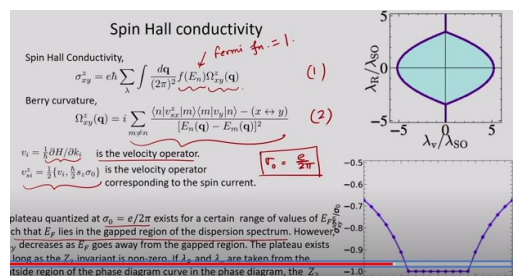


So, here we just show that the graphene only with the Rashba term there is no Holden term and so on. So, you see that this is just the tight binding graphene and this is the Rashba term. So, you see that there are this semi Dirac or semi metallic nature not semi Dirac semi metallic nature at the k and the k prime points which also that there is a band touching because without a σ V or the Holden term there will be no lifting of gap, but now you see the spin resolved bands ok.

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

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 ok.

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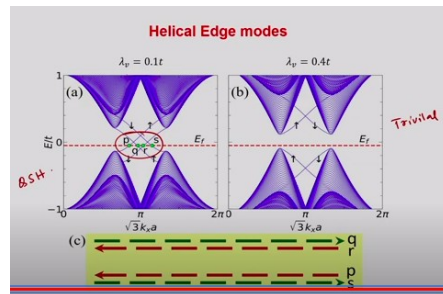
So, finally, the spin hall conductivity which is obtained using. So, this is the spin hall conductivity with you can call it a S also, but it is written with a Z because you are talking about the Z component of the velocity. So, this is really the spin hall not the charge hall conductivity which is equal 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 kx and ky or you differentiate. So, for Vx you take a del kx and for Vy take a del ky 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 si and the Z component which requires one to calculate the anti-commutation relation of these quantities. So, it is a if you want V sx Z then you take a Vx and then h cross by 2 Sz sigma 0 sigma 0 is simply e over 2 pi this is just the scale of the conductance ok. 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.

$$\sigma_{xy}^z = e\hbar \sum_{\lambda} \int \frac{dq}{2\pi^2} f(E_n) \Omega_{xy}^z(q)$$

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 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 very symmetric and so on. So, this is e over 2π 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 goes away and the spin hall conductance becomes dispersive or it 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 ok. And so, in this so, if λ_r and λ_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 ok. So, this is by and large what one gets from the Ken Milley model and the explicit calculations of all the quantities that are of importance are presented here ok.

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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 that light blue region that is sky blue region inside and for the right panel you are outside ok. This is what completes the discussion on the Ken Milley model.

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Let me do a summary slide for the quantum spin hall phase the mercury telluride and the cadmium telluride quantum wells and the Ken Milley 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 Ken Milley 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 Bernawieck. So, these people and later on many other people have contributed immensely to the development of the field.

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Why II-VI?

Periodic Table of the Elements

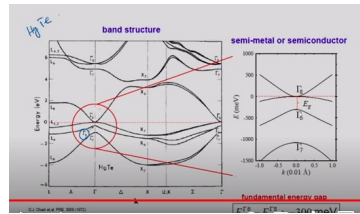
Comp. ---	12	13	14	15	16
2	Be	B	C	N	O
3	Li	Be	B	C	N
4	Na	Mg	Al	Si	P
5	K	Ca	Sc	Ti	V
6	Rb	Sr	Y	Zr	Nb
7	Cs	Ba	La	Hf	Ta

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.

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 Bi_2Se_3 etcetera where only one orbital is near the Fermi level there are 2 orbitals involved in the in making up the energy levels close to the Fermi level.

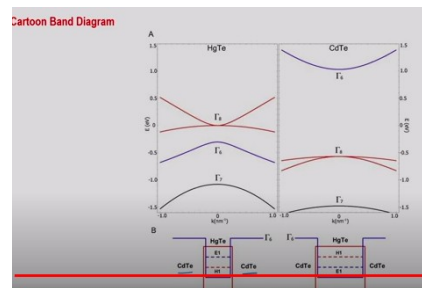
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And even though this has been discussed I mean in the sense that this is this gamma is actually the high symmetry point in the Brillouin zone and these gamma is subscripted with these 6, 7 and 8 you see that there is a 6 here there is a 7 here and 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 CDT 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. Very interestingly the mercury telluride HgT 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 HgT 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.

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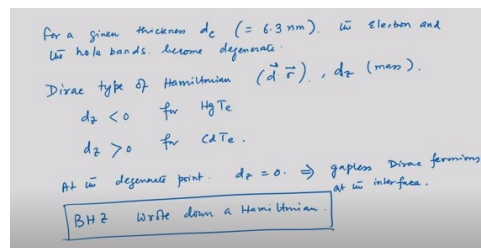


So, this is interesting and when you make a structure out of it when you make a sandwich the mercury telluride in between two cadmium telluride slabs when the mercury telluride start starts dominating the phase diagram or dominating the physics and that's when there is a interesting thing happens and 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 HgT is inside and there are these CdTs outside. So, the electron and the hole bands are shown by blue and red colors and so on and when the width of the well it is increased.

So, this way you increase the electron is 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.

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Now there are 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 hole bands they become the same. So, this is the electron and the hole band they become degenerate. So, this one so $E1$ and $H1$ they merge so this basically is shown one electron band and hole 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 $E D$ 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 $d \cdot \sigma$ then the d_z which is the mass term. So, this d_z is a less than 0 for a GTE which means it's negative that's why the inverted band structure comes and d_z greater than 0 for CDT.

So, at the degenerate point the mass term d_z is equal to 0. So, where one sees the gapless Dirac fermions at the interface. So, based on this BHZ wrote down a Hamiltonian. So, this is the Hamiltonian. So, this is the 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 γ_6 and the γ_8 levels which are connected by time reversal symmetry because this has time reversal symmetry. So, they are basically the Cramer's pairs and the spin split Cramer's pairs.

And so, in the same spirit the Ken Milley Hamiltonian is also block diagonal without the Rachmaninoff term and that gives rise to a spin hall quantum spin hall phase. So, there is a connection between this and the Ken Milley Hamiltonian and this is the same which also is block diagonal in the spin space and one can calculate and that is what we have shown here. Thank you.