

Quantum Hall Effect
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Lec 17: Quantum spin Hall insulator, Kane-Mele Model

We have seen Haldane model or the Chern insulator which is characterized by a nonzero Chern number and the insulator is characterized by a time reversal symmetry broken. There is no time reversal symmetry in the system which is induced by the second neighbour complex hopping which we have mentioned and is this picture of Haldane and later on in about 2004-2005 Kane and Mele this is Charlie Kane and Eugene Mele they have understood that it is possible to recover the time reversal invariance and this would create another insulator which is called as a quantum spin Hall insulator. In fact what they have realized was very profound that if we include the spin degrees of freedom in the system actual spin degrees of freedom not the pseudo spin that we have been talking about so far then it is possible to regain back the lost time reversal symmetry. Of course the system would not have Chern number or it is not will not be called as Chern insulator but it will be another kind of insulator which is known as the quantum spin Hall insulator which is what we will see. So, Kane and Mele they proposed this model which is known as the Kane Mele model and these are the papers that you see that which were published in 2005 in the physical review letters by both Kane and Milley the one of them is called as the quantum spin Hall effect in graphene which they realized that because along with the spin orbit coupling term there is the Hamiltonian respects all symmetries of that of graphene. So, it is quite likely that it will be there in graphene and then they wrote another paper in the same year or rather this paper came earlier than the next one which says about a Z_2 topological order and the quantum spin Hall effect.

So, Z_2 index or the Z_2 topological invariant is the new topological invariant for this system which is distinct from the Chern number because in this system the Chern number is 0 because the system has time reversal invariance. So, this is what we are going to study which goes by the name quantum spin Hall insulator. So, here of course as I said earlier that the time reversal invariance is not lost it is in fact preserved in the systems and the system will show protected boundary modes or edge modes very similar to the Haldane model or the Chern insulator, but here it will be spin resolved modes and they are called as a helical edge modes that are present in the system and as I said that they will be characterized by a Z_2 invariant. So, let me write down these two points.

So, helical edge states that are spin resolved and characterized by Z_2 invariant and we will see what the Z_2 invariant is and we will of course stick to a simpler situation in which the system has inversion symmetry and there the calculation of the Z_2 invariant is easier than of course without a translation or rather the inversion symmetry in the problem. So, the main ingredient of this kind of quantum spin Hall insulator is what is known as the spin orbit coupling and in the most simple way that one can understand is that the angular momentum and the spin are coupled and if the scenario is like this then we know that neither of L or S are good quantum numbers and one actually talks about J which is a good quantum number in this case and one can find out the eigenvalue of this $L \cdot S$ operator in the eigen basis which is spanned by you know J, J_1, J_2, M_1, M_2 and so on so forth. So, the spin orbit coupling is as I said it is an important ingredient in this problem and this special kind of spin orbit coupling is what we shall be talking about it is called as a Rashba spin orbit coupling and it has a special place in graphene because graphene is two-dimensional which has the inversion symmetry about the Z axis is broken and Rashba is a very possible candidate in graphene. So, we will be talking about that and so what kind of spin orbit coupling are we talking about here we are talking about a spin orbit coupling let us write down a Hamiltonian which looks like we may use a different notation but right now we are using a λ SO which is nothing but that second neighbor hopping t_2 that we have talked about in the Haldane model and then there is a σ_Z and then there is a τ_Z and then there is a S_Z okay and we will actually derive this term a part of it is already derived like this term is there in the Haldane model we just have gotten this S_Z extra. Now the σ_Z just to remind you is the sub lattice degrees of freedom τ_Z is a valid degree of freedom and S_Z is a real spin so spin degree of freedom so S_Z equal to a plus or minus 1 for a spin half particle.

So, why this term respects time reversal symmetry it respects time reversal symmetry because under time reversal symmetry the τ_Z changes sign that is one is taken from the K Valley to the K' Valley or K Dirac point to the K' Dirac point so that changes sign so under time reversal this τ_Z goes to minus τ_Z and we will see in a while that S_Z also goes to minus S_Z so an up spin goes to down spin and σ_Z does not change sign because that is the sub lattice degree of freedom and under time reversal it does not change sign so there is no net let me also write that σ_Z does not change sign. So, there is no net sign change and this is the main thing about this quantum spin Hall insulators and we now have taken into account the real spin degrees of freedom. So, if you take this S_Z equal to 1 and minus 1 separately so plus 1 and S_Z equal to minus 1 so this is one copy of the Haldane model and this belongs to another copy of the Haldane model okay such that the Chern number or the Hall conductivity will be a plus e^2/h and minus e^2/h that is equal to 0.

Quantum Spin Hall insulator.

- (1) Helical Edge states
- (2) characterized by a \mathbb{Z}_2 invariant.

Spin-orbit Coupling. $\vec{L} \cdot \vec{S}$

$$H_{SO} = \lambda_{SO} \underbrace{\sigma_z \tau_z}_{\text{valley}} S_z.$$

σ_z : sublattice degrees of freedom.

τ_z : valley " " "

S_z : spin " " "

$S_z = +1 \rightarrow$ one copy of Haldane Model

$S_z = -1 \rightarrow$ Another " " "

Under time reversal

$$\left. \begin{aligned} \tau_z &\rightarrow -\tau_z \\ S_z &\rightarrow -S_z \end{aligned} \right\} \begin{array}{l} \sigma_z \text{ does} \\ \text{not} \\ \text{change} \\ \text{sign.} \end{array}$$

There is no net
sign change !!

$$\left. \begin{aligned} \sigma_{xy} &= \frac{e^2}{h} - \frac{e^2}{h} \\ &= 0. \end{aligned} \right\}$$

But nevertheless one has a quantity called as the spin current which is defined as J_s which is equal to \hbar over $2e$ J_{\uparrow} minus J_{\downarrow} so this will be nonzero and we will have a σ_{xy} a spin Hall let us write it with the s this is equal to a nonzero e over 2π . So it is a distinct topological insulator compared to Haldane model and 2d electron gas we have used this abbreviation several times in presence of an external magnetic field okay. So this is the new thing that is going to come and it is a new form of topological insulator the second kind so to say after the ones that we have seen for either 2d electron gas in an external field or a Haldane model where time reversal symmetry is broken by a second neighbour complex hopping okay.

$$J_s = \frac{\hbar}{2e} (J_{\uparrow} - J_{\downarrow}) \neq 0.$$

$$\sigma_{xy}^s = \frac{e}{2\pi}.$$

It is a distinct topological insulator, compared to Haldane Model.
and 2DEG in presence of an external magnetic field.

So in order to understand this better let me talk about the time reversal symmetry in a spinful model okay I mean spinful model means a Hamiltonian that includes spin real spin or let me write it as in presence of spin. Let me remind you that the time reversal

symmetry operator without any spin present in the problem is the complex conjugation operator. So without spin we will write for this time reversal symmetry or symmetric system as TRS so without spin TRS operator is simply K which is the complex conjugation okay. So we can write it with a slightly tilted T which is nothing but equal to K but with spin this is not sufficient and let me tell you that why it is not sufficient okay and the reason that it is not sufficient is that because this complex conjugation operator will act on the Sigma x let me write it with just K acting on Sigma x will give Sigma x will not change its sign K acting on Sigma y will give you a minus Sigma y because Sigma y is complex and K acting on Sigma z will give you a Sigma z without changing its sign but why do we want it to change sign. So let us go back to that the spin orbit coupling and which is written as $\vec{L} \cdot \vec{S}$ now under this time reversal L goes to minus L and S goes to minus S so that there is no change in sign.

Now you see that since we are talking about spin half particles we have resorted to the Pauli matrices now you see that both Sigma x and Sigma z do not change sign but we want them to change sign. So there is some other operator that we need to think about which will give us a change in sign for all of Sigma x Sigma y and Sigma z and that can be done in the following sense I am drawing a coordinate axis but this is in the spin space so this is say x this is y and this is z so this is actually s x s y and s z if you like and then if I do a rotation by pi about the y axis then x become minus x and z becomes minus z. So rotation by pi x becomes minus x and z becomes minus z and y remains as y because it is a rotation about the y axis.

Time reversal symmetry in presence of spin.
(TRS)

Without spin TRS operator is K (complex conjugation).

$T = K$.

But with spin, this is not sufficient! Why?

$K \sigma_x \rightarrow \sigma_x$ $K \sigma_y \rightarrow -\sigma_y$ $K \sigma_z \rightarrow \sigma_z$

Spin-orbit coupling. $\vec{L} \cdot \vec{S}$

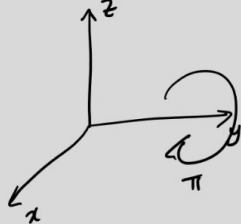
Under time reversal

$\vec{L} \rightarrow -\vec{L}$
 $\vec{S} \rightarrow -\vec{S}$

} No. change in sign.

A rotation by π

$x \rightarrow -x$
 $z \rightarrow -z$
 $y \rightarrow y$



Now this is as I said that this is in the spin space which means that such a rotation will make σ_x to minus σ_x and σ_z to minus σ_z and will not do anything to σ_y but σ_y by virtue of being complex will change a sign under the complex conjugation. So we are looking for an operator that does this rotation about the y axis by π and if you remember the quantum mechanics angular momentum of quantum mechanics such a rotation is written as so this rotation operator is written as exponential say for example $e^{-i\pi S_y/\hbar}$ okay and now the time reversal operator will be this into k okay and since we are talking about this Pauli matrices or other spin half objects we can make a simplification that S_y is equal to \hbar cross by 2 σ_y and or rather all components will follow this relation that is S_x equal to \hbar cross by 2 σ_x and S_z equal to \hbar cross by 2 σ_z .

So if we do that then this complex conjugation operator will be like exponential minus $i\pi$ by 2 σ_y okay and then of course we will have to write down this. So let me deal with this for the moment and this is easy to work out so this will we can write this as a cosine of π by 2 σ_y and a minus i sine π by 2 σ_y . So let me show how this simplification is done so cosine π by 2 σ_y is equal to so cosine of π by 2 σ_y is equal to 1 and minus these π by 2 σ_y whole square there is a half factor here which is $1/2$ factorial and then there is a $1/4$ factorial and π by 2 σ_y to the power 4 and so on. So there is a plus minus plus minus now this can be written as if you remember the properties of the Pauli matrix then this σ_y squared equal to 1 and that gives you that σ_y cube is equal to σ_y and so on so forth okay. So each even power of σ_y will give us 1 and each odd power will give us just simply σ_y okay.

So that tells you that this becomes equal to 1 minus there is a $1/2$ factorial and then there is a π by 2 and so on so forth square plus $1/4$. So it is a π by 2 whole to the power 4 and so on and this is nothing but cosine of π by 2 which is equal to 0 okay and similarly but the sine of π by 2 σ_y will have these all the odd terms which are there so this is equal to a π by 2 σ_y minus $1/2$ factorial π by 2 σ_y cube and a plus $1/4$ factorial I am sorry this 5 factorial π by 2 σ_y whole to the power 5 and so on okay. So this is nothing but equal to so because your σ_y cube is σ_y and there are σ_y so that σ_y into a σ_y sine π by 2 σ_y which gives you so this operator is exponential minus $i\pi$ by 2 σ_y is nothing but minus i the sine π by 2 equal to 1 so it is minus $i\sigma_y$ and that tells you that this time reversal operator for a spin full case which is what we wanted to derive is nothing but a minus σ_y and a k okay so that complex conjugation will be there. So this is a quite a known so that is the operator there and so on.

$$\begin{aligned}
 T &= e^{-i\pi s_y/\hbar} K = e^{-i\pi/2 \sigma_y} K. & \sigma_y^2 &= 1, \\
 s_y &= \frac{\hbar}{2} \sigma_y \Rightarrow T = e^{-i\pi/2 \sigma_y} K. & \sigma_y^3 &= \sigma_y \\
 e^{-i\pi/2 \sigma_y} &= \cos\left(\frac{\pi}{2} \sigma_y\right) - i \sin\left(\frac{\pi}{2} \sigma_y\right). \\
 \cos\left(\frac{\pi}{2} \sigma_y\right) &= 1 - \frac{1}{2!} \left(\frac{\pi}{2} \sigma_y\right)^2 + \frac{1}{4!} \left(\frac{\pi}{2} \sigma_y\right)^4 - \dots = 1 - \frac{1}{2!} \left(\frac{\pi}{2}\right)^2 + \frac{1}{4!} \left(\frac{\pi}{2}\right)^4 - \dots \\
 \sin\left(\frac{\pi}{2} \sigma_y\right) &= \frac{\pi}{2} \sigma_y - \frac{1}{3!} \left(\frac{\pi}{2} \sigma_y\right)^3 + \frac{1}{5!} \left(\frac{\pi}{2} \sigma_y\right)^5 - \dots \\
 &= \sin \frac{\pi}{2} \sigma_y. \\
 e^{-i\pi/2 \sigma_y} &= -i \sigma_y. \\
 T &= -i \sigma_y K.
 \end{aligned}$$

Now what do we do with this in the sense that how is it useful and what are the consequences of time reversal symmetry in a spin full model and a priori the consequences are quite significant it gives you what is called as a Kramer's degeneracy okay.

So let us see what Kramer's degeneracy is okay alright. So now we have of course written down that this is equal to a minus $i \sigma_y$ K if you take a square of that then it is equal to minus i square and σ_y square equal to 1 and K square of course equal to 1 as well because you do twice complex conjugation it comes back so this is equal to minus 1. Now there is something very important that in a spinless system where there is no spin τ square equal to 1 or these time reversal t square equal to 1 for spinless system. Now this minus 1 actually has a lot of interesting thing to go along with and let me see that and how does it lead to the degeneracy. What happens is that suppose if ψ is an eigenfunction of a Hamiltonian with energy E well this Hamiltonian is TRS invariant that is time reversal symmetry invariant with energy E then $T \psi$ is also another eigenfunction or rather $T \psi$ is actually perpendicular to or orthogonal to this it is also another eigenfunction with the same energy and this degeneracy is called as a Kramer's degeneracy.

So how do we see that that this $T \psi$ is and what is the nature of $T \psi$? $T \psi$ is a perpendicular or orthogonal to this so you take a inner product of ψ and $T \psi$ so this is just the T is written with a slight bit of you know curvature if I forget that you carry on with your notation. So this is equal to a T square ψ because so $T \psi$ okay T square ψ

because T you do this time reversal twice and should come back to the ψ and so this is nothing but a minus ψ because T^2 is equal to minus ψ and $T\psi$ and this is equal to minus of ψ and $T\psi$ and now this cannot be possible unless ψ and $T\psi$ is equal to 0 because if you take this the last term on this side then becomes twice of this and then so that means that I mean 2 cannot be 0 so this ψ and $T\psi$ are orthogonal okay. So this is one of the important implication of the time reversal symmetry in a spin full system that they are orthogonal to each other but they have the same energy and this is called as Kramer's degeneracy so this is Kramer's and the ψ and $T\psi$ are called as Kramer's doublets. Alright so let me come back to this band theory that is Bloch states so let us talk about the Bloch states which has you know K as a good quantum number of course the system has crystalline symmetries and so on.

Kramer's degeneracy:

$$T = -i\sigma_y K, \quad T^2 = -i^2 = -1.$$

$T^2 = 1$ for spinless system

If ψ is an eigenfunction of a Hamiltonian (TRS invariant) with energy E , then $T\psi$ is also another eigenfunction with same energy. \rightarrow Kramer's degeneracy.

$$\langle \psi | T\psi \rangle = \langle T^2 \psi | T\psi \rangle = \langle -\psi | T\psi \rangle = -\langle \psi | T\psi \rangle$$

$$2\langle \psi | T\psi \rangle = 0 \Rightarrow \langle \psi | T\psi \rangle = 0.$$

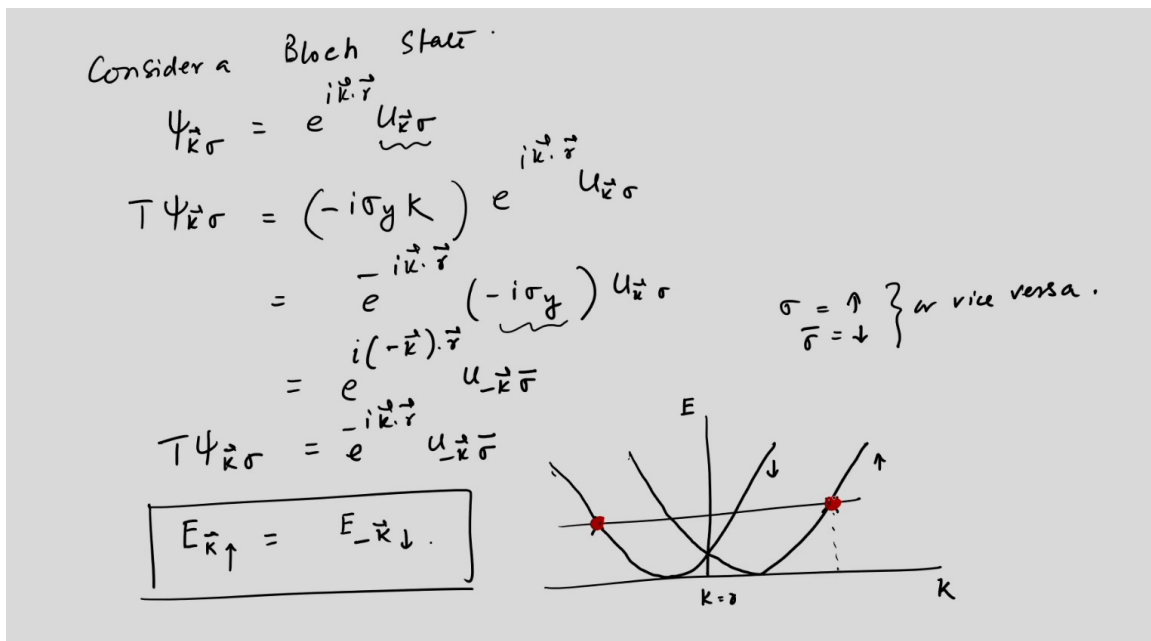
$|\psi\rangle, |T\psi\rangle$ are called as Kramer's doublets.

So if you consider a Bloch state which means that we are talking about a ψ_K with a spin σ this is equal to an exponential $iK \cdot r$ and $u_{K\sigma}$ where σ is a spin and σ can be up or down this is according to Bloch's theorem so this contains the periodicity of the potential and there is a free wave or there is a plane wave term there.

Now if I operate this $\psi_K \sigma$ then what happens is that so I will have to operate it by $i\sigma_y K$ on this $iK \cdot r$ $u_{K\sigma}$ and so this K will act on this and will make this exponential minus $iK \cdot r$ the plane wave part and we can write this as so exponential minus $iK \cdot r$ and then we have of course a minus $i\sigma_y u_{K\sigma}$ and now you see that this can be written as exponential of i minus $K \cdot r$ and then the job of this $i\sigma_y$ will be to invert the spin. So if there is a σ spin then there will be a $\bar{\sigma}$ spin where σ if σ is up then the $\bar{\sigma}$ will be down okay and because this looks like a minus K so this becomes equal to a minus K and a σ

bar and the bar so Sigma equal to up Sigma bar equal to down or vice versa. So this is equal to exponential minus i K dot r and a u minus K Sigma bar okay so that's what happens when you apply psi K Sigma on this. So which implies that there is of course a degeneracy such that E K up is equal to E minus K down and this is called as a Kramer's degeneracy okay. So there's a degeneracy of these up and down states for one given value of K but if it is plus K for the up spin then it's minus K for the down spin or vice versa and this of course has we know that this has a lot of implications on the topological insulators.

So what it means is the following that let me show this just a picture so we'll sort of see it like this there is so I'm just drawing parabolic bands for up and down spins they could be I mean you can interchange them doesn't matter so this is E as a function of K and you see that at K equal to 0 they sort of touch each other but the degeneracy is here So there is these two points let me use a color to mark them so this point and these points are degenerate but they correspond to two diametrically opposite points in the Brillouin zone and that's where the degeneracy comes. So for up spin it's at a K well we have done it just the other way around let me change the spin indices that way so this is down and this is up so this is that K so E at a K is degenerate with E at a minus K E at K for an up spin is degenerate with E at minus K for the down spin.



And this gives the rigidity of the edge modes in this particular spin full system or the Kane Mele model that we are going to discuss in just a while. So the back scattering from state a K upstate to a minus K downstate are forbidden and that's why these edge

states are these these are robust states. So let me come to this model the model is a very intuitive model and which has been introduced by Kane and Mele and that's the name that appears in the model and so on. This is the usual tight binding term that we all are familiar with and we have been seeing this in the context of graphene several times it's just a $\sum_i \sigma_i \sum_j C_i^\dagger C_j$ we haven't written any spin index here because it doesn't matter it's a spin polarized term which is just the tight binding kinetic energy of graphene.

Now this is what we have done just one small change that has occurred is that there is a $\sigma_i \sigma_i'$ term where $\sigma_i \sigma_i'$ can be up or down and this λ SO was nothing but t_2 in the Haldane model. So, Haldane model there is exactly the Haldane term but rather two copies of the Haldane term one corresponding to spin up with the flux which is given by $\pi/2$ and the down spin corresponds to a flux which has exactly equal and opposite magnitude which is equal to $-\pi/2$. And this is of course the term that we are familiar with that's the inversion symmetry breaking term and the term that was there in graphene because if we had sort of different chemical potentials at the two carbon atom sites which are say which are analogous to the hexagonal boron nitride. So, that's the term which is inversion symmetry breaking term. This term without the $\sigma_i \sigma_i'$ there it would have been just the normal Haldane model but now you see that this part is taken into account that's spin S_z is taken into account and they are taking sort of components of that and this of course the chirality.

So, that tells you that if the second neighbour hopping is clockwise then it has a positive sign or if it's anti-clockwise it has a negative sign and this we have taken the flux to be exactly equal to $\pi/2$ and that's what is done excepting when we wanted to generate the phase diagram which is flux versus the these this term. This term means the with the λV term which is the mass term that opens up a gap inversion symmetry breaking term. So, it's basically two copies of the Haldane model. Okay? So, this is you know hold model with flux $\pi/2$ for the spin up and for spin down it's $-\pi/2$. So, this Kane Mele term so this is called as a Kane Mele term.

Okay? This Kane term is actually up up Haldane Hamiltonian for Φ equal to $\pi/2$ Φ is the flux which is due to the you know so this flux is exponential $i\Phi$ I mean it's called as a Haldane flux but this is that term that you know comes with the t_2 term so that if Φ equal to $\pi/2$ then it becomes equal to $i t_2$ and so on $i t_2$ or $-i t_2$.

Kane Mele model

$$H_{KM} = \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + i \lambda_{SO} \sum_{\langle\langle i,j \rangle\rangle, \sigma, \sigma'} v_{ij} c_{i\sigma}^\dagger S_z^{\sigma\sigma'} c_{j\sigma'} + \lambda_v \sum_i \xi_i c_i^\dagger c_j$$

Two copies of the Haldane Model

Equivalent to : $|Haldane|^2$ (conserves S_z)

Spin \uparrow : The Haldane model with $\phi = \frac{\pi}{2}$
 Spin \downarrow : The Haldane model with $\phi = -\frac{\pi}{2}$

$t_2 e^{i\phi}$
 $\phi = \pi/2 \rightarrow i t_2$

$$H_{KM} = H_{\uparrow} \left(Haldane, \phi = \frac{\pi}{2} \right) + H_{\downarrow} \left(Haldane, \phi = -\frac{\pi}{2} \right)$$

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

Hamiltonian obeys time-reversal symmetry.

So, in the absence of any Rashba kind of spin orbit coupling term the Kane Mele Hamiltonian looks like the H up and H down and so on. So, it obeys time reversal symmetry how that's not difficult to understand we have done that here so this was the term so λ_{SO} S_z and τ_z and S_z so this was there in the Haldane model. So, this was Haldane term which was time reversal symmetry broken term and this S_z has returned or recovered the time reversal symmetry. So, now what can happen is that one can also add a term which is called as a Rashba term that will sort of detail about this later the Rashba term is written as $i \lambda_R$ and then there is a $\mathbf{C} \cdot \mathbf{D}$ and then there is a $\mathbf{S} \cdot \mathbf{D}$ vector so this \mathbf{D} vector is basically some vector it just looks like a vector kind of coupling but then you see that we have taken a Z component and of course that there is a λ_V term etc.

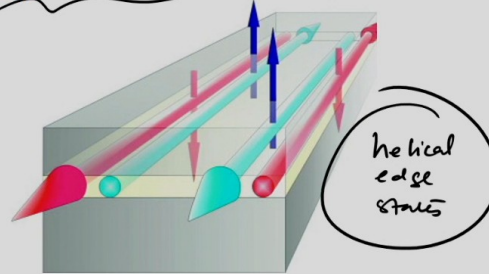
So, what one can get is that now with this term there one actually gets the spin filtered edge states in the problem. So, which means that at each edge you will have a up and down the spin states or edge modes corresponding to up and down. So, at each edge there are two spins up spin and down spin and so on so these are called as a helical edge states. So, a quantum spin Hall effect can be observed in the system and the system will show a quantum spin Hall conductance of e over 2π but we will have 0 charge Hall conductance for the reason that we have already said before having a Hall conductivity you need to have the time reversal symmetry broken for the charge Hall the usual Hall effect that we talk about.

Kane-Mele Model with Rashba spin-orbit coupling

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

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

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



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.

So, this is the full tight binding Kane-Mele Hamiltonian in the momentum space these are the diagonal term which are something like second neighbour hopping or on-site potential and these are the kinetic energy nearest neighbour kinetic energy terms and so on. So, each one of the terms are written carefully here there is a full tight binding model. So, this tight binding model has term you know I mean this one in the low energy limit this Hamiltonian looks like other than so there is only the Kane-Mele term that looks like this $\lambda_{SO} \sigma_z \tau_z$ and $\lambda_R \sigma \cdot \vec{d}$ and this is what we have discussed. If you do all these expansion then this is of course the kinetic energy term or rather than near tight binding nearest neighbor tight binding term and so on and these are the term which is coming from the Kane-Mele term so this is the Kane-Mele term and this is the Rashba term okay and this Rashba term does not do anything to the time reversal symmetry heuristic argument has been already put forward there that is when you have a $\vec{L} \cdot \vec{S}$ kind of coupling both \vec{L} and \vec{S} change their signs and one does not have any net sign emerging out of that. So, this is a time reversal invariant Hamiltonian and this Hamiltonian now had to be we sort of discuss about a little more about the Hamiltonian but before that let me show you the calculation of the Z_2 invariant. So, given that it is a 4 by 4 Hamiltonian in the K space it can easily be diagonalized in order to calculate the eigenvalues and eigenvectors and once when we get the eigenvalues and eigenvectors we know that we can calculate the topological invariant and let us just think that you know let us take two occupied band corresponding to two spins which are ψ_i and ψ_j these are the occupied band wave functions and the overlap of the time reverse block states are calculated using this formula okay.

Kane-Mele Model in momentum space

The momentum space Hamiltonian is given by,

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

Where,

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

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

and

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

(KM)
Rashba

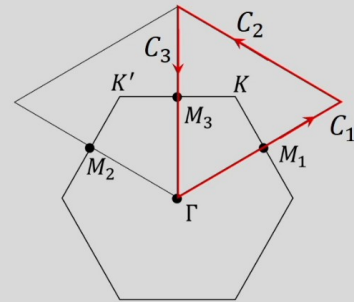
In the low energy limit
 $H_{\text{KM}} \sim \lambda_{\text{SO}} \sigma_z \zeta_z s_z.$

Calculation of Z_2 Invariant

$|\psi_i(\mathbf{k})\rangle$ and $|\psi_j(\mathbf{k})\rangle$ are two occupied band wave functions. The overlap of time reversed Bloch states are calculated as

$$\langle \psi_i(\mathbf{k}) | \mathcal{T} | \psi_j(\mathbf{k}) \rangle = \epsilon_{ij} P f(\mathbf{k}) \quad \mathcal{T} = -i\sigma_y \mathcal{K}$$

$P f(\mathbf{k})$ is '0' at K and K' points, while at the four symmetry points, $P f(\mathbf{k})$ has a value '1'.



The Z_2 invariant is defined by,

$$Z_2 = \frac{1}{2\pi i} \oint_C d\mathbf{k} \cdot \nabla \log[P f(\mathbf{k}) + i\delta]$$

So, what is important is that one has to calculate this thing which is nothing but minus i sigma yk which is what we have shown and they have to be calculated between the two occupied band wave function and what turns out that there is some epsilon function and then the Pfaffian of which is a function of K now this Pfaffian I will just come in a moment what is a Pfaffian but this Pfaffian is 0 at K and K prime points and while at the four symmetry points that is these K and the K prime points this Pfaffian is equal to 0 once one calculates this this matrix element this matrix element will come in the form of

you know I mean this will have numbers and so on and these numbers for a 2 by 2 will give me a Pfaffian there and so this is a 0 at the K and the K prime points in fact if you calculate it over this entire you know rhombus which is that red triangle plus the black triangle then the Pfaffian would come out to 0 and the topological invariant will not be there okay. But if you calculate it only over half the triangle which is denoted by red which are the C1 C2 C3 then it has a value equal to plus 1. So, it is actually defined as the Z2 is defined as $\frac{1}{2\pi i}$ and these closed contour integral over this red curve C that is C1 plus C2 plus C3 and it is a dk dot these the gradient of the log of this quantity this is just taken for convergence by Ken and Millie but one can actually put that equal to 0 it still works. So, it is a log of the Pfaffian that is important. Now what is Pfaffian? So, if you take a 2 by 2 Hamiltonian Pfaffian is just the that off diagonal element okay.

What is a Pfaffian?

$$A = \begin{bmatrix} 0 & a \\ -a & 0 \end{bmatrix}. \quad \text{pf}(A) = a. \quad \text{2} \times \text{2 Matrix}$$

$$B = \begin{bmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{bmatrix}. \quad \text{pf}(B) = 0. \quad \text{3} \times \text{3 Matrix}$$

$$\text{pf} \begin{bmatrix} 0 & a & b & c \\ -a & 0 & d & e \\ -b & -d & 0 & f \\ -c & -e & -f & 0 \end{bmatrix} = af - be + dc. \quad \text{4} \times \text{4 Matrix}$$

So, this is the off diagonal element and for a 3 by 3 Hamiltonian if you have such a matrix structure then the Pfaffian is 0 and for a 4 by 4 matrix with the diagonal elements to be equal to 0. So, this is actually a purely off diagonal matrix all the made the diagonal elements are strictly equal to 0. So, this is equal to A into F minus B into E plus C into D and so on. So, but of course we are interested in only these Pfaffian which is of a 2 by 2 matrix. So, we need to do this integral this integral and this integral needs to be so this is a C1 $\int_{C1} f(x) dx$ and $\int_{C2} f(y) dy$ and so on and then over this C2 so this C1 and then C2 and then C3.

So, this along C1 and then C2 and along C3 the same kind of integrals that will be there. Now I am just showing you integral 1 that is I1 and for I1 you cannot do this integral simply because there is a k_x and k_y dependency and these integrand of course is a function of k_x and k_y . So, along C1 and C2 it is slightly you know non-trivial because of this k_x and k_y dependencies but along C3 of course your k_x is constant and it is only k_y that changes. So, if you take C1 and equation of this line that goes through this point gamma through m_1 it is nothing but k_y equal to k_x by root 3. So, in this integrand that is I1 integrand we have f_x which is a function of k_x and k_y .

So, this is actually k_x and k_x by root 3 and the integral has to be done this has been found out carefully that this is that gamma point is 0 0 and the x coordinate of this point here that is let us call it as OAB and so on. So, it is a OABO integral. So, this integral is that you see here is over this OABO. Okay. So, that is the thing that needs to be substituted here and then this integral is from 0 to 6π by $3\sqrt{3}$ this has been found as 6π by $3\sqrt{3}$ and so on.

And if we substitute k_x equal to root 3 k_y that is what the equation tells you and then this becomes equal to root 3 k_y and k_y over dk_y and dk_y goes from 0 to 2π over 3 and so on. So, these are the double integral is calculated in two steps. So, this step number one in which first you do the k_x integral and then you do the k_y integral. Okay. And similarly one has to do the C2 over I2 and for I3 only dk_y is nonzero because k_x is constant.

The integration has the form, $\left[\int_{C_1} f_x(k_x, k_y) dk_x + f_y(k_x, k_y) dk_y \right] + \int_{C_2} \dots + \int_{C_3} \dots$

Find the equation of the straight line C_1 .

$$k_y = \frac{k_x}{\sqrt{3}};$$

Substitute $k_y = \frac{k_x}{\sqrt{3}}$ in the first part, that is,

$$\int_{C_1} f_x(k_x, k_y) dk_x \rightarrow \int_{k_x=0}^{6\pi/3\sqrt{3}} f_x\left(k_x, \frac{k_x}{\sqrt{3}}\right) dk_x$$

Substitute $k_x = \sqrt{3}k_y$ in the second part, that is,

$$\int_{C_1} f_y(\sqrt{3}k_y, k_y) dk_y \rightarrow \int_{k_y=0}^{2\pi/3} f_y(\sqrt{3}k_y, k_y) dk_y$$

I_1 is the sum of this two integrations

So, k_x is fixed at a value 0. So, we need to only calculate this. So, now you calculate over this C_1 contour and this is that C_2 contour and this is that C_3 contour and then you add integral over C_1 plus C_2 plus C_3 and that should give you a topological invariant. Okay. And this is exactly the plot that one gets from this you see that there's a dark blue line which is like a contour of this enclosed region and this blue line the dark blue line that represents a gap closing scenario for this Ken Milley model which means that there is everywhere on that plot or on that line contour the gap is equal to 0 at the Dirac points.

C_2 . Similarly, find the equation of C_2 and calculate I_2 .

For I_3 , only $\int_{C_3} f_y(k_x, k_y) dk_y$ is non-zero. Since along C_3 , k_x is fixed at zero. Hence we need to compute

C_3

$$\int_{k_y=4\pi/3}^0 f_y(0, k_y) dk_y$$

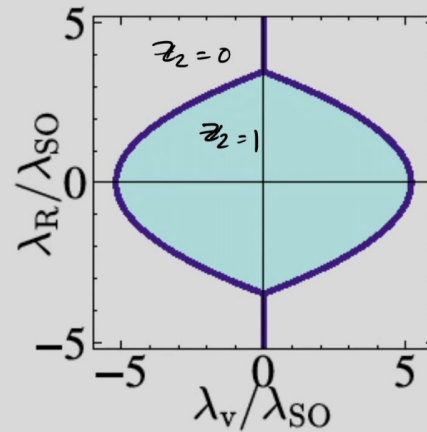
$$I_{C_1} + I_{C_2} + I_{C_3}.$$

Okay. And the gap is nonzero only inside in the sky blue regime. Okay. This sky blue place or these inside this is the Z_2 invariant calculated using the formula that we had given above. So, this is equal to 1 and it vanishes outside. So, Z_2 is equal to 0 here and Z_2 equal to 1 here and there is a blue line that separates.

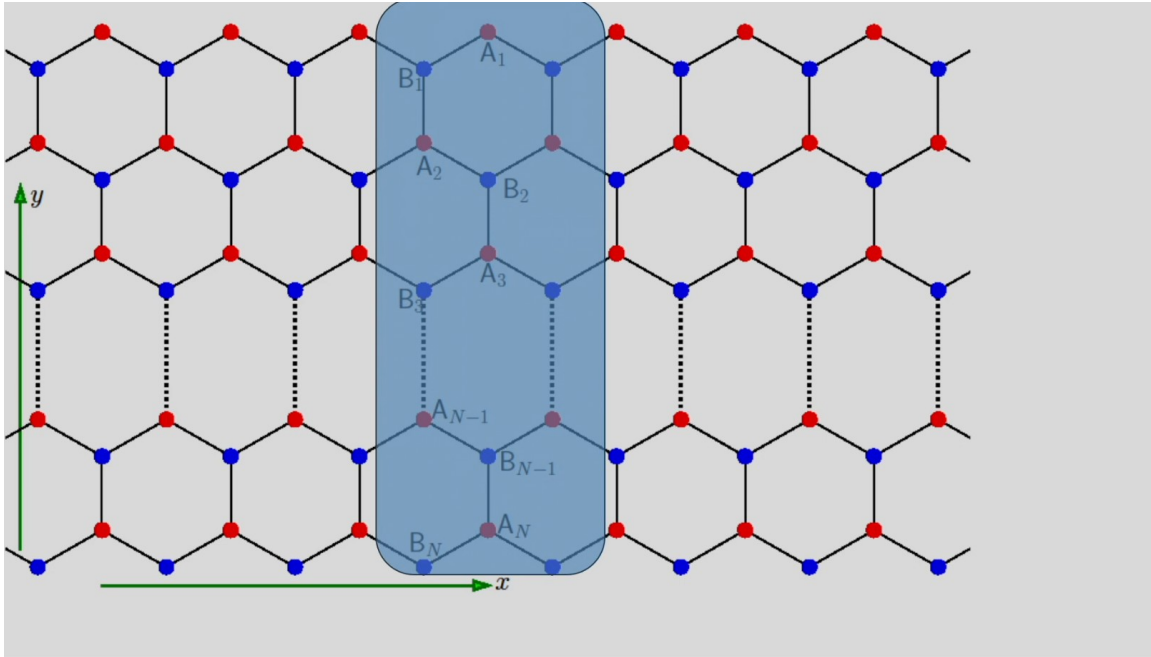
Phase diagram

The outside contour (in deep blue) represents the semi-metallic phase of the system, where the band gap vanishes in the dispersion spectrum.

The region enclosed by the curve (the sky blue region) has a Z_2 invariant equal to 1, while it vanishes outside. Therefore, the system shows non-trivial spin Hall insulating phase ($Z_2 = 1$) inside the curve, while it is a trivial insulator ($Z_2 = 0$) in the outside region.




So, that topological phase transition occurs from the invariant being 1 inside or in the enclosed region and it's 0 outside in the outside region. Okay. So, how do we know that it is a topological or it has edge states it's not a normal insulator and we do the same thing that we have done earlier we take a zigzag edge ribbon or ribbon with a zigzag edge and well one can do also an armchair which is a little different and I believe that one had to or one has to take a larger system but now you write down the Hamiltonian according to the hopping all the hoppings that we have between red to blue and red to red and blue to blue and so on so forth. Okay. And if you want more details on this there's a very recent paper 2023 who have calculated there's an explicit derivation of the helical edge modes for the Ken Milley model and so is elaborate paper that one can actually look at.



We have calculated the same things now you see that we see the spin filtered edge modes. So, the spin filtered edge modes of the Kane-Mele insulator are shown for two different values of λ . λ equal to some value and λ equal to some other value which are taken as $0.1 t$ and $0.4 t$ remember that 0.1 in unit of t means the unit of the nearest neighbour hopping that's a little larger value and just to make sure that one corresponds to the topological phase this is the topological and this is the trivial.

Explicit derivation of the chiral and generic helical edge states for the Kane-Mele model: Closed expressions for the wave function, dispersion relation, and spin rotation

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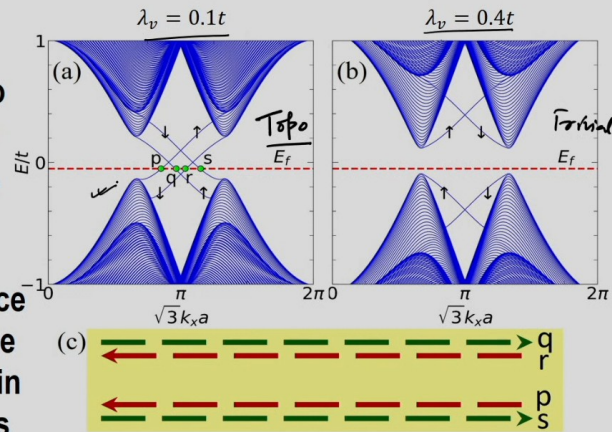
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Although one of the most important and intriguing features of the topological insulators is the presence of edge states, the closed-form expressions for the edge states of some famous topological models are still lacking. Here, we focus on the Kane-Mele model with and without Rashba spin-orbit coupling as a well-known model to describe a two-dimensional version of the Z_2 topological insulator to study the properties of its edge states analytically. By considering the tight-binding model on a honeycomb lattice with zigzag boundaries and introducing a perturbative approach, we derive explicit expressions for the wave functions, energy dispersion relations, and the spin rotations of the (generic) helical edge states. To this end, we first map the edge states of the ribbon geometry into an effective two-leg ladder model with momentum-dependent energy parameters. Then, we split the Hamiltonian of the system into an unperturbed part and a perturbation. The unperturbed part has a flat-band energy spectrum and can be solved exactly, which allows us to consider the remaining part of the Hamiltonian perturbatively. The resulting energy dispersion relation within the first-order perturbation, surprisingly, is in excellent agreement with the numerical spectra over a very wide range of wave numbers. Our perturbative framework also allows deriving an explicit form for the rotation of the spins of the momentum edge states in the absence of axial spin symmetry due to the Rashba spin-orbit interaction.

Because you see there are edge modes coming out from the conduction to the valence band and they are cutting the Fermi energy at these green dots the points that you see there which are named as PQRS. So, all these PQRS are here so at one edge we have P and S the other edge we have Q and R and of course there is no edge modes here. So, there is a bulk gap so this acts like a band insulator the figure on your right is a band insulator and the figure on your left is a topological insulator. So, this thing this is chosen because we have chosen plot that is here that is inside this sky blue region. So, inside the sky blue region we make sure that it's a topological insulator with spin filtered edge modes the and the topological invariant is equal to 1 while on the right figure which corresponds to λv equal to 0.

Edge modes

The spin filtered edge states of the Kane-Mele insulator are shown for two different values of λ_v . $\lambda_v = 0.1t$ lies inside the curve in the phase diagram, that is, the Z_2 invariant is 1 and we observe a pair of edge modes from conduction bands goes into the valence bands and vice versa. As a result, if the Fermi level lies in the bulk gap, the spin currents will flow along both the edges of the ribbon and hence we will observe spin Hall conductivity.



4 t which we have taken this thing equal to 0. So, the λ_v equal to 0.4 is somewhere here somewhere here and so on and of course your λ_R values such that it is Z_2 equal to 0. So, in the Z_2 equal to 0 case we do not have any spin filtered edge modes and just to remind you that in this situation we have taken the K_X to be a good quantum number and K_Y is not a good quantum number. So, the Hamiltonian is written in the Y direction is written in the real space. So, the size of the Hamiltonian depends on how many unit cells we take in the Y direction and in the X direction of course it's an infinite.

So, this called as a semi-infinite nano ribbon which is what we have talked about earlier and we see these edge modes and these edge modes are cartoon of that is has been shown earlier here that you see that these are the edge modes these red and the light green they correspond to down spin and up spin respectively at each of the edges and that's exactly similar to what we get here you see. So, these correspond to the P correspond to the down. So, P corresponds to up, S corresponds to down, Q corresponds to down and R corresponds to up. So, this is exactly the picture that we have shown it's been reproduced using numerical simulations by us. So, this to summarize you know this represents a completely new kind of topological insulator which is marked by a new or a different topological invariant it has time reversal symmetry the states have you know Kramer's degeneracy.

So, these Kramer's degeneracy is what we are talking about we have talked about that there are up and down states which are degenerate. So, these up and down states at the k

values you see that that there are these P and S are degenerate states at you know but they are differ by a momenta which is on diametrically opposite parts of the Brillouin zone I mean they differ by the momentum there and so on and then you also have these other set of things are which differ by these momenta across the Brillouin zone. So, this is a different kind of scenario where spin orbit coupling plays an important role we have talked about two kinds of spin orbit coupling one is a Haldane term with spin term added to it or rather you know it is a spinful Haldane term which is also sometimes called as intrinsic spin orbit coupling and the Rashba spin orbit coupling has been added both respect time reversal symmetry system has time reversal symmetry and there are instead of chiral modes there are spin filtered edge modes which are there present in the system. So, we have been able to show another topological insulator or topological insulating state which is different than the ones that we have seen earlier either in the context of 2D electron gas in a magnetic field or the Haldane model. I will stop here. Thank you. Thank you.