Topology and Condensed Matter Physics
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Lecture – 28

3D Topological Insulators

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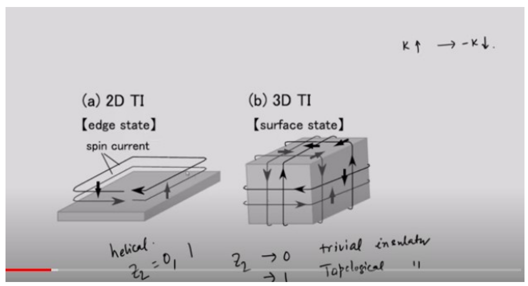

So, far we have seen how the features of topological insulators that is they have the conducting edge states and they have an insulating bulk and we have seen that a reverse scenario that is all the bulk states are localized whereas they are conducting or rather just other way around that there are all the bulk states are conducting whereas the edge modes are localized. So, these are the scenarios that we have seen in 1D topological insulators which are Schur-Schrufer-Hieger model or the Kitaev chain that we have studied in presence of P wave superconducting correlations. Then we have done a similar situation studied a similar situation in 2D where we have looked at graphene and importantly we have looked at the both the integer and fractional quantum Hall effect and all these are two-dimensional systems both of them that is showing either that this 2D electron gas showing integer quantum Hall effect or fractional quantum Hall effect and we have also looked at crystalline systems such as graphene and so these have certain topological properties which have been discussed. Now to wind up our studies on the topological insulators we do 3D topological insulators.

So, in three dimension we will have surface states as it shown here in the right picture whereas there are in the 2D material we have these edge states which go around the edges of the sample and we are particularly interested in the time reversal symmetric systems. So, we see that there are spin currents being present in the system and they are helical edge modes which appear in pairs that is there are these each mode will correspond to one kind of spin and there are two spins or rather two modes per edge for both the spins being present there and these are called as the helical modes we have looked at them and so on and a similar scenario translated to three dimension will have these surface modes being present whereas the bulk would still be gapped and non-conducting whereas the surface will be conducting and each surface will have such these helical modes which are for the two different spin varieties.

These are the new 3D topological insulators and we learn that how actually from a 2D topological insulator we can go to 3D insulators and so on and in particular as I said that we will be talking about non-magnetic topological insulator which means that the time reversal symmetry is intact and there is no magnetic impurity or there is no magnetic perturbation that is present which would have broken the time reversal symmetry.

So, in this 2D we have learned that there is an invariant called as a Z2 invariant and the Z2 invariant can take values which are 0 and 1 and Z2 invariant 0 is called as the trivial insulator or band insulator or usual normal insulator that we are familiar with and it is equal to 1 that corresponds to topological insulators and they are also called as Z2 topological insulators because the Z2 index being non-zero and these insulators are as I said characterized by the helical edge modes present in the system. And these helical edge modes are nothing but the Cramer's partners and we have discussed this in details about the Cramer's degeneracy that is present in a time reversal symmetric system. So, the Hamiltonian has time reversal symmetry then there will be Cramer's partners that is a K corresponding to an up spin will be degenerate to a minus K corresponding to a down spin and that is called as a Cramer's partners and these states that you see on the left in 2D these are the Cramer's partners or the Cramer's doublets and so on.

And in particular we can also assume that there are these inversion symmetry or the parity being present in the system and this calculation of the Z2 invariance become particularly simple when these inversion symmetry being present. And in that case we will have a set of points which are called as a time reversal invariant points and these presence of this time reversal invariant points make things much easier.

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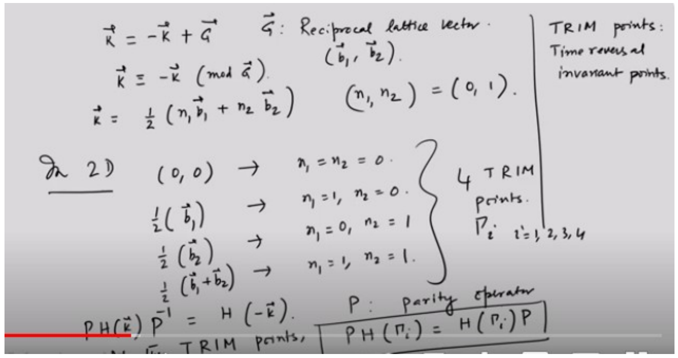

And when we go over to the 3D topological insulators will still consider that the time reversal invariant points are present and just to remind you that what these time reversal invariant points are. So, you have a K which is equal to so K is a momentum and this is equal to a minus K plus a G where G is a reciprocal lattice vector. And in principle reciprocal lattice vector is formed of these unit or rather these basis vectors in the reciprocal space let us call it as B1 and B2. So, this equation that we have written so K equal to so this K is not capital we just meant a small k. So, this means that this K is equal to minus K mod of G these statements are equivalent it says that and so it is when you divide it by the reciprocal lattice vector. So, it just talks about the remainder of this division. So, these K is equal to let us say that this is like half n1 B1 plus n2 B2 where these n1 and n2 are numbers which are 0 and 1. So, in 2D system so we are trying to calculate the trim points.

$$\vec{k} = \vec{k} + \vec{G}$$

$$\vec{k} = -\vec{k}$$

$$\vec{k} = \frac{1}{2}(n_1\vec{b_1} + n_2\vec{b_2})$$

So, let me write down so this trim points mean that time reversal invariant points. And so in 2D there are 4 trim points corresponding to these n1 and n2 being 0 and 1. So, these trim points would be like a 0 0 corresponding to both n1 equal to n2 equal to 0 and it can be equal to so it is like half of B1 this corresponds to n1 equal to 1 n2 equal to 0 or it is equal to half B2 and this is equal to n1 equal to 0 and n2 equal to 1 or it is equal to half of B1 plus B2 and so n1 equal to 1 and n2 equal to 1. So, these are the 4 trim points present in 2D systems which has time reversal symmetry and so on. So, we just coming to 3D in just a while because that is what we want to discuss here.

$$(0,0) \rightarrow n_1 = n_2 = 0$$
$$\frac{1}{2}(\vec{b_1}) \rightarrow n_1 = 1, n_2 = 0$$
$$\frac{1}{2}(\vec{b_2}) \rightarrow n_1 = 0, n_2 = 1$$
$$\frac{1}{2}(\vec{b_1} + \vec{b_2}) \rightarrow n_1 = 1, n_2 = 1$$

So, now the presence of the inversion symmetry makes things a little easier. So, for a block Hamiltonian an inversion symmetry means that it is P H P inverse is equal to minus H k where H k is the block Hamiltonian and this P denotes the parity operator and parity operator means that it changes x to minus x y to minus y and z to minus z. So, at the trim points so, P H and let us call this trim points as gamma i.

$$PH(\vec{K}P^{-1}) = H(-\vec{k})$$
$$PH(\Gamma_i) = H(\Gamma_i)P$$

So, i from 1 2 3 4. So, let us call one of them as gamma 1 the other is gamma 2 gamma 3 and gamma 4. So, P H at these trim points is equal to H at these trim points and multiplied by P. This is the definition of these trim points that are this relationship is valid where P is parity operator ok.

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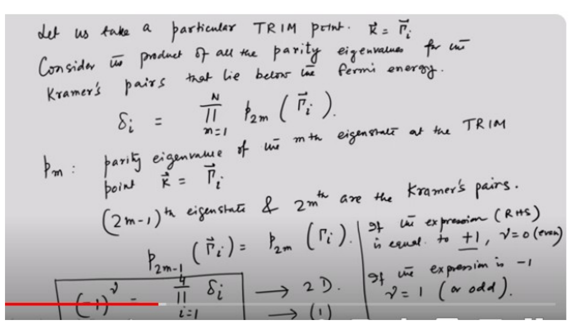

So, now let us take one trim point which means that let us take a k equal to 1 of the 4 trim points and we consider the for the Kramer's pairs that lie below the Fermi energy ok. So, then we define a quantity which is let us call it as a delta i which is equal to m equal to 1 to n and then a P 2 m and gamma i here. So, we define this quantity and what is this P 2 m or P m.

So, P m it denotes the parity eigenvalues of the mth eigenstate at the trim point k equal to gamma i ok. So, the Cramer's pairs are the 2 m minus 1th eigenstate and 2 mth eigenstates are the Cramer's pairs ok. So, what it means is that so, you have a P 2 m minus 1 at the gamma i point this is equal to P 2 m at the gamma i point and so on. So, and then what do we do? So, we get this delta i which is a product of the parity eigenvalues and we use this to define the topological invariant so to say by this formula. So, it is minus 1 to the power nu and it is a product of all these 4 trim points and the parity eigenvalues of these things over of course, all the occupied states.

$$\delta_i = \prod_{n=a}^{N} p_{2m}(\vec{\Gamma}_i)$$

So, this is how the topological invariant is defined in 2D and it is very clear that if this expression is so, let me write it here. If this expression that is let us call it as equation 1, if the expression I mean basically the either of the sides. So, we are particularly talking about the right hand side expression in RHS this is equal to 1 plus 1 then of course, nu is equal to 0 or even or even and if the expression is minus 1 then of course, the nu is equal to 1 or it is odd, it is odd. So, you see if this product if this product gives you a plus 1 it because these delta i's are plus 1 and minus 1. So, over all the trim points when you multiply the product can either give you plus 1 or minus 1.

$$p_{2m-1}(\vec{\Gamma}_i) = p_{2m}(\Gamma_i)$$

$$(-1)^{\nu} =_{i=1}^{4} \delta_i \qquad \text{(Equation 1)}$$

So, if it is plus 1 then of course, this nu is equal to 0 or it is some even value and if this product is minus 1 then of course, nu is equal to 1 or it has some odd value. And why this nu is called as the topological invariant is because this nu equal to 0 that corresponds to a trivial insulator and nu equal to 1 corresponds to a topological insulator.

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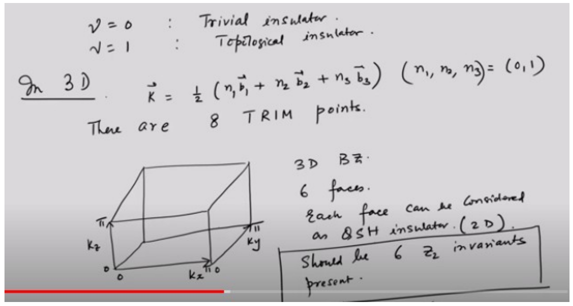

So, this is the story in 2D. So, we have a Z 2 invariant equal to 1 which we knew that it is called as a topological insulator and the Z 2 invariant being 0 is a trivial insulator. Now we are casting it in the form of this nu, but the meaning remains the same.

Now what happens in 3D is the question. So, in 3D we have these this wave vector is written as n 1 b 1 plus n 2 b 2 plus n 3 b 3 ok, where n 1 n 2 n 3 are 0 and 1 ok. So, you can have just b 1 when the other 2 are 0 b 2 when n 1 and n 3 are 0 or just b 3 when n 1 and n 2 are 0 and so on and then you can have 2 of them to be 1 and the third one to be 0 or you can have 1 to be 1 all 3 to be 1 and so on. So, there are for all these choices there are 8 trim points and corresponding these choices of n 1 n 2 n 3 being 0 and 1. So, as opposed to 4 trim points in 2D in 3D there are 8 trim points ok.

$$\vec{k} = \frac{1}{2}(n_1\vec{b_1} + n_2\vec{b_2} + n_3\vec{b_3})$$
$$(N_1, N_2, N_3) = (0, 1)$$

And how do we then talk about this topological invariance and this topological invariance let us try to understand let me draw a cube that is a just a Brillouin zone it is a simple cubic Brillouin zone. So, let us call this as K x this as K y and this as K z and this is 0 to pi 0 to pi and 0 to pi ok. So, the that is a 3D B z ok. So, there are 6 faces of this Brillouin zone and each face can be used as a or it can be considered as as a quantum spin hall insulator ok. Because each one of them is has time reversal symmetry and I mean basically the Hamiltonian has time reversal symmetry.

So, if we take a slice of that say in the K z equal to 0 plane or K x equal to 0 plane or K x equal to pi plane and so on so forth. So, each of the 6 faces can be considered as a topological is a 2D QSH insulator in 2D ok. So, there should be 6 this independent z 2 invariants corresponding to each of this. So, should be 6 z 2 in-variants present ok, but all 6 of them may not be independent.

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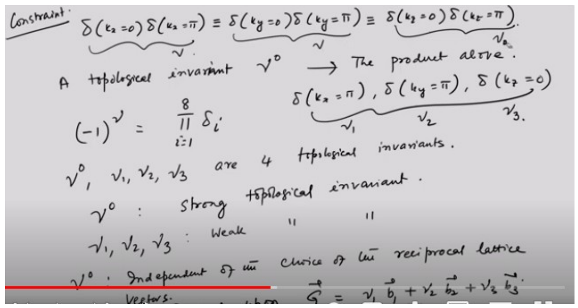

And in fact, we can see that so, this delta K x equal to 0 into delta K x equal to pi is identical to delta K y equal to 0 and delta K y equal to pi and is identical to delta K z equal to 0 and delta K z equal to pi. And so, this is a constrained condition and this constrained reduces the number of z 2 invariants from 6 to 4 and this particular the product of such of these these deltas they correspond to a topological invariant. They are same a topological invariant which is called as a nu 0. So, this product the product above ok. So, what we had was that we had a minus nu minus 1 whole to the power nu that was over these all these deltas and now there are 8 of them.

$$\delta(k_x = 0)\delta(k_x = 0) = \delta(k_y = 0)\delta(k_y = \pi) = \delta(k_z = 0)\delta(k_z = \pi)$$

$$(-1)^{\nu} = \prod_{i=1}^{8} \delta_i$$

So, it is 1 to 8. So, now, because of this condition there are these nu 0 and nu 1 nu 2 and nu 3 are 4 topological invariants that are present in the system ok. So, now, this nu 0 is called as the strong topological invariant and nu 1 nu 2 nu 3 are called as a weak topological invariant ok. So, basically this nu 0 is independent of the choice of this reciprocal lattice vector. And, whereas this nu 1 nu 2 nu 3 they depend upon the choice of the reciprocal lattice vector G which is equal to a nu 1 b 1 plus a nu 2 b 2 plus a nu 3 b 3 ok. So, that is the difference between the strong topological invariant and the weak topological invariants that are present in the system.

$$\vec{G} = \nu_1 \vec{b_1} + \nu_2 \vec{b_2} + \nu_3 \vec{b_3}$$

So, in this language so, you have a delta k x equal to pi delta k y equal to pi and delta k z equal to pi. So, these correspond to nu 1 nu 2 and nu 3 ok and the product correspond to nu 0. So, these are nu 0s it is usually written above. So, let me write it above. So, there are 4 topological invariants which are nu 0 and then nu 1 nu 2 and nu 3. So, that is the story for a 3 dimensional topological invariant.

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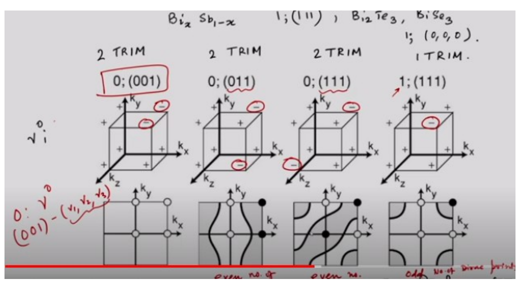

So, these are some of the pictures of these topological invariants. So, there are 2 trim points here you see that these are 2 negative signs here. So, that is called as a 2 trim points again 2 trim points here this taken from a Fu and Kane their paper in 2007 physical review B. So, 2 trim points there are 2 trim points as well.

So, there are these 2 this negative signs which means that these are the trim points. So, there is a negative the 2 trim points here and there is just 1 trim point here ok. So, there are 2 trim here 2 trim here and there is just 1 trim here ok. So, these 2 trim points make it weak topological insulator. So, this is exactly given in the same way as we have just said. So, there is a nu 0 and with a colon. So, we should change our so, maybe this one and so, these are the representations. So, a nu 0 which is a strong invariant and these are the weak Ti invariant ok. So, in this particular case this nomenclature that you see here this nomenclature this 0 corresponds to the nu 0 and then these inside the bracket that you see there. So, 0 0 1 inside the bracket these are set of nu 1 nu 1 nu 2 and nu 3.

So, these are the weak topological invariants and so on. When you have even number of trim points then this index that is the strong topological index is equal to 0 and it is only when you have odd number of trim points which is the case the last case that is the fourth one the topological invariant the strong topological invariant is 1 whereas, the weak topological invariants along the k x k y and k z directions are 111 here which is same as 111 here as well and there are 0 1 1 and so on. So, they again depend upon the various this delta k x equal to pi delta k y equal to pi and delta k z equal to pi. So, these the parity eigenvalues. So, what happens is that so, there are these in this particular case there are even number of Dirac points and there are even number of Dirac points here and there are odd number of Dirac points even Dirac even number of Dirac points these are even number of Dirac points and there are odd number of Dirac points.

So, like for example, we have this the first topological insulator which is B i x S b 1 minus x that is a Bismuth x and antimony 1 minus x, x is usually around 10 percent basically around anything between 0 to 12 percent. So, this has it is a strong topological insulator. So, it is like a 1 1 1 and so on. So, this. So, this is and then the second generation of topological insulators such as B i 2 te 3 and B i 2 Se 3 these are the second generation 3D topological insulators and they have again it is a 1 and 0 0 0.

So, the strong topological invariant is 1 and the 3 weak topological invariants are 0. So, these are the classifications of strong and weak topological insulator. Just to remind you that a strong topological insulator will have odd number of Dirac points at the surface and it will have odd number of trim points here we have shown the odd number to be equal to 1. Whereas the when the strong topological invariant is 0 then there are even number of the trim points and there are even number of Dirac points present in the system. So, there are 2 Dirac points present in these cases and so on. So, let us see how we can generate 3D topological insulator from what we already know we know already the 2D Bernoulli Hughes and Zhang model the BHZ model.

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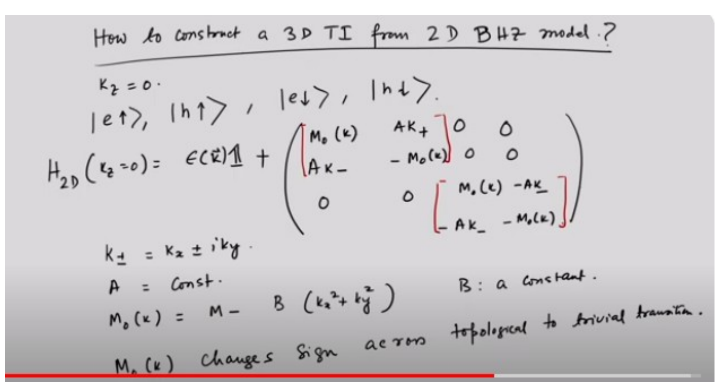

So, how to construct a 3D TI 2D BHZ model and please have a look at the BHZ model discussion. We will have a discussion once more and so what we do is that BHZ model is basically it is a 2D model and say it is taken for kz equal to 0. So, the third dimension is frozen out because you have decided to take it at a particular value of kz and say kz equal to 0 and just to remind you that the basis in which the BHZ model was written. Now this BHZ model just to remind you that it is the model for these strain structures CDT, HGT, HGT that is mercury telluride and cadmium telluride. So, this mercury telluride has an unconventional band structure which has band inversion properties at the gamma point and these CDT of course is a usual semiconductor and now for a certain critical width or rather beyond a certain critical width larger than that these HGT this squeezed between sandwiched between two CDT slabs shows unconventional topological properties which are called as a quantum spin hall phase and this band inversion that occurs. So, we write down the Hamiltonian in the electron hole and the spin basis. So, it is E up, E means electron and up is up spin.

$$k_z = 0$$

$$H_{2D}(k_z = 0) = \epsilon(\vec{k})1 + \begin{pmatrix} \begin{bmatrix} M_0(k) & AK_+ \\ AK_- & -M_0(k) \end{bmatrix} & \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} M_0(k) & -AK_- \\ -AK_- & -M_0(k) \end{bmatrix} \end{pmatrix}$$

So, it is E up H up and E down H down basis and this Hamiltonian in 2D. So, this is let us call it a 2D and for kz equal to 0 is written as epsilon k and there is a unit vector and plus. So, there is a m naught k which is called as a mass term and a k plus a is a constant and a 0 0 a k minus minus m 0 k 0 0 and 0 0 m 0 k and a minus a k minus and a minus a k minus and a minus m 0 k ok. So, this is the 2D.

$$k_{\pm} = k_z \pm ik_y$$
$$A = constant$$
$$M_0(k) = M - B(k_x^2 + k_y^2)$$

So, let me remove this and write it ok. So, that is the BHZ model and you see that there is a nice block diagonal form that you have here. So, the up and down spins are not mixed and it can be diagonalized easily and one can get the solution which is what we have discussed earlier. So, what is our k plus minus? So, this is equal to kx plus minus i ky a is a constant and this m 0 k is given by it is equal to m minus some constant B and kx square plus a ky square and a B is a constant ok. So, that is the 2D BHZ model and so, how it undergoes from topological to a trivial transition as these width of the HGT slab that exceeds certain critical width which is let us call it DC which has some value 6 point something nanometer. So, this model if it has to capture the essential physics of that transition then it has to undergo a topological to trivial transition and in fact, across that transition m 0 k ok.

So, what it means is that if your m minus B kx square plus ky square is greater than 0 then you have a certain kind of phase and when it is less than 0 then it undergoes a phase transition and that is the topological phase transition that we are familiar with we have seen that earlier ok. Now, what happens if we want to generalize it to 3D can we generalize it to 3D and still hope to see similar transition happening there ok.

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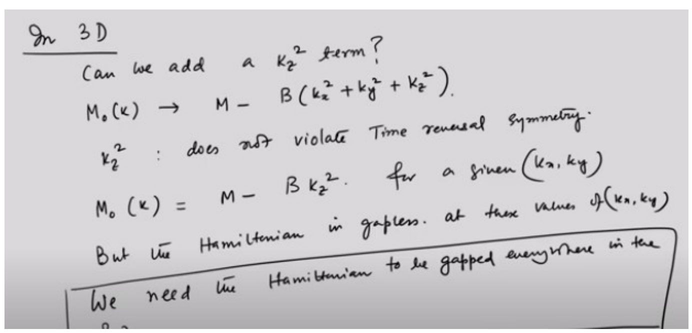

So, one of the usual way of doing it is so, can we add kz square term ok. So, that your m naught of k that becomes equal to. So, there is a m minus B kx square plus ky square plus kz square ok. Now, if this is going to solve the problem then of course, the system should remain gapped everywhere and as this thing this m 0 k changes sign you should again see a phase transition from a topological to a trivial happening there. In fact, when m is equal to positive it is a trivial phase and when m naught is negative then it is a topological phase and remember these kz square term this does not wireless time reversal symmetry. But, this is not going to solve the problem and why it is not going to solve the problem is the following that if you take a particular value of kx and ky that is you freeze the kx and ky then this m 0 k that takes a form which is equal to m minus B kz square and these this term of course,it does not break the time reversal symmetry, but the Hamiltonian remains gapless. I mean this is for a given kx ky. So, that we have frozen that value and have absorbed that constant.

$$M_0(k) \rightarrow M - B(k_x^2 + k_y^2 + k_z^2)$$
$$M_0(k) = M - Bk_z^2$$

So, the Hamiltonian is gapless whereas, you want gapped values. So, the Hamiltonian is gapless at at these given values at these values of kx ky right because if you put kz equal to 0 the gap goes to 0, but you want you want the Hamiltonian to gap to be gapped at every point in the Brillouin zone. So, we need in the Brillouin zone ok. So, this is a requirement that we have, but clearly this choice that we have taken that is a B kz square adding that to this problem does not help because at kz goes to 0 the gap will go to 0 ok. So, but you want the Hamiltonian to be gapped.

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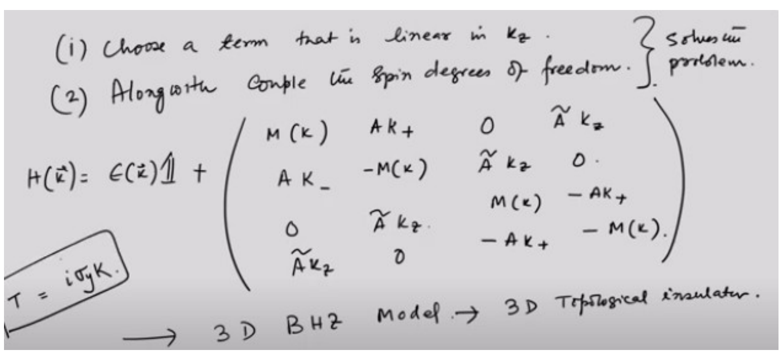

So, is there a different way of doing it? There is indeed another way of doing it and you have to keep two things in mind. So, choose a term that is linear in kz ok, but this has two problems. One is that again at kz equal to 0 the Hamiltonian or the energy spectrum becomes gapless and that is what you do not want and the other problem is that under time reversal symmetry the kz will go to minus kz. So, this kz will be odd in the time reversal symmetry. So, you are breaking time reversal symmetry ok and that is not allowed in this particular case ok, but there is a solution to this problem that is if you can couple the two spin degrees of freedom via this linear term in kz then it will the

Hamiltonian will be gapped everywhere and you would be able to access a topological to trivial transition by in the mass changes ok.

So, along with couple the spin degrees of freedom ok. So, these two together solves the problem. So, the problem is that that we are able to go from 2D to 3D and retain all the features that we have seen there that is a time reversal symmetry being intact and as well as the Hamiltonian is gapped everywhere in the Brillouin zone ok. So, the Hamiltonian takes a form which is equal to epsilon k this is the that is the band structure of the problem. So, this is mk ak plus then we have a 0 and then we have a a tilde kz and we have ak minus and you have a minus mk and a tilde kz and 0 and 0 a tilde kz and mk and this is a minus ak plus. So, and then we have a tilde kz and 0 here and a minus ak plus and a minus mk ok.

$$H(\vec{k}) = \epsilon(\vec{k})1 + \begin{pmatrix} M(k) & AK_+ & 0 & \tilde{A}k_z \\ AK_- & -M(k) & \tilde{A}k_z & 0 \\ 0 & \tilde{A}k_z & M(k) & -AK_+ \\ \tilde{A}k_z & 0 & -Ak_+ & -M(k) \end{pmatrix}$$

So, this is the Hamiltonian and this is known as the 3D BHZ model and this denotes a 3D topological insulator ok. So, that is your Hamiltonian that we get now there is very important thing that one should take a note here that is the Hamiltonian is no longer block diagonal. So, earlier here this is for the up spin and this is for the down spin ok. So, the spins were not mixed, but here the spins are mixed ok because of this off diagonal terms coming in, but and this off diagonal terms have a linear in kz. So, that would break the time reversal symmetry, but then also remember that the spins would also change under time reversal symmetry.

So, an up spin goes to a down spin under time reversal symmetry because the time reversal symmetry operator is exponential i sigma y and k ok or it is simply i sigma y k and so on. And so, this is the time reversal symmetry operation and because a k changes sign under time reversal and spin changes sign under time reversal. So, the whole thing would be again time reversal invariant ok. So, just some plot to show.

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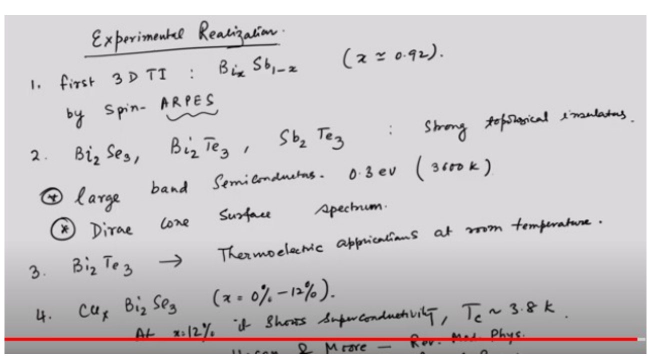

So, this is a topological insulator. So, we have taken some result that is published in the net. So, it is a energy spectrum of a thin slice of BHZ model. So, you see that we have taken m to be negative. So, which means that it is a topological phase and this is the band structure corresponding to this Hamiltonian ok. So, this is a 3D TI Hamiltonian and this is how the and for the time reversal symmetric insulator topological insulator and it shows transition as these m changes sign from being positive to negative ok.

So, at the end let me talk about some experimental realization ok. And so, as I said that the first 3D TI was this B i x S b 1 minus x and so, this is x around 0.92 this was people have done the spin R-PES study I am not going into detailed this called as a angular resolve photo emission spectroscopy and there is this angular resolve photo emission spectroscopy. So, the subsequent ones are Bi2 Se3 Bi2 Te3 Sb2 Te3 and all these are strong topological insulators and in addition to that these are stoichiometric compounds and so, that they can be prepared with high purity and that is why these are very good quality samples ok. And so, these have also large band gap semiconductors I mean what is this about 0.3 electron volt and it is called large because it is about 3600 Kelvin is the band gap and they have Dirac cone surface spectrum. So, there are at the surface there are single Dirac cone or odd number of Dirac cones and these Bi2 Te3 is known to have applications in thermo electricity, thermo electric applications at room temperature and in addition to that there are these Cu X Bi 2 Se 3 which are non stoichiometric compounds. So, there is a X Cu X added where X can be from 0 percent to 12 percent and particularly at 12 percent it shows superconductivity at X equal to 12 percent it shows superconductivity with about 4 Kelvin.

So, Tc is about 3.8 Kelvin ok. In fact, there are very good reviews on 3D topological insulators by Zahid Hasan and Joel Moore. So, it is Hasan and Moore in it is there in various journals I mean one of them is the reviews of modern physics and plus there are annual reviews in condensed matter physics ok. So, I will not elaborate more on this, but there are a number of experimental realization of these materials and so on. Thank you.