Electronic Theory of Solids

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Lecture - 60
Topological state of matter, XY Model, Topological Insulators

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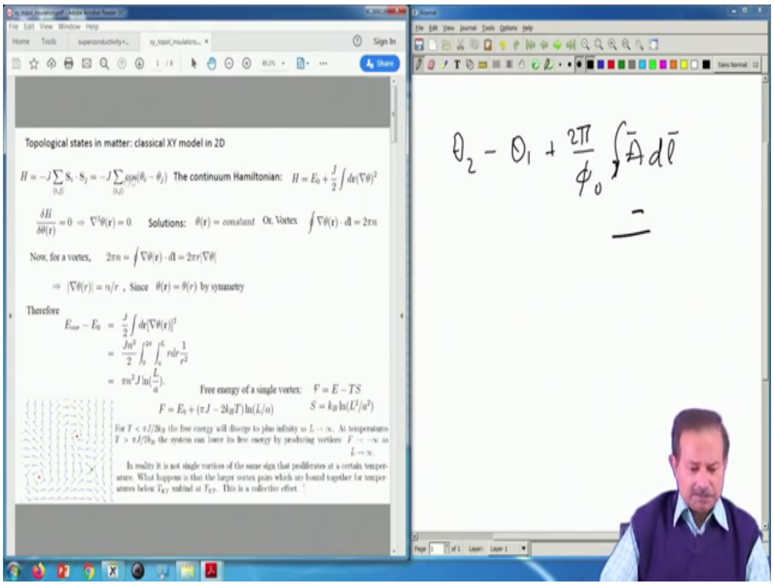

As I promised that we will discuss a bit about these topological states in matter which have become extremely important in condensed matter physics of late in the last 15 years and some of these were actually known for a long time. And then only recently last year 3 physicists got Nobel prize for bringing this topological aspect of systems to for and bringing peoples attention on to these systems and these were Kosterlitz, Thouless and Duncan Haldane. And the first such example was actually done by Kosterlitz and Thouless in the US and Berezinskii in the former USSR and what they showed was really remarkable.

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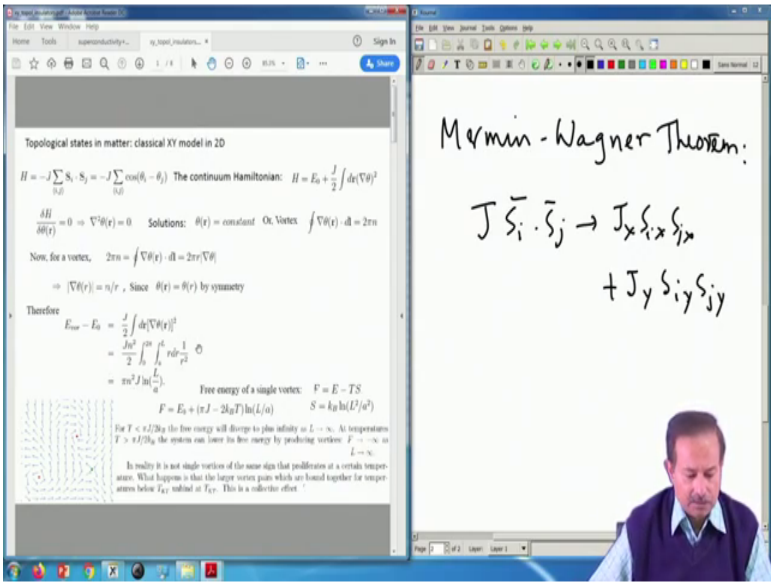

As I said that Mermin Wagner theorem for example, tells you Mermin Wagner theorem this we discussed a bit while we were doing spin systems magnetism and long range order and so on. What where we mentioned that if the order parameter which means this for example, the average spin here or magnetization has a continuous symmetry, then you cannot have long range order in any dimension less or equal to 2. So, for example, that means, that of course, Ising model does not have this continuous symmetry it is only up or down spins can have 2 values.

So, that can have an order state in 2 dimension also and that was a famous solution whereas, take for example, the next higher model. So, suppose you have J Si dot S J Si dot Sj. This is S Sx Sx Sy Sy Sz Sz and out of which ising was only the Sz Sz part, but the other 2 were thrown out because the J has huge anisotropy and Jz was much larger. But now a suppose Jx and Jy are both large and Jz is very small then this model will become Jx Si x Sj x plus Jy Si y S jy. And then if I can put Jx and Jy if they are similar or same, I can put them as just J and some J and that model is called a called a XY model because it has only x and y component of the spin.

So that means, the spins have is can rotate in the xy plane; that means, they have a continuous symmetry. And in such cases you are told by Mermin and Wagner that you should not have a long range order. Of course, you go one more which is Heisenberg model where all components exists that is a that has full SU 2 rotational symmetry of the spins and of course, and classically it has it can be anywhere on a on a sphere the spins can point in any direction on a sphere and; that means, you have a continuous symmetry and you cannot have order according to Mermin Wagner theory theorem. Of course, what was shown by Kosterlitz and Thouless was really remarkable.

They showed that indeed that is true that you do not have order of this type that long range order, but certain correlations become algebraic below the certain temperature in 2D XY model. And what they found out that there is a there is a phase transition of a different kind of a topological kind where vortices start forming inside the in a XY model in 2 dimension. And these vortices and anti vortices I will show you what that means, bind themselves at the particular temperature and that temperature they called TC a transition temperature.

So, it is a transition of a very different kind. It is a vortex binding unbinding transition and a very simple argument shows how a classical XY model in 2 dimension has this kind of vortices and state with vortices is actually of lower a free energy than the normal state were without vortices. And this argument can be presented very simply although the actual transition is much more complicated it is a vortex binding unbinding transition at a finite temperature and that finite temperature.

That means it in terms of Mermin Wagner theorem, you should not have any transition at any finite temperature. So, therefore, this was a first example that was worked out where you indeed have a transition of a topological nature at a finite temperature in a 2d XY model where Mermin Wagner theorem prevents long range order at finite temperature. So, let us see how it works. The 2D model and the classical model is very simple; the S is a constant length.

So, it is like a like a moment it is a vector Si and Sj and therefore, you absorb the S square term inside j and write cos theta i minus theta j and these S i dot S j is just the cosine of the angle between the two and the S square term is absorbed inside the j. Now, of course, nearest neighbor model i j are summed over nearest neighbors. The continuum Hamiltonian you can write after from this where the theta i minus theta j is very small. So, you can expand it and you can then get a grad theta square right. Because if you expand cos theta it will give you theta i minus theta j square is the first theta dependent term. So, that is basically gradient of theta square. Now you can sum E 0 plus j by 2 grad d r grad theta square ok.

So, now we know how to tackle such problems. We minimize with respect to theta set to 0 and the equation that you get is del square theta r equal to 0. Now we know from that such situations where you can have a trivial solution like theta r equal to constant does not depend on r at all that is of course, an a solution. But there is another solution possible where grad theta r integrated over a closed loop around a singularity which is called a singularity is 2 pi times n and that defines the vortex actually.

So, let us see if what this solution gives. Again this is basically the again this is the single valuedness of the you can think of in terms of theta changing over a circuit and it comes back to the same place. So, it should be 2 pi times n. So, for a vortex in a vortex this is interesting that grad theta r dot dl is basically 2 pi r which is in a circle over a circle times the magnitude of change in theta. Since a theta r is not dependent on the angle by the symmetry of the problem because the problem has whole xy symmetry it is symmetric on a plane. The Hamiltonian if you look at the Hamiltonian J x and J y at the same. So, nothing to distinguish any particular direction over a circle in the plane.

So, that means you can just write theta of vector r is actually theta of r only. There is no angle dependence. So, that means, over a circle it remains a constant circle of radius fixed radius. You change the radius, it will change again. Therefore, you can your solution is grad theta mod of grad theta is n by r because there was this 2 pi r ok. So, now, you can evaluate the energy because this is this is the Hamiltonian.

So, that if you evaluate you can immediately show that this is pi n square and J log l by a where l is the size of the system and a is the size of this vortex. So, how does this vortex look like? This is a picture of two vertices actually. So, these and these for example, these two vertices you can look at; these two have spins moving around them in a in and changing their direction of directions you see.

So, it goes around in this fashion and changes to 2 pi when it comes here comes a full circle. In this one it changes the same way, but in opposite sense of rotation. So, the sense of rotation here in this one and in this one are just the different. So, these are called vortex and anti-vortex and if you come bring them together, you can easily see that these 2 rotations will cancel each other and you will again have a background spin which has no rotation. So, this is these are the vertices, the solution is grad theta is 1 over r or n by r that is well known and then that is what the singularity I was talking about r going to 0 is a singular point. Now if the energy then is log L by a.

So, a is the size of this vortex you can think of the size of the vortex beyond which the spins have all healed up to they have no idea there was a there was a vertex here. So, they have healed basically. They said they have healed back to their original states and that size is called the a. So, the size of the vortex basically and L is the side of the size of the system. So, that is the energy of forming one vortex ok. So, E vortex minus E 0 is this much. Now of course, this is a this is positive if as L is greater than a, but look there is a entropy correction you have to take care at finite temperature.

So, that is the free energy is E minus TS the Helmholtz free energy is E minus TS E o you already got. So, the F is E 0 plus this pi n square J log L by a minus this entropy contribution. So, kb. So, minus TS now how is S? How does one find out S is very simple? How many ways how many places can you put this vortex in size is L. So, the linear dimension of the system is capital L. So, L square is this area. The typical area of a vortex is a square. So, L square by a square is the number of ways you can put it in and log of that into kb is the entropy. This as simple as that and then you just multiply by T and subtract and this is what you get. So, this is the total energy. Now you can see that for T less than pi J by 2 kappa beta.

So, you set this to 0 this coefficient to 0. The free energy will diverge to plus infinity as l goes to infinity. At temperatures T greater than pi j by 2 kb the system can lower it is free energy by producing vortices. F goes to minus infinity, then as L goes to infinity. So, there is this possibility that you can have vortices and you can lower your energy by having vortices. But of course, this is a very simplified way of looking at it in reality it is not a single vortex that forms. There are vertices of plus and minus both sign the vortex and anti-vortex proliferates at certain temperature. What happens is that the large larger vortex pairs which are bound together for temperatures below T kt. This temperature is called T kt unbind at T kt.

So, this actually in the real system they showed that there is a transition from vortex binding to vortex unbinding and this is basically a collective effect. But this is the first example that we know of where a topological transition has been predicted where the Mermin Wagner theorem actually predicts it is also a rigorous theorem. It produced there is no usual long range order at any finite temperature, but of course, there is a topological order and that is there. So, this is fundamentally important concept in physics brought about by these 3 physicists Kosterlitz Thouless and Berezinskii. Kosterlitz and Thouless are still alive and they got this they got the Nobel prize for this discovery for this work along with some other work on topological features of materials which let me just come to discuss.

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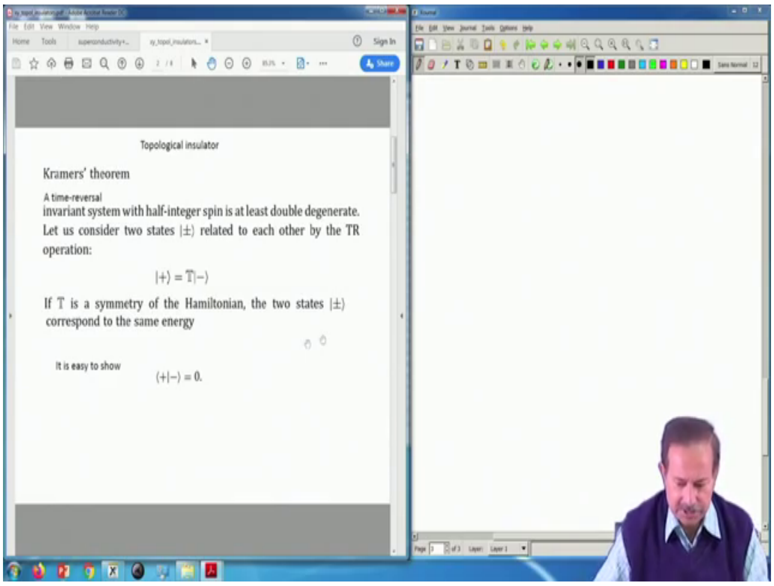

There is this topological insulator that you must be hearing for quite some time and this is this has taken us by storm actually. But it was already there when one the concept was already there when one discussed Quantum Hall effect because if you remember in the Quantum Hall effect we were discussing states which were moving about at the edge of the system even when we discuss born from (Refer time: 15:23) both ideas of absence of magnetism we discussed this skipping orbits at the boundary.

So, those are called edge states, we will come to that. So, it starts from this Kramers theorem. It says that a time reversal invariant system with half integer spin is at least double degenerate. So that means, that if you have this time reversal operator which is an anti unitary operator introduced by Wigner actually it converts a plus state to a minus state. So, let us. So, this is the time since time reversal operation is a symmetry of the system.

So, we can define a state as an Eigen state of time reversal operator and it converts a minus state to plus state. T has two Eigen states. So, we will not get into the details of this if T is a symmetry of the Hamiltonian the two states plus and minus are degenerate and it also and one can also show that plus minus are orthogonal. So, they are two independent states ok.

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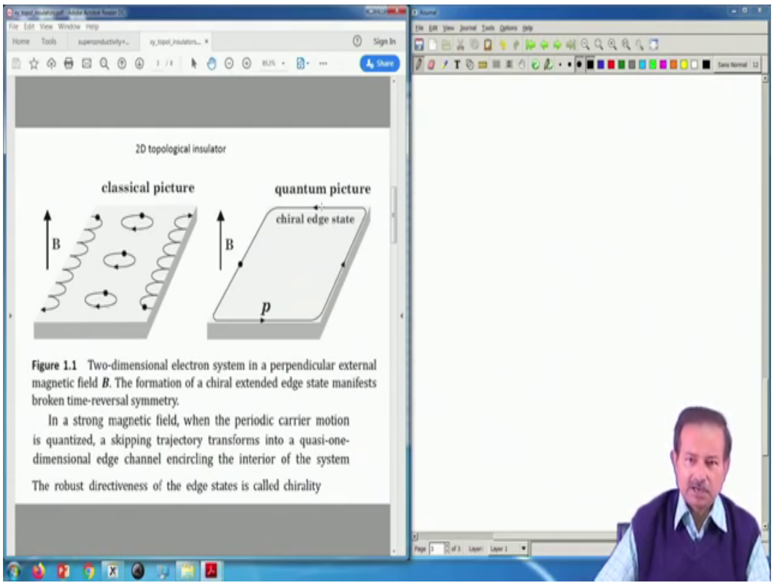

So, that is Kramer's theorem. Basically it says a spin half system with time reversal symmetry is double degenerate. So, that is all we need to know. So, the classical picture I had outlined long back that there are these so called skipping orbits and the bulk there are this bulk orbits they their effects get cancelled out and this effect of skipping orbits cancelled the B orbit coming from the bulk.

So, that was the classical picture. In the quantum picture, these are called these edge states are called chiral edge states they have a chirality. I will come to it what it means. Chirality means they have a direction dependence I mean. So, we will we will show it we will show you what it is. So, they let us discuss in presence of magnetic field at the moment. So, magnetic field violates time reversal symmetry. So, we are not yet at the Kramers degeneracy level, but we are just discussing a time reversal symmetry violated situation like in integer quantum Hall effect where we these edge states are important.

And I will show you in a strong magnetic field, the periodic carrier motion is quantized and that is what we found out in quantum hall integer quantum hall effect. A skipping trajectory transforms the classical skipping trajectories now transform into a quasi one dimensional edge channel encircling the interior of the system. So, the what the analog of this in a quantum situation of the skipping orbits classical skipping orbit is the this edge this basically quantized skipping trajectory into a quasi one dimensional edge channel. So, it is an edge current as you can see that is flowing encircling the entire system.

So, this is directive because you see magnetic field is in this direction. So, the motion has to be in this current has to be in this direction the rotation has a particular sense.

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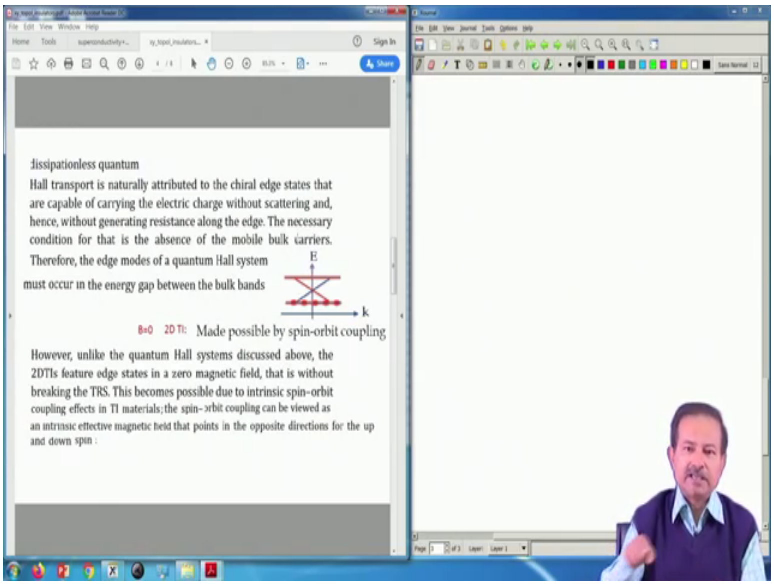

So, the directiveness of this edge state is called the chirality. So, the dissipationless quantum hall transport is naturally attributed to the chiral edge states. Of course, we have seen that Quantum Hall Effect is a quantized current quantized conductivity and that means this is basically due to this chiral edge states that are capable of carrying the electric charge without scattering. Remember that Quantum Hall Effect was so well quantized using 1 part 3 parts in a billion or so in the initial experiments it is much more now.

So, that means there is no scattering. So, tau was set to infinity remember and hence without generating any resistance along the edge and the necessary condition for that is the absence of mobile bulk carrier. So, that means in the bulk you should not have mobile carriers of which these edge channel electrons can exchange energy by scattering. The if the bulk has a gap then the even if you scatter of those electrons the those electrons will not be able to take any energy from you because they have a gap at the fermi level. So, they cannot go up.

There is a large energy transfer that has to happen to take them out of the beyond the gap and that is exactly what this is. And therefore, these edge modes of Quantum Hall effect must occur in a in the energy gap between the bulk bands and that is the picture that yeah is shown here. So, with a B strong B this is the situation that there are these edge modes chiral edge modes which carry the current and they do not do not dissipate energy with the carriers in the bulk because the bulk carriers are all gapped.

Now, the question is there of course, I have to set B equal to 0 to have real interesting physics here because the topological insulators are situation where the there is no B externally applied. So, this is made possible by spin orbit coupling and that is what is interesting. So, the unlike the quantum hall systems discussed above the 2d topological insulators feature edge states in 0 magnetic field that is without breaking the time reversal symmetry. This is possible due to intrinsic spin orbit coupling in TI materials. The spin orbit coupling can be viewed as an intrinsic effective magnetic field that points in the opposite directions for up spin and down spin.

So, this is really interesting. So, something called a spin orbit coupling which we remember in Hund’s rule we discussed it. Third Hund’s rule was about spin orbit coupling and in that case you can think of that as an effective magnetic field, but in opposite directions for spin up and spin down.

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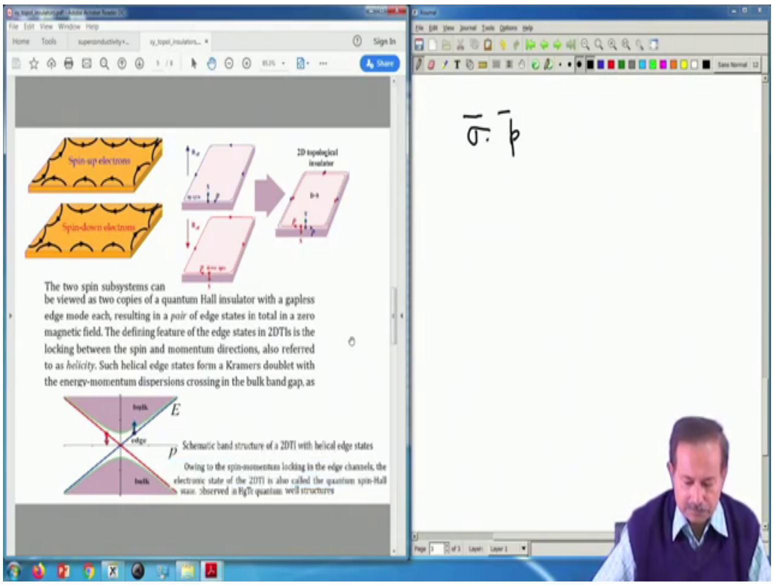

So, this is the picture that for spin up electrons the sense of rotation, then will be in one way at the edge for the chiral edge state and spin down electrons have the others. And so, you can think of it as two quantum Hall integer quantum Hall systems 1 for spin up 1 for spin down moving in opposite directions. And they are they do not talk to each other because they are protected. So, so these gapless edge modes uses two copies of a quantum hall insulator with gapless edge modes resulting in the pair of edge states in total in a 0 magnetic field.

So, this the defining feature of the edge states in 2d topological insulator is the locking between the spin and momentum direction. So, the this is this is what happens if you have spin orbit coupling sigma and p are no longer good quantum number so it is a sigma dot p which is conserved and that is that results in the locking of sigma and p. As you see if sigma dot p is conserved then their directions the direction is locked. If p changes direction sigma has to change direction also and vice versa to keep this dot product constant. So, this is referred to as helicity ok. Such a helical edge state form a Kramer’s doublet. Now because there is no time reversal symmetry violation these 2 are degenerate states and they are the Kramer’s doublet to degenerate Kramer states that I mentioned at the beginning.

So, the energy the E versus momentum looks like this. The bulk is of course, gap full. There is a gap there is and the edge states are these 2 edge states now with spin up and spin down moving in opposite directions. So, that is the band structure. So, this is schematic band structure of 2D TIs with helical edge state. This can also be thought of at as a spin hall effect because the 2 spins are moving in 2 different directions up and down. So, there is spin directions are different. So, up spin is moving this way down spin is going the other way. So, there is a spin imbalance that can happen. Of course, in a closed loop that will get that will it not happen, but there is a at any point at any point of time you will see that the two spins are moving in opposite directions continuously.

So, that is a remarkable situation and it is actually it is also called quantum spin Hall effect. So, this is going to be the spin momentum locking in the edge channels the electronic state of the 2 d TI is also called quantum spin Hall Effect observed in HGTE quantum well structures. So, this picture actually shows it in B equal to 0 this p s up. So, s dot p when is conserved. So that means, p has to maintain is if s remains up then p has to maintain in this direction and then if is s is down in the red then p has to maintain in this direction. So, the again the momentum the electrons are moving in two different directions that is also that is the hallmark of Hall system right. But it is due to the spins and spins are forcing the up and down spin are forcing the momentum to be in two opposite direction and that is this logic is the locking that is being talked about and this is also called quantum spin Hall effect.

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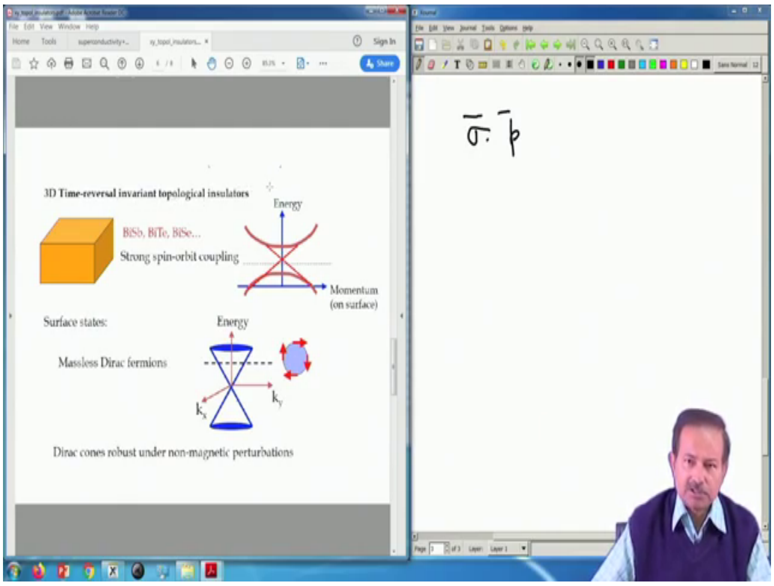

So, the 3 there is of course, the 2d is a is already known in the sense that when one did Quantum Hall effect one actually realized this that there are these edge states which are chiral edge states and they have this feature. They are gapless at the edges and the in the bulk there is a gap and so on. All that was serve understood in the eighties and early nineties, but about 15 years back the 2 3d time reversal invariant topological insulators was predicted. And remember when I mentioned quantum Hall and edge state we still had no time reversal symmetry.

So, the quantum spin Hall Effect is when the B was 0. So, time reversal symmetry was intact. So, that is different from quantum Hall, but that is attributed to spin orbit coupling. So, that was understood now this was understood late. The fact that edge states are the ones carrying current in quantum Hall effect was understood in 1980s and early in and there on, but the fact that spin orbit coupling can do the same in a time reversal symmetry invariant system was understood in the early 2000s by Charlie Kane and Mele had series of papers and many others Burne (Refer time: 27:18) and so on and so forth.

The there are beautiful reviews on this you can look up the literature. So, there is there now a 3d time reversal invariant topological insulator which is basically transfer the bulk the whole thing that was happening at the edge will now happen at the surface. So, that is the; that is how it is done. So, these are materials where strong spin orbit coupling gives these surface states. These 2 states are the surface the bulk is gapped and these are for example, from graphene we actually knew that there are massless Dirac fermions Dirac kind of spectrum right and so this massless Dirac spectrum has this such features and you can write a Hamiltonian for that for this kind of a situation.

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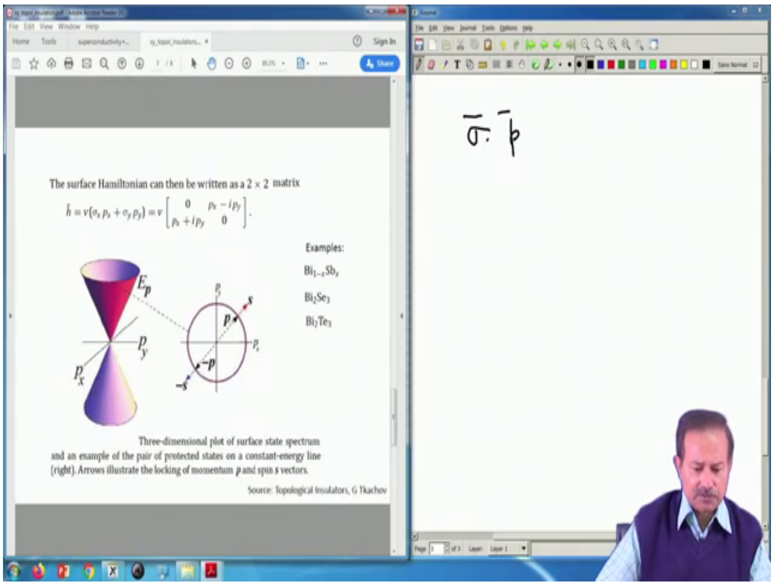

So, dirac these dirac cones are robust under non-magnetic perturbation. So, all that happening is that there is there are these edge states at the surface which are gapless whereas, the bulk is gap full. So, these are 3d topological insulators and there are systems where people have found it BiSb,BiTe,BiSe and so on. So, one can write the surface Hamiltonian for these kind of systems which is very much like graphene and. So, this is this is the massless Dirac mold and as you can see that here also you have this spin and momentum locking and the minus S and plus S have different directions of momentum.

So, there are two such states pair of protected states. These are p states are topologically protected because they by Kramer’s theorem. They are they have the same energy and by the fact that Hamiltonian has this helicity which is conserved they have to maintain it and because the bulk is gap full there is nothing to scatter with and that is exactly an analogue of this 2d edge states which was a one dimensional edge. Here it is a surface two dimensional surface where the same thing more or less happens and the Hamiltonian is this and for example, and then you have these surface states which are protected and their momentum and spin are locked.

And as I said they have a gapless metallic region at the surface because of these states and these are called topological insulators. So, in 3 dimensions. So, this is now an active area of research and if you are interested you can go up and look at lots and lots of literature on this.

So, this basically ends the discussion of Electronic Theory of Solids. I only could give a glimpse of what is happening and how things are happening. I have avoided discussing experiments in detail because this is to give you the microscopic theories and our basic understanding of all the electronic processes of the ones which are important and which should be discussed in a condensed matter course.

And then of course we also discussed this physics of spins and of course, super conductivity and topological systems a bit and all this is basically electronic all these are electronic processes. The spin is tied to the electron and every process that we discuss is an electronic process. So, and in some cases the degree of freedom is such that the charge degree get gets quenched the spin degree is the only manifested degree that one should look at. For example, in insulators in magnetic insulators and so on so, this these kind of ideas that in a real system this beautiful quantum mechanical physics plays out and all these degrees of freedom can be manipulated can be used and they have their manifestations in beautiful new exotic properties is what I wanted to convey to you. We will end here and I hope you enjoyed it. I did it myself and thank you so much.

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