Topology and Condensed Matter Physics
Prof. Saurabh Basu

Department of Physics

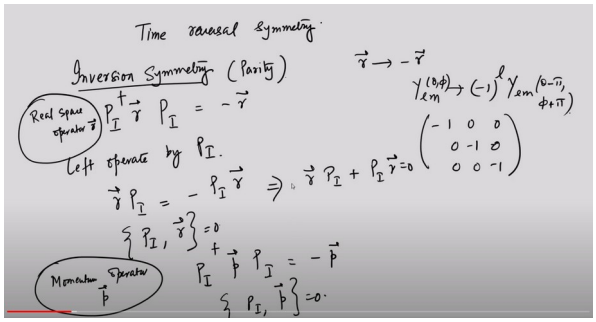
Indian Institute of Technology Guwahati

Lecture – 05

Symmetries and SSH - model

Welcome to the fourth lecture on Topology and Condensed Matter Physics course. We have been talking about discrete symmetries and how these symmetries actually are responsible for the topological phases of matter. And if you actually destroy one of the symmetries then the system may not remain topological or may make a transition from one topological state to a trivial state or a topological state to another topological state which will happen via you know the gap closing of the energy spectra of the Hamiltonian.

(Refer Slide Time: 1.26-7.50)



So while we were discussing the discrete symmetries and we have talked about these time reversal symmetry which has been you know discussed in the previous day and we have done it for both spinless systems that is the Hamiltonian does not explicitly involved spin or even in the case when it does explicitly involved spin because if particularly if the system has this spin orbit coupling then you need to take into account spin degrees of freedom else it can be considered as spin polarized which are both the cases we will see over as we progress through the course. Alright so now since we have done this time reversal symmetry the one that is remaining a few of them are remaining we will now talk about the inversion symmetry this is also called as parity. So what is an inversion symmetry if you change x to minus x or r to minus r then that is called as inversion symmetry I mean r to minus r what I mean is that so the vector r goes to minus r that

means the magnitude r remains same theta changes by certain angle and phi changes by certain angle and that is what is called as a parity operation this you might have learned when you did hydrogen atom and or the angular momentum.

$$\vec{r} \to -\vec{r}$$
$$Y_{lm}(\theta, \phi) \to (-1)^l Y_{lm}(\theta - \pi, \phi + \pi)$$

So in fact you wanted to know that what are the sort of inversion symmetry or parity of the spherical harmonics and the spherical harmonics actually pick up a minus 1 whole to the power L under parity transformation. So this is like minus 1 whole to the power L Ylm so this theta phi and so this is equal to theta plus pi and phi minus so it is probably minus here or plus here anyway this can be settled if you look at the relevant discussions in hydrogen atom. Here we are talking about discrete symmetries that is under these transformation the let's talk about this parity or the inversion symmetry operators by a pi, i stands for inversion and p stands for parity why I am writing both the with a subscript is that we will also use the particle whole symmetry with p that is why I am just writing it with a pi. So if you have a pi acting on you know r and a pi so this is a dagger then this becomes equal to minus r so r is the position operator so this is the definition of that.

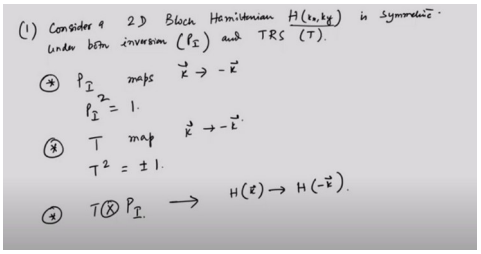
$$P_I = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
$$P_I^\dagger \vec{r} P_I = -\vec{r}$$
$$\vec{r} P_I = -P_I \vec{r}$$
$$\implies \vec{r} P_I + P_I \vec{r} = 0$$

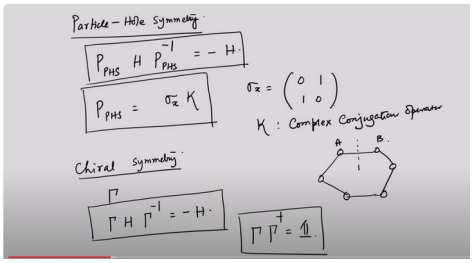
So in a simple case you know pi could be just a matrix like minus 1 0 0 0 minus 1 0 and 0 0 minus 1 which inverts all the r to minus or the x to minus x y to minus y and so on. So if you write it like that then pi r these are unitary operators which means that uu dagger equal to 1 so pi dagger equal to 1 so this becomes equal to minus r pi and so on so what I do is that I write multiplied by the pi dagger on both sides and the pi pi dagger becomes equal to 1 and that tells you that I mean this or what you can do is that you can also write left multiply by p let us just do that instead of this step. So I will write it so left operate by pi and that will become r pi because pi pi dagger will become equal to 1 and minus pi r and so that tells you that they anti commute because r pi plus pi r equal to 0 and hence they anti commute so pi and r anti commute.

$$\{P_I, \vec{r}\} = 0$$
$$P_I^\dagger \vec{p} P_I = -\vec{p}$$
$$\{P_I, \vec{p}\} = 0$$

And what happens to the momentum variable in fact we mostly talk about the position variable momentum variable and if it concerns spin now of course parity has got nothing to do with spin so it will leave it unchanged. So this is for the real space operator R and for the momentum operator p it has a very similar thing because p is nothing but dr dt which means that it's proportional to the velocity multiplied by the mass so this will also give rise to this pi then p and then pi equal to minus p okay and so the p is the momentum operator and then again you we have these pi and p that anti commute and will give to 0. This what it means by when a Hamiltonian has p and r Hamiltonian contains p and r and this is individually how the inversion operator or the parity operator acts on each of R and p and will transform them. So if Hamiltonian has both R and p so you can check whether you know it changes sign under this inversion operation.

(Refer Slide Time: 7.52-15.00)





So let me write down a few important points so if you consider say a 2D block Hamiltonian just for an example what I mean by 2D block Hamiltonian is that it's a *H which is a function of k and k is a function of kx and ky* just a 2D thing and if it is symmetric under both function which is what we have seen just now and time reversal symmetry I'm in short I'm writing it as a trs which is t then the inversion of course maps to so pi maps k to minus k, k is nothing but the wave vector which is related to the momentum by just multiplying it by h cross and it also satisfies that p square is equal to 1 because if you do the inversion twice it comes back to the same configuration and then if we have trs as well then it sort of so trs does the same thing so trs also maps k to minus k and t square of course will square to 1 or minus 1 depending on whether we have the spin variable in the problem or not because the spin is not included here explicitly as we can see in this block Hamiltonian then we can write it as t square equal to plus 1. So if a Hamiltonian has both t and pi okay then H of k remains as H of k I mean that so they remain invariant under this both time reversal and the inversion operation okay so let me now look at in brief we'll talk about it we'll talk about the particle hole symmetry.

$$H = H(K) = H(k_x, k_y)$$
$$\vec{k} \to -\vec{k} \quad P_I^2 = 1$$
$$\vec{k} \to -\vec{k} \quad T^2 = \pm 1$$
$$T \otimes P_I \to H(\vec{k}) \to H(-\vec{k})$$

So this means that if we convert a particle into hole then the Hamiltonian whether the Hamiltonian remains invariant it's a property of a superconductor to have particle hole symmetry okay so the number of particle states will correspond to exactly the same number of hole states and so on and corresponding to a particle of energy E particle state of energy minus E there will be a whole state of energy plus E and so on. So let's write a P H S less that the operator be for the particle hole symmetry and then a Hamiltonian will have this kind of operation which is minus H okay so this is the symmetry operation of that so we can write down this P P H S usually as a sigma x and a k where sigma x is a Pauli matrix which is written as 0 1 1 0 and k is the complex conjugation operator okay and as I said that this is inbuilt in the in the case of the superconductors. Now to wind up the discussion we'll talk about the chiral symmetry this is a very important symmetry of the Hamiltonian and vis-a-vis its relation to topology and in a very simple model which we are going to see just after this discussion say a model has like for example graphene has chiral symmetry which means that both the A and B sub lattice they are like this so it's a honeycomb lattice and there are two unit cells two atoms per unit cell and both the atoms we name them as A and B but both the atoms contain carbon.

$$P_{PHS} H P_{PHS}^{-1} = -H$$
$$P_{PHS} = \sigma_x K$$
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

So if A changes over to B or B changes over to A it's like an inversion about this dotted line then the Hamiltonian remains invariant because both of them correspond to carbon atoms okay. This is a particular example in graphene but we'll see more examples particularly tight binding Hamiltonians and at this moment I do not want to elaborate on it much but a similar operation which we do it by tau so this is a chiral symmetry operator it has a similar effect as the particle hole symmetry so this is equal to minus H okay. So this is the operator and these are how it sort of transforms now I'm just saying that chiral symmetry for a very simple case is the inversion symmetry or it's a this called as a sub lattice symmetry so the chiral symmetry for graphene is a sub lattice symmetry what graphene is we haven't said yet but we'll make that clear as we you know go along

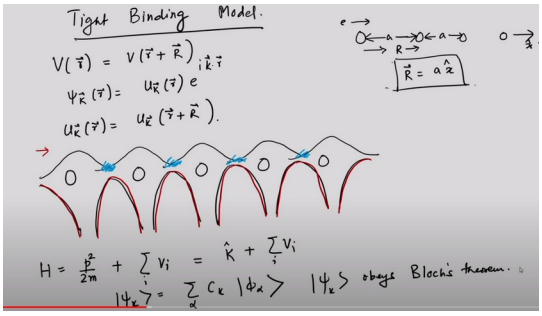
the course and of course all these symmetries are unitary symmetries or anti unitary.

$$\Gamma H \Gamma^{-1} = -H$$

$$\Gamma\Gamma^{\dagger} = 1$$

So these gamma, gamma dagger is equal to 1 and so on okay. So these are some of the discrete symmetries that we'll be needing in during the course and let's now go into a simple problem which is a tight binding model that shows topological features and it's the simplest paradigmatic model for seeing topology and is widely studied in this context it's simple and as well as it's quite intuitive for us to understand okay.

(Refer Slide Time: 15.09-21.44)



So we'll do that and but before that let's do a quick recap of the tight binding Hamiltonian or tight binding model and to understand what that is it's a method of calculation of the energy spectrum for a particle that is subjected to a periodic potential and what I mean by periodic potential is that we talk about crystal lattice where there are presence of ions or atoms at regular interval and this regular interval is called as a lattice constant okay. And as if I consider an electron to be you know moving in this array of ions or atoms these ions say for example are going to sort of exercise or the electron will actually see perceive this interaction or rather a potential due to this presence of these ions or the atoms okay. And since these are periodically placed one can write down V equal to V of R equal to V of R plus capital R where capital R is the vector that connects from one lattice point to another okay.

$$V(\vec{r}) = V(\vec{r}+\vec{R})$$

$$\vec{R} = a\hat{x}$$

So this is the R and this is equal to if you write so R vector is equal to a say R R cap or something okay. So this direction is R or you can write it simply as X cap okay. So this is called as a periodic potential and Bloch has said that the wave function of a particle is subjected to such a potential has a form which is psi k of R this is equal to u k of R exponential i k dot R this k is a vector. So where is the periodicity information embedded the periodicity information is embedded here in this u of k which is equal to u k of R equal to u k of R plus R okay. Now this is well known and the proof is also quite simple

and straightforward will not follow that this is the first course of solid state physics would teach you that this is the wave function but just getting the wave function is not enough to arrive at the solution of a problem we also need to know the energies.

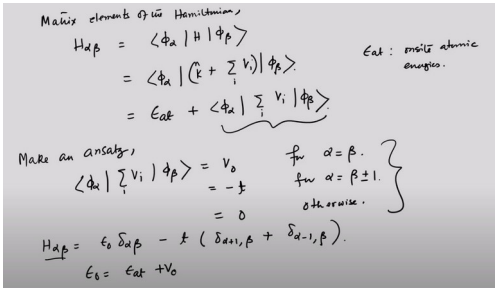
$$\psi_{\vec{k}}(\vec{r}) = U_{\vec{k}}(\vec{(}r))e^{i\vec{k}.\vec{r}}$$
$$U_{\vec{k}}(\vec{r}) = U_{\vec{k}}(\vec{r} + \vec{R})$$

And in order to get the energies we need to resort to some approximations and tight binding approximation or tight binding model is one such approximation in which it is assumed that the electronic wave function is tightly bound to this these ionic cores I am just for a moment I am consider them as iron so that the electron feels a potential it could be an atomic potential also but let's just consider that there's a potential like this like this that is an attractive potential given by these ions. So these ions are positively charged and then it gives a potential which is which is given by this let me use a color so that overwrite on this so this is the potential on in red that you are seeing so an electron that's going passing through these potential so the electron will be passing like this and it sees a potential a series of potential which are periodically placed which means they are placed at regular intervals which are given by this a which called as a lattice constant. Okay so the assumption is that this electrons are they have the majority of the amplitude of the wave function is centered at the core ionic core that is it peaks here where the ion is and so on at all of them it has very little overlap between the wave function at the next core as the next ionic core. So you see this overlap region of overlap and this region of overlap is very small and that's why it's called tight binding it's tightly bound to the ionic core and these small overlap renders a mobility to the electron because the electron has to go from one ion to the next ion and to the next time it will move around it's a mobile charge. So it is tightly bound to this and in this approximation one can work out what the energy is as I said that the energy is still missing into this this blocks theorem which gives you the form of the wave function.

$$H = \frac{p^2}{2m} + \sum_i V_i = \vec{K} + \sum_i V_i$$
$$|\psi_k >= \sum_\alpha C_k |\phi_\alpha >$$

So H is in this particular case H is equal to say for example a p square over 2m which is coming from the electrons and plus a Vi. Okay and so this can be written as the kinetic energy plus the Vi where Vi are these ionic potentials at a site i so i equal to 1 to n whichever the number of sites are. Okay and one can write down the wave function as psi k and it can be expanded in the basis of phi alpha this is equal to Ck and a phi alpha. Okay so this is like a expanding it in a complete set of states where phi alpha is the basis. Okay psi k obeys blocks theorem.

(Refer Slide Time: 21.44-26.24)



So I am trying to give you a very simple derivation of the tight binding Hamiltonian and which is going to be essential for a lot of the discussion that is going to follow and phi alpha of course are the basis states. So if we write down the matrix elements of the Hamiltonian that is H alpha beta where alpha and beta are two orthogonal basis phi alpha H phi beta we have already written H and this is equal to a phi alpha k plus Vi and a phi beta. Okay and this is so the kinetic energy is a one body term which we have discussed so this can be written as the atomic energies so let us write it as epsilon At for the atomic energies and what is important is this term to calculate which is equal to i and a Vi phi beta.

$$H_{\alpha\beta} =< \phi_\alpha | H | \phi_\beta >$$
$$=< \phi_\alpha | (\hat{k} + \sum_i V_i) | \phi_\beta$$
$$= \varepsilon_{at} < \phi_\alpha | \sum_i V_i | \phi_\beta >$$

Okay this basic quantum mechanics so these epsilon At are the onsite atomic energies basically because of the kinetic energy of the electrons and this is the thing that one needs to compute and one can make an ansatz as follows phi alpha sum over i Vi and a phi beta so this is equal to V0 for alpha equal to beta it is equal to minus T for alpha equal to beta plus or minus 1 we are talking about one dimensional system and it is 0 otherwise. Okay so what I mean is the following that the matrix element for this Vi will this Vi will vanish if these i and j or rather these alpha and beta are not these wave functions that correspond to the neighboring sites and at the site for alpha equal to beta that is the onsite that term can be of course absorbed in this epsilon At.

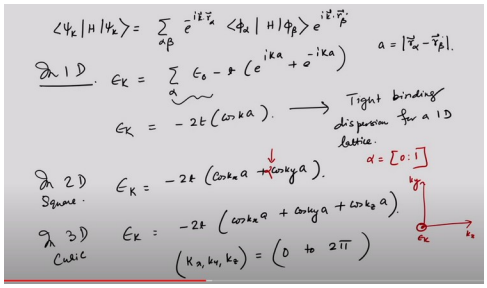
$$< \phi_\alpha | \sum_i V_i \phi_\beta >= V_0 \quad for \quad \alpha = \beta$$
$$= -t \quad for \quad \alpha = \beta \pm 1$$
$$= 0 \quad otherwise$$

Okay and so if we leave these epsilon At and V0 which we can all combine that is we can write down H alpha beta equal to some epsilon 0 delta alpha beta and then we can write down a minus T, T is the amplitude for that matrix element for which alpha equal to either beta plus 1 or beta minus 1 where alpha and beta here refer to of course they refer to the basis indices but the basis is written in terms of the onsite indices the site indices for the system.

$$H_{\alpha\beta} = \epsilon_0 \delta_{\alpha\beta} - t(\delta_{\alpha+1,\beta} + \delta_{\alpha-1,\beta})$$
$$\epsilon_0 = \epsilon_{at} + V_0$$

So this is equal to delta alpha plus 1 beta plus delta alpha minus 1 beta and so on. Okay so and where epsilon 0 is of course this epsilon At plus a V0. Okay that's a constant that we don't need to worry about that anyway this gives you the diagonal elements of H alpha beta and minus T they lie on just the band above the diagonal and below the diagonal and this is the form of the this Hamiltonian and the energies are these are basically nothing but the energies and these energies are obtained within this tight binding approximation as this. So this is the tight binding approximation and this is the energy corresponding to that so when I write down H alpha beta which means that I'm writing down the matrix elements of the Hamiltonian.

(Refer Slide Time: 26.24-32.42)



Okay so this can be written as so your psi k H psi k which gives you the energy it can be written as alpha beta exponential minus i k R alpha I'm writing it as a vector but in one dimension it will be a scalar so phi alpha H phi beta and exponential i k dot R beta so this is nothing but equal to sum over alpha epsilon 0 which takes into account the delta alpha beta and a minus T exponential i k a where a is equal to R alpha minus R beta so this is I'm writing it in one dimension so in 1D it becomes just a so a is the magnitude of this okay plus exponential minus i k a that comes from so this alpha R alpha minus R beta and if you leave this term which is just a diagonal term then this becomes equal to minus 2T cosine k a that's the tight binding dispersion for a 1D lattice. And very soon we are going to use this so in 2D square lattice square lattice so these are 1D chain result and so this is like epsilon k that is its dependence on this k, k is a wave vector that you know runs over the first Brillouin zone and this is equal to minus 2T and then you have a cosine

k x a plus a cosine k y a and so on okay in a 3D cubic lattice this can be it's a simple cubic lattice so epsilon k will be minus 2T cosine k x a plus cosine k y a plus cosine k z a okay and in all these cases the k x y z etcetera they run from 0 to 2 pi okay they are sort of in this interval or you can call it a minus pi over minus pi to plus pi okay.

$$< \psi_k|H|\psi_k >= \sum_{\alpha\beta} e^{i\vec{k}.\vec{r_\alpha}} < \phi_\alpha|H|\phi_\beta > e^{i\vec{k}.\vec{r_\beta}}$$

$$a = |\vec{r_\alpha} - \vec{r_\beta}|$$

So this is a simple tight binding model that gives you the energy of the electrons in a periodic potential the wave function of the electrons they have already been given by the Bloch's theorem okay so we are more or less ready to treat a tight binding Hamiltonian the main motive of us in this particular course is not to look at the electronic dispersion and talk about transport properties etcetera but to look at the topological characters from these dispersion and a priori without doing any calculation yet we can say that you know these topological properties are intimately connected to the band dispersion or the spectral dispersion that is these they are embedded into this epsilon k. So if you change the epsilon k somehow if you do some band engineering or if you change the say you put a say for example an alpha here okay where alpha is varies from 0 to 1 so this alpha and let me write it with a different color I do not intend to put it but just in case that you have an isotropic dispersion for some reason then these alpha will go from say 0 to 1 so alpha is 0 to 1 and you can clearly see that if alpha equal to 0 it becomes a one-dimensional chain and for alpha equal to 1 it becomes a regular 2d square lattice okay. So any nonzero value of alpha that is between 0 and 1 it will correspond to an anisotropic dispersion in which bands will be deformed if you draw the bands between minus pi and plus pi or 0 to 2 pi then the bands will be deformed okay. The standard way of doing this is that you take a kx and ky so this kx and ky and you calculate these quantity which is minus 2t cosine kx a plus cosine ky a and then plot that in the you know the z direction your epsilon k is in the z direction and then when you take the projection onto the kx ky plane will give you the contours or the energy dispersion and this dispersion can be represented by colors which will show you know the color will code values that are either higher or lower depending on you know the variation of the dispersion.

$$In \;\; 1D \;\; \epsilon_k = \sum_\alpha \epsilon_0 - t(e^{ik\alpha} + e^{ik\beta})$$

$$\epsilon_k = -2t(\cos k\alpha)$$

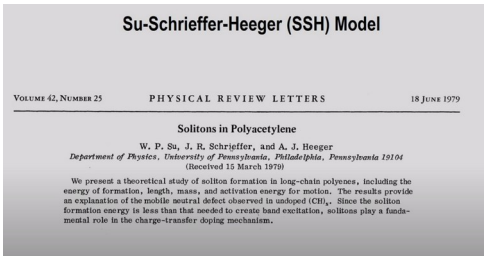
$$In \;\; 2D \;\; \epsilon_k = -2t(\cos k_x a + \cos k_y a)$$

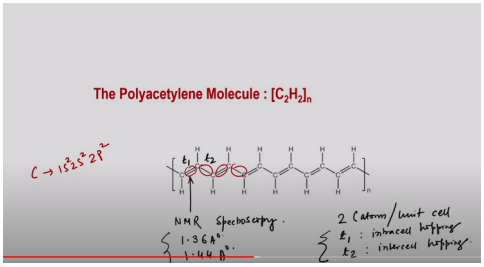
$$In \;\; 3D \;\; \epsilon_k = -2t(\cos k_x a + \cos k_y a + \cos_{k\ z} a)$$

$$(k_x, k_y, k_z) = (0 \;\; to \;\; 2\pi)$$

So coming back to the point that if you change alpha or you somehow deform the band structure by some chemical pressure or some mechanical pressure or something on a lattice then the topological properties are bound to change and these topological invariants that we have talked about at length they also will change.

(Refer Slide Time: 32.49/33.26-37.50)





Okay so let me show you one very simple paradigmatic model which is called as a Schur-Schrieffer-Higer model okay. This widely studied in the context of topology and it was pretty long back more than 40 years back it was proposed in a paper by Schur-Schrieffer and Higer Schrieffer is the same one who's in the BCS theory of superconductivity. So this is in physical review letters on 18th of June 1979 and it is about these they say that these long chain polyenes which are polyacetylene and they have this form C2H2N and this is how a long chain polymer that is polyacetylene molecule would look like this C2H2. So you see there is a double bond here and then there is a sort of single bond there is a double bond and then there is single bond and so on so forth okay and each of the carbon is attached to a via single bond to a hydrogen.

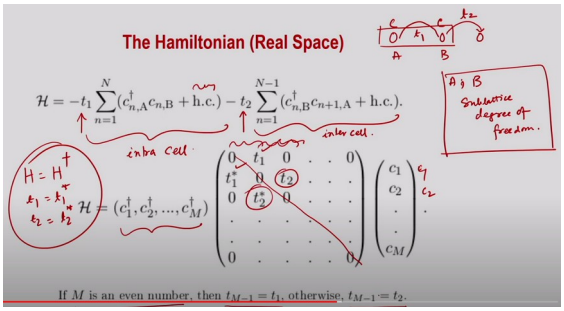
For us it's not important the hydrogen is not important for us what's important is this carbon-carbon-carbon bonds. So if we forget the hydrogen for the moment and only look at these carbon-carbon chain and carbon is in the it has carbon has 1s2, 2s2, 2p2 that's a 6 electrons and then these one of the p electrons that are available for conduction and the other p electron they sort of give rise to the sigma bonds which is to the stability of this long chain polymer okay. So it is you can you can take it as a 1 electron per atom and 1 electron per atom should be a metal because the electron is allowed to you know move from one carbon atom to the next and to the next and so on will give rise to its conducting behavior. However what happens is that these bonds are being probed by NMR spectroscopy and when they are probed they show that they have different length this 1.36 angstrom and 1.44 angstrom okay.

So they have these double bonds have different length as compared to the single bonds and these lengths being different as a physics you know a person trying to find out the properties of this model one can actually say that this corresponds to a hopping T1 and this corresponds to a hopping T2 just to remind you that this is the same T that we are

talking about the T here which is the hopping amplitude or the amplitude of the kinetic energy for the electron to you know go from one ionic site to the next ionic site. So this is the same thing here we are talking about so there is a T1 and a T2 so this model consists of two atoms per unit cell two carbon atoms per unit cell and T1 is intracell hopping and T2 is inter cell hopping okay.

Now as it is there is no surprise in this model or the properties do not seem to be anything very different or would yield any topological feature that we are interested in but it does it you know when you tune T1 with respect to T2 or T2 with respect to T1 you see that the system makes a transition from a topological state to a trivial state and once again I want to remind you that the topological state is like the like the doughnut and the trivial state is like the orange and the difference between them come from the fact that one has a hole that is a genus which the doughnut has and the orange has no such hole and that it denotes a trivial state of matter. So whether T1 greater than T2 or T1 less than T2 will give rise to such topological state or trivial state it cannot be a priori you know figured out. So that's why this model is interesting it's a model in 1D tight binding chain and that's the simplest one can think of and then we'll see that depending on a topological invariant called as a winding number this model shows different properties.

(Refer Slide Time: 37.59-42.25)



So the discussion is like this that we'll write down the Hamiltonian in the real space which we have written it down and then of course we'll Fourier transform it and take it into momentum space calculate the energy plot the energy find out the topological invariant which is a winding number here plot the winding number and see that the system winds the you know here it's called as an exceptional point but we have introduced this as a singularity. So that point of singularity whether your system is it encloses or not that will decide if it does then it is a topological state and if it doesn't it denotes a trivial state. So I write down so this is the intra cell hopping so these carbon atoms that you saw there they correspond to A and B sub lattices this is a C and a C a carbon atoms but since it's a two atoms per unit cell that's why we have labeled them as two different sub lattices so A and B are sub lattice degree of freedom.

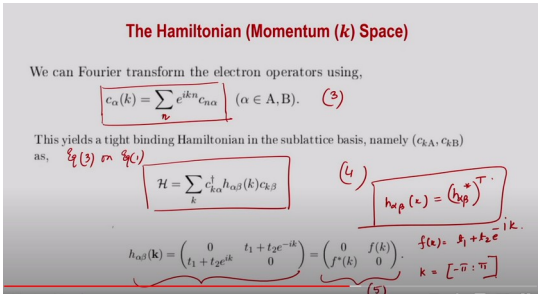
$$H = -t_1 \sum_{n=1}^{N} (c_{n,A}^{\dagger} c_{n,B} + h.c.) - t_2 \sum_{n=1}^{N-1} (c_{n,B}^{\dagger} c_n + 1, A + h.c.)$$

So this is the intra cell term that is inside a cell from A to B sub lattice so N is the the unit cell index is the unit cell index and this is within the cell hopping of the electron from one carbon atom to another and this one is the inter cell hopping which comes with a T2 this one comes with a T1 so which means that this hopping is T2 and this hopping is T1 and this precisely we have said about that polyacetylene molecule long chain molecule and this is there the Hermitian conjugate this is the Hermitian conjugate is always used in such tight binding models and if you do not use the plus Hermitian conjugate then the Hamiltonian will come out to be or rather the energies will come out to be complex.

$$H = H^{\dagger}$$
$$t_1 = t_1^*$$
$$t_2 = t_2^*$$

So there is a T1 and there is a T1 star for the Hamiltonian which means that H equal to H dagger your T1 equal to T1 star and T2 equal to T2 star which means their Hermitian these things conjugates are same. Alright so you have no term along the diagonal because you see no term that connects there is no potential at the on-site potential and these are between the same unit cell this is the hopping between A and B sub lattices and this is the hopping that is between this and this is the hopping which is T2 and T2 star and so on so forth. So this is written in this the first line indicates the Hamiltonian written on the site basis and in the second term we wanted to make sure that you know how to write it in the basis which are formed by these site operators. So C1 dagger, C2 dagger, C3 dagger, Cm dagger are the creation operators for electrons at the sites 1, 2, 3, 4 till m and similarly C1, C2 here they correspond to operators annihilation operators at the site C1 to Cm. There is you have to be careful if you keep m to be an even number then you use you know the Tm minus 1 is equal to T1 and if you take m to be an odd number then the last one that is or the one that is you know one before the last but one hopping are will change accordingly because you want to end it at the with the right kind of hopping.

(Refer Slide Time: 42.31-45.10)



Alright so because this system has transnational invariance one can do a Fourier transform this is the operator for the Fourier transform where so this n here and then there is an alpha here there is n, n is the site index if this is n alpha is sub lattice index and it yields a when you do that apply to this Hamiltonian equation number 1 let us call it equation number 2 then you get a Hamiltonian which is like this.

$$c_\alpha(k) = \sum_n e^{ikn} c_{n\alpha} \quad (\alpha \ \epsilon \ A, B)$$

$$H = \sum_k c^\dagger_{k\alpha} h_{\alpha\beta}(k) c_{k\beta}$$

So if you apply 3 on equation 3 on equation 1 then you get this you get a nice and compact form for the Ck alpha H alpha beta K Ck beta where H alpha beta has a nice form which is like this of diagonal form that is it does not have any diagonal term 0, 0 are the diagonal elements and the off diagonal elements has a real term and an imaginary term and these off diagonal element is actually the complex conjugate of that.

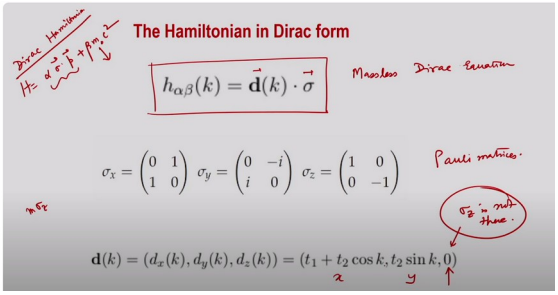
$$h_{\alpha\beta}(k) = (h^*_{\alpha\beta})^T$$

$$h_{\alpha\beta} = \begin{pmatrix} 0 & t_1 + t_2 e^{-ik} \\ t_1 + t_2 e^{ik} & 0 \end{pmatrix} = \begin{pmatrix} 0 & f(k) \\ f^*(k) & 0 \end{pmatrix}$$

$$where \quad f(k) = t_1 + t_2 e^{-ik}$$

So in the sense that if you change so H alpha beta K is equal to H beta alpha you know this and so on okay I mean I can write this as H alpha beta star and transpose okay so this tells you that it is a Hermitian matrix and so I write f of K is equal to t1 plus t2 e to the power minus ik. K is it runs from minus pi to pi it is a one-dimensional Brillouin zone you can connect it you know using periodic boundary conditions but this is a very simple model which we are almost at the last stage of calculating the energy but as we know that calculating only the energy is not sufficient we have to also talk about the topological properties at least first calculate the energy.

(Refer Slide Time: 45.13-49.10)



And very interestingly this Hamiltonian that we have written here let us call it equation 4 so the 4 and 5 combined you can see that we can write down the Hamiltonian in terms of this called as a massless Dirac equation and why it is called a massless Dirac equation is that usually the Dirac equation is written in terms of so your H is equal to alpha sigma dot p plus beta m naught c square that is a form of the Dirac Hamiltonian.

$$h_{\alpha\beta}(k) = d(\vec{k}).\vec{\sigma}$$

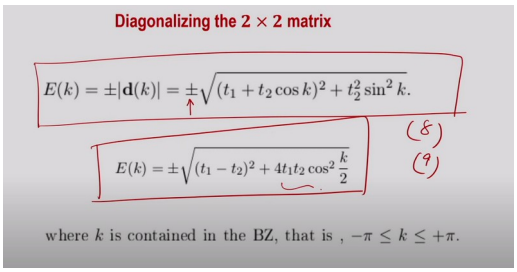
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

And in this particular case the Hamiltonian is this term does not arise here and it is only this term p is nothing but h cross K if you take h cross equal to 1 its sigma dot K or K dot sigma and there is a this alpha which is usually it is a matrix in the case of Dirac equation but here that is equal to 1. So it is a d dot sigma so where these p is replaced by d and these d is a function of K so that is a vector there is a vector and the sigma x sigma y and sigma z are nothing but the Pauli matrices. So in the first course of quantum mechanics you might have seen them and have read a lot about their commutation relations and their properties and so on okay many things and the problems concerning this Pauli matrices must have been taught okay. So what is this d vector? d vector has got of course three components because we are writing it as d dot sigma but fortunately for us the one component is equal to 0 that means that sigma z is not there okay and this is a very important thing in this study of topology that if you have the d vector to only have two components like here x and y component but it may have y and z component or x and z component in that case it is easy to find the winding number. If it is not the case that is if you are include a term say let us call it as some m sigma z and in that case you will have a plus there is a m here and this m will make the definition of the winding number to be ill-defined in the sense that you will not be able to show the winding unless you do something to the problem that is do a unit rate transformation to you know take away one of the components it is very difficult to visualize the winding number.

$$d(k) = (d_x(k), d_y(k), d_z(k)) = (t_1 + t_2 \cos k, t_2 \sin k, 0)$$

In this particular case we will take this d vector and vary k over the Brillouin zone which means that we change k from minus pi to plus pi and see that the 0 0 point see the 0 0 point when you have k equal to 0 that is I mean 0 it means that k equal to 0. So, k equal to 0 is it becomes t 1 plus t 2 and 0 0. So, the d vector becomes you know just a one component thing which is just like a point. So, this 0 point that is the k equal to 0 which is a center of the Brillouin zone is called as an exceptional point and this we want to see whether the d vector encloses the exceptional point. So, this is the idea and then we diagonalize the 2 by 2 matrix which is very easy for us to do.

(Refer Slide Time: 49.06-50.30)



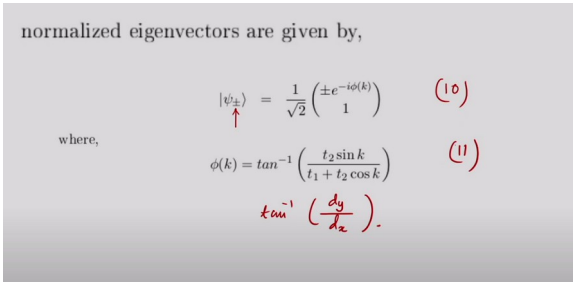
So, this is the matrix that you diagonalize equation number 5 f k and f star k and then we find out that this e k is the energy dispersion for these problem where it is and square root of t 1 plus t 2 cos k plus t 2 square sine square k and there are 2 bands coming from the plus and the minus sign. If we open the bracket inside we can write it in a little more convenient fashion which is you know convenient for our discussion it is a plus minus root over of t 1 minus t 2 square plus 4 t 1 t 2 cos square k by 2 and say this is equation 5. So, this is equation 6 say this is equation 7 and let us call this as equation 8 and this is equation 9 ok. So, k is as I said is contained in the in the first Brillouin zone. So, it is minus pi less than equal to k less than equal to plus pi.

$$E(k) = \pm|d(k)| = \pm\sqrt{(t_1 + t_2\cos k)^2 + t_2^2\sin^2 k}$$

$$E(k) = \pm\sqrt{(t_1 - t_2)^2 + 4t_1t_2\cos^2\frac{k}{2}}$$

So, this is the form of the these Schur Schrieffer-Hegel model the energy dispersion of particles in the Schur Schrieffer-Hegel model it contains as expected the 2 hopping t 1 and t 2 and the k dependence is here that how it varies with k ok and so on ok.

(Refer Slide Time: 50.38-51.00)



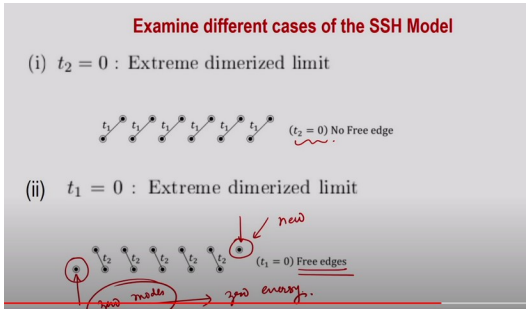
So, you can solve the matrix and find out the eigenvectors as well we have calculated the eigenvalues and here are the eigenvectors. So, these are corresponded this plus and minus sign that you see here correspond to the plus and minus eigenvalues of this Hamiltonian or these energies that you see here and so, this is a equation 10 and this phi k is nothing, but the tan inverse of this t 2 sin k. So, this is nothing, but a tan inverse of d y by d x ok

that is the d y means you know this is like y component of the d vector divided by the x component of the d vector ok it is not derivative or anything. So, this is the complete solution of the problem, but we are far from the topology that is embedded here.

$$|\psi_{\pm}>= \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{-i\phi(k)} \\ 1 \end{pmatrix}$$

$$\phi(k) = \tan^{-1}(\frac{t_2 \sin k}{t_1 + t_2 \cos k}) = \tan^{-1}(\frac{dy}{dx})$$

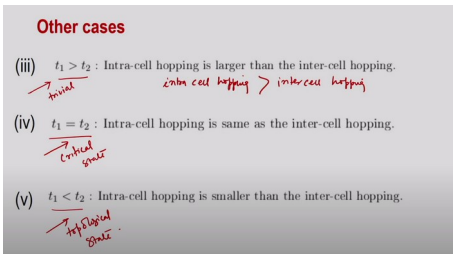
(Refer Slide Time: 51.40-53.50)



Now, in order to see the topology let us examine few different cases one of them is let us call it as a t 2 equal to 0 that is these model does not have any t 2 which means that these inter cell hopping is equal to 0. So, if you have inter cell hopping equal to 0 it looks like this. So, there is nothing here ok. So, this is absent and this is absent and so on and in this case it is called as a extreme dimerized limit. So, these are dimers are formed and you have a perfect dimer and there are no free agents.

So, t 2 equal to 0. Now, you see if you take the other extreme dimerized limit which means that t 1 equal to 0 that is this hopping is equal to 0 if that is not there then you get a form which is like this ok. Again there are dimers, but there are two important digrations here which are not there in the earlier plot or earlier picture ok. So, there are free ages present and why I am showing them as free ages is that now adding them to the system will not alter the energy or you take them away from the system it will not alter the energy and that is why these are called as 0 these will give rise to 0 modes 0 modes means with 0 energy ok. They correspond to 0 energy for the reason that if you take them away or put them back really it does not make any difference in a finite size chain the edges or the edge atoms whether they are there or whether they are not there it hardly makes a difference to the energy of the system which means that they have 0 energy ok.

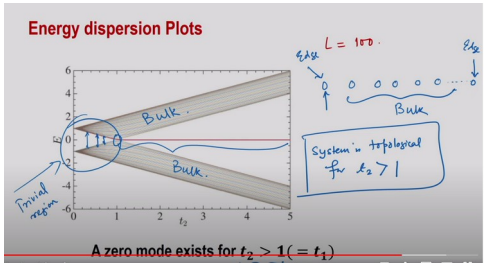
(Refer Slide Time: 53.53-55.17)



And this is what is important that they have 0 energy and there are other cases which are like this t 1 greater than t 2 that is the intracell hopping is greater than the intercell hopping ok and when they are same and when the other thing happens that is the intracell hopping is smaller than the intercell hopping ok.

Now a priori without going into the results this case is not interesting topologically not interesting and it denotes a trivial state that is like an orange which does not have a genus ok. This is the critical state where the system undergoes from a trivial to topological by a gap closing scenario. If you remember that we have talked about the Hamiltonian undergoes you know a gap closing scenario this gap has to close and open again for the topology to be visible to us or it is to be perceptible we can perceive it. So, t 1 less than t 2 is the topological state and let us see how we understand them. If we understand them in a simple way that is the triumph of this model.

(Refer Slide Time: 55.22-59.00)



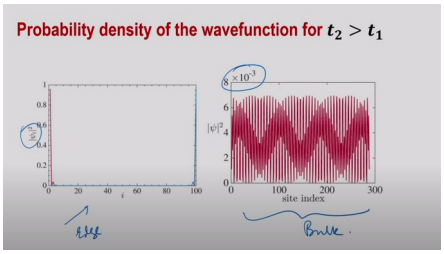
So, the energy dispersion this is a real space for certain you know L that is we have chosen certain L some value which is say 100 or 200. So, there are these say for example, 100 or 200 whatever we have say 100 and then we have solved it with t 2 with t 1 equal to 1 ok. So, t 1 equal to 1 you see that there is a 0 mode that is visible let me use a color there is a 0 mode that is visible here. So, that is beyond 1 that is t 2 greater than 1 you see there is a 0 mode and there is no 0 mode prior to that and the this is the bulk of the system.

Bulk means all the states that are in between. So, this is say this is equal to 100 ok. So, this is the last one. So, from t 2 equal to 1 and above so, that is t 2 greater than 1 these 2 becomes like this case like this case where there are these free edges and there are 0 modes present in the system. So, there are 0 modes bulk has a gap in both the cases that is the bulk states that is these states these are bulk and this is edge the left edge and this is a right edge ok. So, these are the bulk states which are here and here.

So, the system is topological here. Ok, because the 0 modes exist because you can add 2 edge modes which are so, it does not matter to the system whether you have added them or you have deleted them they are the modes with 0 energy. Now, you see that before these t 2 equal to 1 or larger we just talk about because t 2 equal to 1 is a critical state that is the gap closing thing which you see here. So, we will talk about t 2 greater than 1. So, t 2 less than 1 you see that there is a gap here at all values the gap is of course, reducing, but there is a gap, but there is no 0 mode.

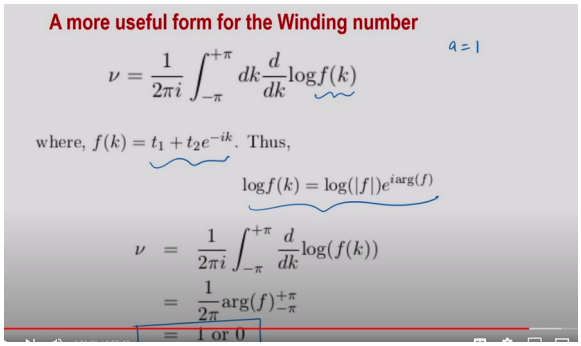
So, there is the trivial region. This region acts like an orange which has no genus ok and the 0 modes come from t 2 greater than t 1 that is t 2 greater than t 1 because t 1 we have taken to be equal to 1 if we take t 1 equal to 2 it will happen at t 1 greater than 2. So, why is it topological because now there is a difference between the edge and the bulk and this is the precisely the distinction of topological insulator. So, in the bulk of the system it looks different than what it looks at the edges ok and that is what is apparent from here it will be more apparent if we calculate the topological invariant.

(Refer Slide Time: 59.04-1.00.10)



We calculate the psi i squared here as a function of the site index site indices and you see that only at the edges we just plot the edges in this left hand side. So, this is the edge probability and this is the bulk. So, the bulk is extended it like a metallic bulk or they are extended states and so on and these are seem to be sort of there are high weights here whereas, the bulk states have almost same weight everywhere ok. So, it is there is a 10 to the power minus 3 which means that it is a very small weight for all the bulk states whereas, at the edges it is almost equal to 1 which means that bulk and edge they behave differently and this is called as a bulk edge correspondence. So, we will calculate the topological property from the bulk properties, but it will show signatures of the edge modes being present and that is called as a bulk edge correspondence or the bulk boundary correspondence ok.

(Refer Slide Time: 1.00.14-1.01.45)



Anyway so, we calculate this winding number it looks a little complicated will sort of simplify this discussion. So, mathematically the winding number which is a topological invariant ok. So, this is the topological invariant and it is some d cap cross d dk of this thing. So, this d dk of this d and then you take the z component and then d unit vector d is the vector d we have talked about and then magnitude of d ok. So, this is a more useful form and that can be used easily you remember that we have defined f of k f of k was defined here yes this is f of k.

$$v = \frac{1}{2\pi i}\int_{-\pi}^{+\pi} dk \frac{d}{dk} log f(k)$$

$$where \quad f(k) = t_1 + t_2 e^{-ik} \quad , \log f(k) = \log(|f|)e^{iarg(f)}$$

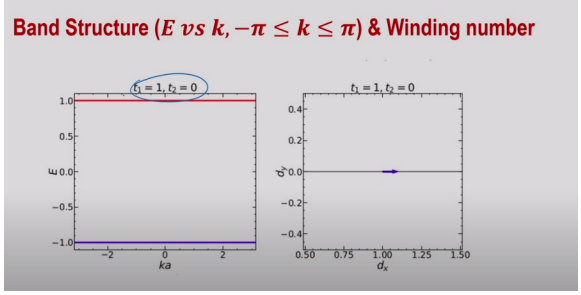
$$v = \frac{1}{2\pi i}\int_{-\pi}^{+\pi} \frac{d}{dk} log(f(k))$$

$$= \frac{1}{2\pi} arg(f)_{-\pi}^{+\pi}$$

$$= 1 or 0$$

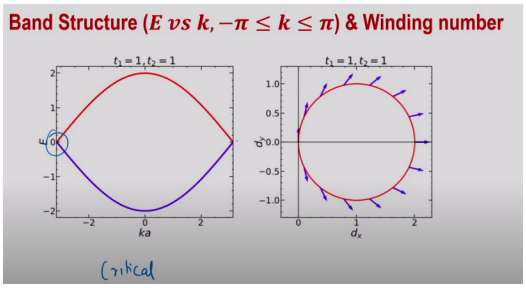
You take f of k and take this you take the log of that take a d dk of that and then integrate over the Brillouin zone which is from minus pi to plus pi ok. This everywhere we have taken a to be equal to 1 where a is the nearest neighbour carbon-carbon distance or the lattice spacing. So, this is if you take this and then log of f k you write it as this and do a little bit of algebra this will give you the winding number to be 1 or 0 depending upon the exceptional point or the singular point is being wound or not ok whether the system winds this thing ok.

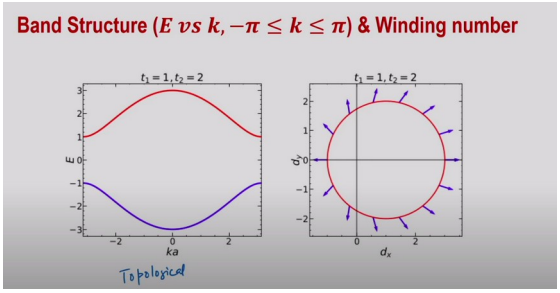
(Refer Slide Time: 1.01.50-1.03.10)



So, we show all these 5 situations that we have talked about here like the ones that are talked about. So, these 2 dimerize limit one being trivial, topological and again this is trivial critical and topological and so on. So, we calculate this winding number that we have just defined by this and calculate it for each one of these things. Of course, this is the dimerize limit where we do not expect any topological properties which is this extreme dimerize limit the top one that we see here this one that we see here that corresponds to this winding. So, we plot both the energy and the winding number. So, energy is on the left panel and the winding number is on the right panel for the same values of these things. So, this d 1 equal to 1, d 2 equal to 0 you see 2 flat bands at 1 and plus 1 and minus 1 and you see that there is no winding of the d in the dy dx plane as you change k from minus pi to plus pi ok.

(Refer Slide Time: 1.03.16-1.06.50)

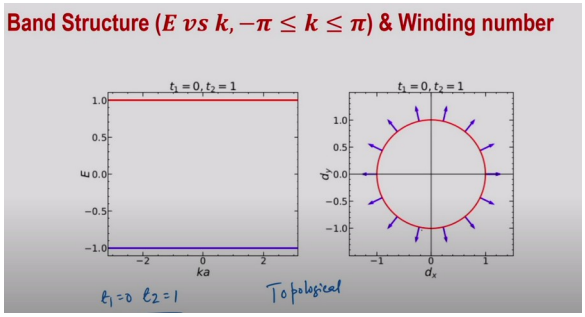




As you see the second scenario that is you have t1 still greater than t2 which means it is a trivial phase and the bands of course, show some dispersion not like this flat ones that you see here it shows some dispersion, but you see the winding this dx dy plane encloses a red circle which does not include the origin which is here. So, this is of course, a trivial phase and by this blue arrows what we show is that the d vector the unit vector d at various points in the dx dy plane as you change k ok that is shown by this blue arrow here ok. So, the winding is actually 0 winding is a point there is no winding here this is the d vector that is being shown ok and here also it is a trivial this is the critical ok and I said that the critical will show a gap closing scenario you see at the corner of the Brillouin zone which are minus pi and plus pi you see that the gaps close ok. Gaps close the dx dy circle just touches the touches the singular point or the exceptional point which is k equal to 0. So, this is the k equal to 0 point and it does not enclose it ok and again these dx dy directions are shown like this. This will correspond to topological phase. Now, if you look at the band structure between this and this that is t1 equal to 1 t2 equal to 0.5 t 1 greater than t 2 the band structure is absolutely identical ok.

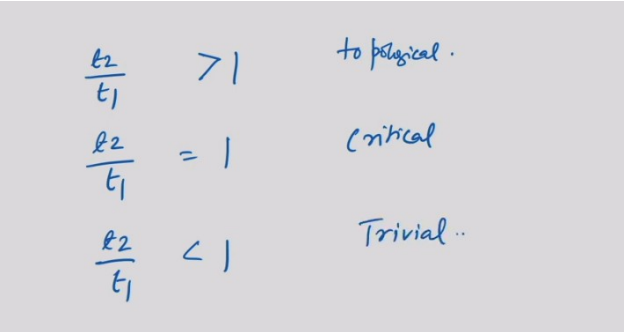
So, the conduction band which is shown by red and the valence band which is shown by blue this correspond to the plus and minus signs of the e versus k they are different, but of course, you see the dx dy curve which is a closed curve in the dx dy plane as you change k from pi to plus pi encloses the origin ok. And that is why the winding is equal to plus 1 or its finite ok and it is not 0 that is what is shown here that you see that the winding is 1 or 0. So, 1 corresponds to topological like your donut or your mug 0 corresponds to trivial like an orange with no genus ok. So, even though the band structure does not say anything that is e versus k we have done it with k a just to take it dimensionless.

(Refer Slide Time: 1.06.56-1.07.50)



So, that it becomes a number, but the winding of this gives you that it winds the origin and this is the other dimerized limit where there are you know t 2 is greater than t 1 or rather this is like t 2 is equal to 1 and t 1 equal to 0 that is the case which we have shown graphically by this plot this one here ok that is shown by this ok. Now you see it is again topological for the reason that your d x d y plane the curve the closed curve actually encloses the origin ok. And so, this of course, shows a topological phase transition as the system you know goes from this dimerization. So, we call a dimerization to be a ratio which is like t 2 by t 1. So, if t 2 by t 1 if t 2 is greater than t 1 or this dimerization is greater than 1.

(Refer Slide Time: 1.07.53)



So, dimerization is greater than 1 then topological or let us not call it dimerization let us call it as you know basically this is t 2 by t 1 ok. And let us not I mean it is a dimerized model of course. So, let us not talk about this as dimerization, but you can call it a hopping anisotropy anisotropy parameter or something ok. So, this anisotropy so, this will be topological and this to be trivial critical and to be trivial ok. So, SSH model thus encodes a very important property which is very important for our discussion it is a very simple model. However, it shows the topological characters that we have talked about it shows a topological phase transition as these hopping amplitudes the ratio of the hopping amplitudes are varied across the value 1 ok. So, we will come back with another model slightly more difficult, but nevertheless an important model which also shows topology ok. We will stop here. Thank you. .