

Topology and Condensed Matter Physics
Prof. Saurabh Basu

Department of Physics

Indian Institute of Technology Guwahati

Lecture – 03

Second quantization

Welcome back. We have been trying to establish connection between topology and condensed matter systems and in general we have done that for quantum mechanical systems such as electrons or the Aharonov-Bohm phase that is you know in the vicinity of solenoid. It is an additional phase that an electron can pick up. We are now more into these the connection to condensed matter physics and let me start with a topic which is quite important for understanding the later parts of this and it is been used heavily in the study of condensed matter and it is called as a second quantization. We will have to understand these the way the Hamiltonian are deformed etc. and why we bring in the topic of topology.

(Refer Slide Time: 1.31-9.00)

Second Quantization

Many particle system \rightarrow Identical particles

1 Particle $|a_1\rangle$

2 particles $\{ |a_1\rangle, |a_2\rangle, |a_3\rangle, \dots, |a_N\rangle \}$

$|a_1\rangle \otimes |a_2\rangle \otimes |a_3\rangle \otimes \dots \otimes |a_N\rangle \rightarrow$ Incorrect !!

2 particles $|\Psi\rangle = \frac{1}{\sqrt{2}} [|a_1\rangle \otimes |a_2\rangle \pm |a_2\rangle \otimes |a_1\rangle]$

$= \frac{1}{\sqrt{2}} [|a_1, a_2\rangle \pm |a_2, a_1\rangle]$

+ : Bosons
- : Fermions

So first we have to learn how to write down the Hamiltonian and these techniques of second quantization will aid us in doing so. So we will start with second quantization that is a formalism and this is a very important formalism in the study of either you talk about condensed matter physics or quantum field theory. It is very similar notations are used quantization. So we this would be also interesting because we would like to write down the Hamiltonian in the tight binding form.

Most of those Hamiltonian that we write later on would be having a tight binding form and then we will see that how a system is topological the parameter regimes in which it becomes topological and the properties that come along with. So why is this formalism important in general? So we are talking about many particle systems which means it

consists of *many particles* and these are *identical particles*. This is the main assumption of quantum mechanics that the particles that we deal with cannot be distinguished one from the other. So they all are absolutely identical and this identical nature creates a problem and in the following sense that when you swap two particles that is exchanged two particles the resulting wave function picks up a sign or may not pick up a sign depending on whether they are *fermions or bosons* respectively. So if you have more than two particles that is three particles so you have to keep a track of two such swaps or exchanges and three such or rather one swap is swapping say A and B and the other swap is a swapping A and C or B and C and so on. So let us just talk about two swaps in a four particle system there will be three swaps and so on. Each time you make a swap and you are dealing with fermions then you have to change the sign in the following sense we will just show that.

So this becomes a big problem to deal with a large number of particles and we often have to deal with large number of particles because the formalism of statistical field theory demands that we are actually talking about macroscopic number of particles so that the statistical mechanics that we are familiar with can be applied. So in that context we need to evolve a mechanism where such swaps between particles and the corresponding changes sign of the wave function can be incorporated. So let us just talk about one you know a particle to begin with let us say the state of the system is determined by these α_1 okay and if you are talking about n particles so this for one particle and say for n particles will have α_1, α_2 and then α_3 and so on and say so we are dealing with n particles and α_n okay and this will form a state okay a complete set of states and so on.

So this will form the Hilbert space. Now can we simply multiply it to write down the resultant ket that is whether this one is a possibility the inner product states and so on okay. So this is incorrect because of the reason that this does not give rise to the these permutation of particles or exchange of particles so we will see how. So let us talk about just two particles to make matters simple. So the either for fermions or bosons we can write down the resultant state as say ψ is equal to we do the normalization as well and we can write it down as say α_1, α_2 and plus minus α_2, α_1 okay.

$$\{|\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle, \dots, |\alpha_n\rangle\}$$

This can also be written as $\frac{1}{\sqrt{2}}|\alpha_1, \alpha_2 \pm \alpha_2, \alpha_1\rangle$ and where the plus sign refers to bosons and the minus sign refers to fermions okay and $\frac{1}{\sqrt{2}}$ is the normalization factor.

$$\begin{aligned} |\psi\rangle &= \frac{1}{\sqrt{2}}[|\alpha_1\rangle \otimes |\alpha_2\rangle \pm |\alpha_2\rangle \otimes |\alpha_1\rangle] \\ &= \frac{1}{\sqrt{2}}[|\alpha_1, \alpha_2\rangle \pm |\alpha_2, \alpha_1\rangle] \end{aligned}$$

(Refer Slide Time: 9.25-13.25)

So this wave function that you see here because of the indistinguishability you have to take combinations but that is indistinguishability also gives you or rather it provides you a solution as well okay and that solution is provided by going into a Fock space and this is discovered by V.A. Fock was Russian mathematician.

So we will discuss very quickly what Fock space is and if you need to understand what Fock space is let us just talk about bosonic system just to begin with so that because the fermionic system the number of particles is 0 and 1. So I already gave you the answer that will not really worry about that which state to put a particle in. So we will just worry about how many particles are there in a state. So we will go from these you know representation of putting a particle in a given state to count the number of particles

corresponding to a given state and this is called as a Fock space okay. So it's also it's called as an occupation number basis and so on.

So let us say that we have a quantum state suppose a quantum state is 1 1 1 2 2 2 3 3 4 5 6 and so on okay. So which means that the you know there are these particles is there is three quantum states containing one particle three quantum state containing two particles and two quantum states containing three particles one quantum state containing four particles one five and one six and so on so forth okay. So and this is like a sort of huge you know redundancy in its in its representation it will be much better if we just number these states in the occupation number basis and write the state in terms of how many particles in a in a given state. So we will just count the number of particles n_1 n_2 n_3 and n_n . So this n particle so there are these subject to of course these things that n_i so i equal to 1 to n has to be equal to n okay.

$$|\psi\rangle = |n_1, n_2, \dots, n_n\rangle$$

$$\sum_{i=1}^N n_i = N$$

So this is the total number of particles. So the Fock space has n_1 particles in state 1 n_2 particles in state 2 and so on just like you know there are three particles that are there three quantum state correspond to one particle and so on okay. So this is a this is called as a Fock basis and this will help us in writing down a second quantized Hamiltonian let us see how okay. So n_i can be anything for bosons okay so this is an important point and n_i is equal to 0 and 1 for fermions okay.

$$n_i = \text{anything} \quad \text{for bosons}$$

$$n_i = 0, 1 \quad \text{for fermions}$$

So either a given quantum state can have 0 particles that is no particle and or it can have at the most one particle okay.

(Refer Slide Time: 13.36-22.45)

Creation and annihilation operators (for fermions).

creation operator c^\dagger
annihilation c

creation $c^\dagger |n_1, n_2, \dots, n_i, \dots, n_n\rangle = (1 - n_i) c^\dagger_i |n_1, n_2, \dots, n_{i+1}, \dots, n_n\rangle$
annihilation $c_i |n_1, n_2, \dots, n_i, \dots, n_n\rangle = n_i (-1)^{\epsilon_i} |n_1, n_2, \dots, n_{i-1}, \dots, n_n\rangle$

$\epsilon_i = \sum_{j=1}^{i-1} n_j$

c_i, c_j^\dagger obey anticommutation relations

$\{c_i^\dagger, c_j^\dagger\} = c_i^\dagger c_j^\dagger + c_j^\dagger c_i^\dagger = 0$
 $\{c_i, c_j\} = c_i c_j + c_j c_i = 0$
 $\{c_i^\dagger, c_j\} = c_i^\dagger c_j + c_j c_i^\dagger = \delta_{ij}$

$[a_i^\dagger, b_j^\dagger] = i\hbar$
 $[a_i, b_j] = i\hbar$
 $[a_i^\dagger, a_j] = \delta_{ij}$

We are not talking about spin at this moment but that can also be incorporated. So this is basically provides you of course a simplification in writing an n particle state and but then we still are not sure that how this representation is doing justice to this exchange of

particles or the swap of the particles and let us see how that is being done. So that is done by using creation and annihilation operators okay. So these are represented by the creation operators are represented by C^\dagger it can be A^\dagger or B^\dagger depending on sort of notations that are used by various authors and the annihilation which is also called as a destruction operator this is represented by C okay. And so how what does this do this really does this so it is C_i it acts on these Fock space which contains $n_1, n_2, \dots, n_i, \dots, n_N$ and n_i so this is nothing but equal to $1 - n_i$ and minus 1 whole to the power epsilon i I just tell you what epsilon i is and n_1, n_2, \dots, n_i plus 1 and n_N okay.

$$C_i^\dagger |n_1, n_2, \dots, n_i, \dots, n_N\rangle = (1 - n_i)(-1)^{\epsilon_i} |n_1, n_2, \dots, n_{i+1}, \dots, n_N\rangle$$

$$C_i |n_1, n_2, \dots, n_i, \dots, n_N\rangle = n_i(-1)^{\epsilon_i} |n_1, n_2, \dots, n_{i-1}, \dots, n_N\rangle$$

So what it does is that it increases the number of particles in the i th level by 1 okay so this is what it does and in the process it picks up this factor and this factor we will just tell you in a moment what this factors are and you have a C_i that is this is for the creation and this is for the annihilation. So $C_i |n_1, n_2, \dots, n_i, \dots, n_N\rangle$ this is equal to n_i into minus 1 whole to the power epsilon i $|n_1, n_2, \dots, n_i - 1, \dots, n_N\rangle$ okay. So what is epsilon i ? Epsilon i is a quantity that considers this swap so it is a sum over all the n_j 's prior to that i so this j runs from 1 to $i - 1$,

$$\epsilon_i = \sum_{j=1}^{i-1} n_j$$

so you count all of them their occupancies we are particularly you know writing in terms of you know fermions such that so these are for fermions. We are not talking about bosons but they can also equivalently be done provided you do a symmetrization of the wave function this is very specific to the nature of fermions and bosons the fermions obey an anti-symmetric property whereas the bosons obey symmetric property wave function is symmetric under the exchange of particles okay and this is one of the reasons that the fermionic wave functions are written as later determinants because you know the properties of determinants are that if you exchange a row and or a column that is you exchange say third row with seventh row and so on or you exchange fifth column to fourteenth column for a given determinant it picks up a sign a negative sign you do two such swaps it picks up another negative sign which means the next sign will be positive and very importantly if you make two of the rows or two of the columns identical then the determinant is equal to 0 which is related to the exclusion principle Pauli's exclusion principle which says that no two particles will be allowed to occupy the same quantum state okay with all their quantum numbers to be identical okay we are at this moment we are not talking about spins but if they have different spins then they can occupy okay so epsilon i which is there in the exponent of this minus 1 whole to the power epsilon i I mean minus 1 so it's in the exponent of this minus 1 that takes care of these swapping of

the particles okay and these $1 - n_i$ in this expression for the creation operator that you see it ensures that if the particle already has an occupancy that is if an electron is already sitting in these state then no more addition can be done or it's allowed and so this is that $1 - n_i$ and this n_i that you see I'm sorry if I were to put an equality sign and this n_i that you see is it makes sure that the occupancy can never be negative okay so it is either 0 or 1. Now these things obey anti-commutation relation what are anti-commutation relations they are just like commutation relation that you are familiar with just to remind you that $x p$ commutator is equal to $i \hbar$ cross that's a commutation relation which means $x p - p x$ is equal to $i \hbar$ cross,

$$\begin{aligned} [\hat{x}, \hat{p}] &= i\hbar \\ \hat{x}\hat{p} - \hat{p}\hat{x} &= i\hbar \\ \vec{L} \times \vec{L} &= i\hbar \vec{L} \end{aligned}$$

these are operators okay so you can if you want you write it with a cap there so all these applies to the operators and so on so these are not just not quantities that we are talking about and similarly there are like all these commutation relations that we are familiar with for the angular momentum which is $i \hbar$ cross \vec{L} so this is like it encodes a number of commutation relation for the components of the angular momentum okay.

So all these quantities that are fermions, bosons and spin etcetera they have their own commutation relations like fermions have this anti-commutation relation which I just said the bosons obey commutation relations and the spins have their own commutation relations okay they are they do not match with the ones for the fermions and the bosons. So what I mean is the following so this is how it is written now there are you know different notations that you might find but mostly it's done written with a curly bracket instead of a square bracket but sometimes a square bracket is followed by a plus sign this also means anti-commutation okay because there are you know opinion about relations that people follow. So this is equal to $C_i^\dagger C_j^\dagger + C_j^\dagger C_i^\dagger$ this is equal to 0 and similarly you have a $C_i C_j$ anti-commutation.

$$\begin{aligned} \{C_i^\dagger, C_j^\dagger\} &= C_i^\dagger C_j^\dagger + C_j^\dagger C_i^\dagger = 0 \\ \{C_i, C_j\} &= C_i C_j + C_j C_i = 0 \\ \{C_i^\dagger, C_j\} &= C_i^\dagger C_j + C_j C_i^\dagger = \delta_{ij} \end{aligned}$$

So anti-commutation very importantly you see that this plus sign is the main thing let me write it with color so that you are sensitized about this the main thing about the anti-commutation relation. So it's $C_i C_j$ plus a $C_j C_i$ and again this is equal to 0 and a $C_i^\dagger C_j$ this is equal to a $C_i^\dagger C_j$ plus $C_j C_i^\dagger$ and this is not equal to 0 but this is equal to a delta function a Kronecker delta with delta ij what it means is that if i equal to j then this is equal to 1 that is if you have $C_i^\dagger C_i$ plus $C_i^\dagger C_i$ then of course this is equal to 1 and so on okay.

(Refer Slide Time: 22.48-31.25)

Handwritten notes on a slide showing the derivation of one and two body operators in second quantization. The top line defines the many-body state: $|n_1, \dots, n_N\rangle = (c_1^\dagger)^{n_1} \dots (c_N^\dagger)^{n_N} |0\rangle$, where $|0\rangle$ is the many-body vacuum. Below this, the one-body operator \hat{K} is derived: $\hat{K} = \sum_{i,j} \hat{c}_i^\dagger \hat{K}_{ij} \hat{c}_j = \sum_{\alpha, \beta, i} |\alpha\rangle \langle \alpha| \hat{K}_{ij} |\beta\rangle \langle \beta| \hat{c}_i^\dagger \hat{c}_j$. This is then simplified using the completeness relation $\sum_i |\alpha\rangle \langle \alpha| = \mathbb{1}$ to get $\hat{K} = \sum_{\alpha, \beta} \langle \alpha | \hat{K} | \beta \rangle \hat{c}_\alpha^\dagger \hat{c}_\beta$. To the right, the orthonormality of the basis states is noted: $\langle \alpha | \alpha \rangle = 1$, $\langle \alpha | \beta \rangle = 0$ for $\alpha \neq \beta$, and $\langle \alpha | \beta \rangle = 1$ for $\alpha = \beta$. The two-body operator \hat{V} is similarly derived: $\hat{V} = \sum_{\alpha, \beta, \gamma, \delta} \langle \alpha, \beta | \hat{V} | \gamma, \delta \rangle \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \hat{c}_\gamma \hat{c}_\delta$.

And there are you know various properties that we can talk about the number operator and so on which you will see okay. So these anti-commutations that you see are they ensure that there is a this plus sign actually or the anti-commutation relation ensures that there is a minus 1 whole to the power epsilon i and that will take care of all the swaps that are affected in writing down the many particle wave function.

$$|n_1, \dots, n_N\rangle = (C_1^\dagger)^{n_1} \dots (C_N^\dagger)^{n_N} |0\rangle$$

So we will write down the ket as $n_1 n_2 \dots n_N$ this is equal to a $C_1^\dagger C_1^\dagger \dots C_N^\dagger C_N^\dagger$ whole to the power $n_1 n_2 \dots n_N$ and multiplying by or rather operating not multiplying it is operating on a 0 and this is actually a many body vacuum which means that it does not have any particles but that particles means in the many particle sector it is a vacuum. So this is how it is written and how these are so useful and why put this we have to learn this is the following when we try to write down 1 and 2 body operators which are all what are there in the Hamiltonian. You see sort of in general these scattering problems are all one body and two body problem a one body problem is that expresses the kinetic energy of the particle the body it is just one body how it moves and so on and when you talk about two body problem then we talk about the interaction between two particles.

Three body onwards it is almost unsolvable in most of the cases because of the phase space that you have for which are defined by the momentum and energy conservation laws they are not enough to find out you know deal with the three body scattering process. There are some specialized techniques which one does but anything more than that of course will be treated as a many body problem where you would talk about them statistically. So what is this one body operator so one body and two body operators. So let me write down a kinetic energy which is equal to sum of the all the kinetic energies so i equal to 1 to n K is the kinetic energy and this can be written as using the complete set of

states we can write this down as α α . So this will give you I will tell you that and this is that k and a β β and so on ok.

$$\begin{aligned}\hat{K} &= \sum_{i=1}^N \hat{k}_i = \sum_{\alpha, \beta, i} |\alpha\rangle \langle \alpha| \hat{k}_i |\beta\rangle \langle \beta| \\ &= \sum_{\alpha, \beta, i} \langle \alpha| \hat{k}_i |\beta\rangle |\alpha\rangle \langle \beta| \\ &= \sum_{\alpha, \beta, i} \langle \alpha| \hat{k}_i |\beta\rangle C_{\alpha}^{\dagger} |0\rangle \langle 0| C_{\beta} \\ &= \sum_{\alpha, \beta, i} \langle \alpha| \hat{k}_i |\beta\rangle C_{\alpha}^{\dagger} C_{\beta}\end{aligned}$$

So α and β are single particle states and these α α this is called as an outer product and these a complete less relation would give this and similarly for the β s they would give this as well ok. So this is why the you know this I should write it with i and so on ok. So these are the so this is an i and so on ok. So I just introduced this complete set of states and then we can write this down as α and β and i and so on and then we can write this as α and then k k i and then β and then we can sort of take α and β and so on ok. So that we use this and it is also α α equal to 1 and β β equal to 1.

So we left multiply by a vector which is α so it is a ket of α so that this becomes equal to 1 and we use a β here which becomes equal to 1 and that is because we can multiply a 1 here and so these are written in terms of the matrix elements. So these are α β and i and this is like α k i β and c α dagger 0 so α is written in terms of c α and a vacuum and the β is written as 0 and c β and this will also become equal to 1 because 0 is as much of an element of that Hilbert space as any other. So this is so finally what you get is α β i is like α k i β and c α dagger c β and this is a form of the one body operator ok. So this is a number which is the expectation value of these k i say for example in a continuum sense this is like minus \hbar cross square by 2 m and $d^2 dx^2$ and then you write down α and β and then this is the operator that comes out so it is a c α dagger c β . So if α and β are say for example states that are they denote say position or something ok then this will be like a c i dagger c j and so on so forth ok.

$$\begin{aligned}V &= \sum_{\alpha, \beta, \alpha', \beta'} \langle \alpha, \beta | \hat{V} | \alpha', \beta' \rangle C_{\alpha}^{\dagger} C_{\beta}^{\dagger} C'_{\beta} C'_{\alpha} \\ &\text{where } (V)_{\alpha\beta\alpha'\beta'} = \langle \alpha, \beta | \hat{V} | \alpha' \beta' \rangle\end{aligned}$$

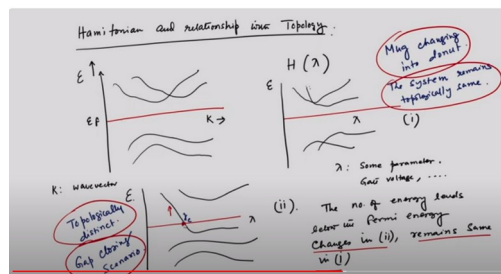
And similarly we can also write down this I will not go in but you can see this we can write this down as for the potential energy so this V is equal to α β α' β'

beta prime so this will be like alpha beta and V alpha prime beta prime and this will be like c alpha dagger c beta dagger c beta prime c alpha prime and so on ok. So this is nothing but the matrix elements of this operator which can be for a coulomb term this is like minus e square over R and so this is like a alpha beta alpha prime beta prime. So the matrix element is this and the operator is here ok so the matrix element is given by this V alpha beta alpha prime beta prime and so on ok. So this is quite helpful and it will help us to write down these tight binding Hamiltonians that will be extensively you know discussing throughout this course ok. Then it will be made clear or rather it will be more clear that why we have introduced these notations and as I said that they take care of this humongously large number of swaps or the exchanges of the particles or these signs arising from these exchanges and they are taken care of very sort of in a very smart way.

$$\begin{aligned}
 |\alpha\rangle\langle\alpha| &= 1 \\
 |\beta\rangle\langle\beta| &= 1 \\
 \langle\alpha|\alpha\rangle &= 1 \\
 \langle\beta|\beta\rangle &= 1
 \end{aligned}$$

So first we write down the Fock states and then we introduce the these C and C dagger operators and their anti-commutation relations we are talking about fermions so but similar way one can talk about bosons as well the formalism leaves is exactly the same excepting that we would be talking about commutation relations instead of anti-commutation relations alright. So these are Hamiltonians now we are slowly you know moving towards condensed matter physics which deals with Hamiltonians for a given system its energy levels and so on and these energy levels are called as the you know the band structure E as a function of K usually we you know plot it as a function of K.

(Refer Slide Time: 31.30-43.00)



So these Hamiltonian and let us talk about the Hamiltonian and relationship with topology okay. So I just just a freehand drawing of bands and say one band is like this another band is say like this this is the conduction band and this is a valence band and so on okay. So this is E versus K for a given system I am just arbitrarily drawing some two bands and it can actually have many bands but something that is too far away from the

Fermi level is not interesting at all because it does not contribute to the physical properties of the system the ones that are closest to the Fermi level are only important for us to consider and I mean what is meant by near the Fermi level so this is the Fermi level so this is called as a Fermi level and this is usually the zero of energy.

So this line let me then draw it with another color okay. So this is the Fermi level and something that's far away from the Fermi level are not interesting the ones that are close to the Fermi level maybe within electron volt or so are important by the way this one electron volt even if it sounds a very small energy especially the students who are familiar with high energy physics and so on we for condensed matter people this one electron volt is a very large energy in fact this is roughly the energy that the typical semiconductors like germanium or silicon they have or is aluminum gallium arsenide etc. maybe having a one point something electron volt one electron volt is 11600 Kelvin okay. You understand the enormity of these energy what I mean is that one electron volt when you write it or equate it to kT , k is the Boltzmann constant to put the value of the Boltzmann constant and do all these homogenizing the units etc and then T comes out to be close to 12,000 Kelvin 11,600 and that's a very large temperature because you know the outside of Sun is about 6000 Kelvin or a little more than that so anything in the world would you know melt at 12,000 Kelvin okay. So even though looks like the one electron volt is a small energy you cannot really you know think of such a large energy in condensed matter system okay.

Alright so what I am trying to get at is that suppose this Hamiltonian is a function of some λ we have used this notation earlier where λ is some parameter of the system and then λ can be tuned say for example λ can be the electric field or the gate voltage for a system for which you are writing down the Hamiltonian and then you are slowly tuning the gate voltage and the Hamiltonian changes and see the Hamiltonian changes in this manner that as a function of λ it sort of there are only two levels that I wrote down and then you know it sort of it these two energy levels in the both in the conduction and the valence band they get slightly they change slightly as it's shown here but they do not cross the Fermi energy again the Fermi energy is at the middle okay. So now I am not plotting it as a function of K , I say I am at a given K and then I am plotting it as a function of λ okay do not mind is just an example that I am giving they the plots look same versus K , K is the wave vector by the way. So let me write that K is the wave vector and λ is some parameter okay some parameter such as you know gate voltage or say spin orbit coupling and which can be tuned by using some external means etc. So it can be anything and I am just showing that this a situation in which it is changing with λ but let me show another situation where again I will show the Fermi energy with red and so it happens like this and so on okay again as a function of λ so this is E versus λ and so on. Now see there's a big difference between this picture let's call this as 1 and let's call this as 2 okay.

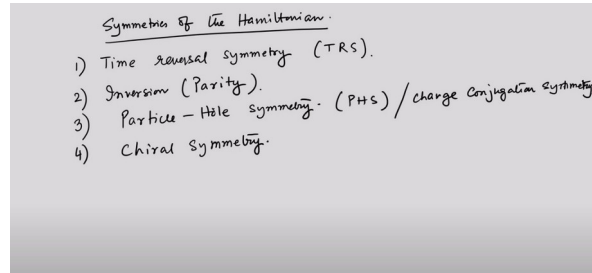
And 1 and 2 the difference is that the number of levels the number of energy levels or the number of bands energy levels below the Fermi energy changes in 2 remain same in 1 okay. So 1 means this 1 and when I say 2 what I mean is this ρ_1 ρ_2 the figure I am referring to okay. Now let me sort of changes in 2 and remains same in 1 we underline and this will decide that whether the system is topologically equivalent as λ is being you know is tuned this parameter λ is tuned in case 1 the system is in the same topological state then topological invariants are same what I mean to say is that if you refer to the lecture in the last one that we have now delivered there the mug changing into doughnut. So this will be so mug changing into doughnut the systems are topologically equivalent I said a number of times that a smooth deformation of the system from the mug to the doughnut leaves the system topologically same that's their identical because there is just one hole it just counts the number of genus present in the system. So where you hold the cup is the hole that it transforms into the doughnut and that's only thing that happens okay the system remains topologically same okay.

So these are the 2 inferences that comes out okay these 2 inferences emerge from this particular plot this just a you know just a schematic plot do not worry too much about this I just shown 2 energy levels 2 below the Fermi energy 2 above the Fermi energy and so on. However here these systems are topologically distinct. Okay because the Hamiltonian for which energy is the eigenvalue of the Hamiltonian it does not remain invariant rather the number of levels below the Fermi energy as a function of λ till this point there are 2 levels above and 2 levels below but this point onwards whatever that point is let's call that as λ_c that point onwards there are 3 levels below and which is not the same as 2 levels. So the system undergoes a topological phase transition which means that there is a gap closing scenario that occurs which means that you are puncturing or you are tearing something in order to create a different either a differently topological system that it has different topological invariant that is you are making a mug into by somehow you know piercing it or breaking it or drilling some hole into it you are creating another genus that is it sort of is equivalent to now a spectacles the pair of spectacles that people were. So they are topologically distinct and this topological distinction is accompanied by a gap closing scenario.

So these are the 2 important features of these 2 things that or these 2 plots that I have drawn. So I hope that if you read more of course you will agree with me more but I hope I have been able to give you this analogy between topology and condensed matter physics that this is how you slowly deform a system and if the system remains invariant that is a sort of becoming a donut then they are topologically equivalent which is farther you know corroborated or supported by this Gauss Bonnet theorem whereas this system you have to make some drastic changes to the system and in language of condensed matter physics it means that there is a gap closing occurs. You see the gap it was earlier gapped it was here gapped but that gap closes with the Fermi energy at this point λ_c this

point is λ_c this is what I mean as λ_c and these gap closing occurs and so on. So then the system does not remain topologically equivalent that is a mug donut sort of you know in that sense the equality or the similarity does not remain and one actually gets a different system okay. So one the Hamiltonian representing the two systems before λ_c and after λ_c are not topologically equivalent okay the topological invariant changes.

(Refer Slide Time: 43.37-48.30)



Okay so now this topology etc. and its relation to condensed matter physics can be understood even better by looking at the symmetries of the Hamiltonian. So let us see what we mean by symmetries of the Hamiltonian. So every day we come across a lot of symmetric objects say for example a circle is a very symmetric object if you sort of turn it make a rotation by some angle θ it you will be not be able to distinguish whether it is a earlier circle or the new circle which is rotated by θ or say a sphere or there are many symmetric objects there are like many things in nature which are symmetric suppose these leaves that you see which have got a you know symmetry there are these alphabets many of the alphabets have got you know symmetries along various lines like for example o has a symmetry about any of the axis or m has a symmetry about the vertical axis and so on okay. So these Hamiltonians also have certain symmetries and these symmetries dictate whether as a function of λ whether the system will undergo a topological phase transition or will remain equivalent to the original system as you know as you change λ okay. So these symmetries are really distinct from the crystal symmetries this crystal symmetries come in say all these group theory that you might have studied in which people talk about symmetries such as C_{4v} symmetry C_6 symmetry and so on so forth.

So these are distinct than that and there are few symmetries which are really important and we will study them and one of them is called as a time reversal symmetry in short we will call a TRS then we will talk about symmetry which is it is called inversion symmetry or it is also called as a parity okay. So this if you invert the coordinates or you know so how does the system or the Hamiltonian behaves with inversion of this that is R going to minus R how does the Hamiltonian behave. So that is called inversion or it is also called

parity then there are these symmetry called as the you know the particle hole symmetry it is called PHS it is short name for that and this is particularly important in the context of superconductors and then we have chiral symmetry and so on okay. And now this particle hole symmetry is also called as a charge conjugation symmetry okay and so on. So let us you know start with the time reversal symmetry and you might wonder that what is reversing time I mean is there anything called time goes in the other way that is not true what we still do is that we want to understand whether the system moving on the towards the right with the velocity V whether that scenario remains unchanged as the particle moves in the other direction with minus V okay.

So if the direction of motion of a certain particle which is expressing you know being expressed by the Hamiltonian if that changes or that changes sign then what happens to the Hamiltonian does the Hamiltonian remain same and so on. And we will see that this has very significant you know effects on the condensed matter physics because there is something called Cramer's degeneracy that will emerge just talk about it you know. So let us talk about time reversal symmetry okay.

(Refer Slide Time: 48.38-55.30)

Time Reversal Symmetry (TRS)

(1) System without spin degree of freedom.

TRS $T : t \rightarrow -t$

$[H, T] = 0$

a) $T \alpha T^{-1} = \alpha$
 b) $T C_j T^{-1} = C_j$
 c) $T i T^{-1} = -i$
 d) $T L T^{-1} = -L$
 e) $T [x, p] T^{-1} = -[x, p] = -i\hbar$

f) $T C_j T^{-1} = C_j$
 g) $T C_j^\dagger T^{-1} = C_j^\dagger$
 h) $T C_k T^{-1} = C_k$
 i) $T i T^{-1} = -i$
 j) $T (-i) T^{-1} = i$

$T = K$ K : Complex Conjugation.

So I will not go into details how the form of the symmetry operator comes but I will just tell that this is the symmetry operator and try to you know justify the behavior of the Hamiltonian on that okay. So under time reversal operator it is usually written with a curly T but it is easier for me to write this straight T under this it is written as T going to minus T okay.

So under time reversal we are talking about a system without spin. So one system without spin degree of freedom and you might wonder that if you are talking about electronic systems or even bosonic systems they have spins okay. So how can you ignore spins and we can ignore spins in a variety of cases suppose the system is spin polarized which means that it has only spins pointing in the say talking about spin half pointing in the positive Z direction in which case you have only that kind of systems and or they are pointing in the opposite direction okay. So now the system does not distinguish between

the particles pointing in the opposite the spins pointing in the positive Z direction or negative Z direction. If it does not do that there is no term that mixes the spin one kind of spin to another then you can just talk about one kind of spin and then extend that analysis to the other kind of spin as well and then the spin really does not arise into the discussion that we carry on later on and you just put if you need to sum over both the spins you to a factor of put a factor of 2 but otherwise the spin does not you know enter into the discussion.

So under TRS this T small t goes to minus t and the Hamiltonian commutes with the time reversal operator okay.

$$T : t \rightarrow -t$$

$$[H, T] = 0$$

So a time reversal operator simply changes t to minus t and the Hamiltonian commutes with that. Now if you want to know that my Hamiltonian may not only contain t it contains x and p and so on so forth it I will show you the all these properties. So a if it is txt inverse this is how it is the operation is talked about or discussed it is txt inverse is equal to x then you have tp t inverse is equal to minus p. So the x that is the position variable does not change sign but p which is equal to V over t or dv dt or dp dt I mean this is like it involves p is equal to mv.

$$TxT^{-1} = x$$

$$TpT^{-1} = -p$$

$$TiT^{-1} = -i$$

$$TLT^{-1} = -\vec{L}$$

$$T[x, p]T^{-1} = Ti\hbar T^{-1} = -i\hbar = -[x, p]$$

$$T = K \quad T^2 = 1$$

So it is it has a V, V has a x by t since t changes sign so p has to change sign. So this is another one and the important thing is that if it gets i anywhere which is i equal to root over minus 1 then it changes it over to minus i okay. So and if you like you know TL t inverse that is L is the angular momentum that also picks up a negative sign okay. So if you want a little more on that it is not required but then x and p is ih cross we know so this is equal to t ih cross t inverse and by the third property or C property ti t inverse will become equal to minus 1. So this becomes equal to minus ih cross which is equal to a minus xp commutator okay.

$$TC_jT^{-1} = C_j$$

$$TC_j^\dagger T^{-1} = C_j^\dagger$$

$$TC_kT^{-1} = C_k$$

So xp commutator does not remain invariant. So let us go to this f so that tells you that if you have a real space second quantized operator T C J for example T inverse so this remains same however T C J dagger T inverse that also of course remains same but if you write it in the k space that is a wave vector space so T C k T inverse this is equal to C of minus k okay and similarly for the k. So this is f, g, h and so on. So I am talking about this C in the k space we have not specified earlier what alpha and beta are they could be you know valid momentum states written in the momentum eigen basis or in the position eigen basis so this is what it does.

$$as \quad T i T^{-1} = -i \quad T(-i) T^{-1} = i$$

So in this thing what it what turns out is that the form of T is equal to the complex conjugation okay so k is complex conjugation and T square that is square of that is equal to 1 or you can write it as a matrix 1 because T is usually an operator. So T square gives you 1 that is if you do twice so T acting on i will give you a minus i which is in C and then when I do it on this other side that is T acting on minus i T inverse that gives you i so T square becomes equal to 1 you know so this is like if I right multiply by T or left multiplied by T then that T square becomes equal to 1.

(Refer Slide Time: 55.34-1.01.30)

(a) Systems with spin degrees of freedom.
 $(s = \frac{1}{2})$.
 $[H, T] = 0$ TRS is a valid symmetry operation.
 $T|\psi\rangle = |\psi_T\rangle$ Both $\psi \rightarrow E$
 $\langle\psi|\psi_T\rangle = 0$ $\psi_T \rightarrow E$
 $H|\psi\rangle = E|\psi\rangle$ $H|\psi_T\rangle = E|\psi_T\rangle$ } Kramers' degeneracy.
 $T = e^{-i\pi\sigma_y} K$ $-i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
 $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$ $e^{i\theta} \vec{r} \cdot \vec{A} = \vec{r} \cdot \vec{A} \cos\theta \pm i \vec{r} \cdot \vec{A} \sin\theta$
 $T = \frac{1}{2} \begin{pmatrix} 1 & \sigma_y \\ -\sigma_y & 1 \end{pmatrix} K$ $\theta = \pi/2$ $\vec{A} = \vec{S}$
 $T = i\sigma_y K$ $-i\sigma_y K = i\sigma_y$
 $T^2 = (i\sigma_y)(i\sigma_y) = -1$ $\sigma_y^2 K = -\sigma_y^2 = -1$.

So this is where k is the complex conjugation this is slightly different when system with explicit spin degrees of freedom is there okay and we are talking about spin half okay. So again I mean H and T should commute if a system has this means that TRS is a valid symmetry operation that means the system has time reversal symmetry okay.

$$[H, T] = 0$$

$$T|\psi\rangle = |\psi_T\rangle$$

$$\langle\psi|\psi_T\rangle = 0$$

So it is written as the operator is now no longer just k or the complex conjugation and we also have you know T acting on the wave function will give me say psi T and the psi T and psi are distinct and so psi and psi T this is equal to 0 both psi has eigenvalues that is E as the eigenvalue and psi T also has E as the eigenvalue what means is that H acting on psi will give you E psi and H acting on psi T gives you E psi T I am telling you all the results a priori and this is nothing but what is called as a Cramer's degeneracy. This along

with this condition okay so for a given system if the system has time reversal symmetry in that case the wave function ψ corresponds to an energy E there is also the time reversed state which is ψ_T here where you apply ψ on the I mean the time reversal operator on the ψ and becomes a ψ_T then the inner product of ψ and ψ_T are is 0 that says that these are orthogonal states ψ and ψ_T and each of them have energy E that is H acting on ψ will give you $E\psi$ and H acting on ψ_T also give you $E\psi_T$ okay.

$$\begin{aligned}\psi &\rightarrow E \\ \psi_T &\rightarrow E \\ H|\psi\rangle &= E|\psi\rangle \\ H|\psi_T\rangle &= E|\psi_T\rangle\end{aligned}$$

So the time reversal operator in this particular case has a form which is exponential TSY this SY is the we talk about spin half I told you that so this is has to be it is a spin half operator Y component of the spin half operator and this K which is a complex conjugation and if you write down you know S is equal to \hbar cross by 2 sigma in order to convert that into Pauli matrices then this becomes equal to e to the power minus $i\pi$ by 2 H cross by 2 yeah sorry I forgot this H cross.

$$\begin{aligned}T &= e^{-i\pi S_y} K \\ \vec{S} &= \frac{\hbar}{2} \vec{\sigma} \\ T &= e^{-i\frac{\pi}{2} \hbar \sigma_y} K\end{aligned}$$

So it is H cross and then a sigma Y and a K okay. So this is the form of the operator for a system with spin degrees of freedom. So if you take a T square now what is this exponential minus $i\pi$ by 2 H cross sigma Y how to calculate this if you remember that it is a exponential $i\theta$ sigma dot \hat{n} this is how the exponentiation of the Pauli matrices are done sigma is the Pauli matrix which has components sigma X sigma Y and sigma Z and \hat{n} cap is just a direction this is equal to by using this De Moivre's theorem and properties of these Pauli matrices it is equal to this and i sigma dot \hat{n} cap sine theta. Now here you see theta is equal to π by 2 and \hat{n} cap is equal to Y cap okay. So the first term goes to 0 and the second term gives you so this is a minus so there is a minus there is a I mean plus minus there is a plus minus. So exponential minus $i\pi$ by 2 H cross sigma Y you can take H cross equal to 1 if you like.

$$\begin{aligned}e^{\pm i\theta \vec{\sigma} \cdot \hat{n}} &= I \cos \theta \pm i \vec{\sigma} \cdot \hat{n} \sin \theta \\ \theta &= \frac{\pi}{2} \quad \hat{n} = \hat{y} \\ e^{-i\frac{\pi}{2} \hbar \sigma_y} K &= i \sigma_y\end{aligned}$$

So this is equal to let me take H cross equal to 1 that will be better and this is equal to $I \sigma_y$ and that is all I mean plus at θ equal to $\pi/2$ the first term is 0 and the second term gives you $\sin \theta/2$ equal to 1 so it is simply $I \sigma_y$ so T is equal to $I \sigma_y K$ okay.

$$T = i\sigma_y K$$

$$T^2 = (i\sigma_y K)(i\sigma_y K) = i^2 \sigma_y^2 K^2 = -\sigma_y^2 = -1$$

So if you want to calculate T square so this is equal to $I \sigma_y K$ into $I \sigma_y K$ this is equal to I square and then σ_y square which is equal to 1 and then K so this becomes equal to a minus I mean this becomes equal to minus σ_y square and this is equal to a minus 1 okay. So that tells you that the system with without spin degrees of freedom T square is equal to 1 and with spin degrees of freedom T square is equal to minus 1. So the square of the time reversal operator changes as you you know talk about spinless particles that is spin half particles or spinless particles okay.

(Refer Slide Time: 1.01.37-1.04.41)

$$T C_{j\uparrow} T^{-1} = -C_{j\downarrow}$$

$$T C_{j\downarrow} T^{-1} = C_{j\uparrow}$$

$$T H(k) T^{-1} = H(-k)$$

So once again I will show you the $C_{j\uparrow} T^{-1}$ and this is equal to minus $C_{j\downarrow}$ and $T C_{j\downarrow} T^{-1}$ this is equal to $C_{j\uparrow}$. So it tells you that if you have a J spin I mean a particle with at a site J with spin up it makes it the spin becomes lowered the it is rendered lower and there is a minus sign and for the lower it becomes up and with no sign there. So now $T H(k)$ suppose you have a tight binding Hamiltonian where the Hamiltonian is written in the k space this is equal to so T inverse is equal to H of minus k okay alright. So this is about the time reversal symmetry and on the next lecture I will be talking about the inversion symmetry and particle hole symmetry and the chiral symmetry and so on okay.

$$T C_{j\uparrow} T^{-1} = -C_{j\downarrow}$$

$$T C_{j\downarrow} T^{-1} = C_{j\uparrow}$$

$$T H(k) T^{-1} = H(-k)$$

So what we have given so far is the first two classes they were concerned with establishing what topology is and the various you know properties etc or through various visual graphic and demonstration we have said that a system remains invariant if it has

the same number of genus as you deform the system. Now what is its relation to condensed matter physics that needs to be understood and when we say that these deformation is nothing but you know driving the system which is a function of certain parameter and then whether the entire property of the system changes that is the number of energy levels below the Fermi energy does that get altered if it does not then the system remains you know it is as a function of λ it goes into or rather it remains topologically identical so a mug becomes a doughnut.

But however if the number of energy levels are altered then you have done something violent to the system and there the system undergoes a topological phase transition from. So it will be a different topological invariant including a 0 okay so which means that system goes from topological to trivial that is non-topological when the this genus or this thing is topologically invariant is 0. We will continue with this symmetry for just a while and then we will go on to materials which shows this topological properties these are called topological insulators most of the course we will be talking about topological insulators. Thank you for your attention.