Advanced Condensed Matter Physics

Prof. Saurabh Basu
Department of Physics
Indian Institute of Technology, Guwahati

Lecture – 01
Propagators I

Good morning everyone. In this course of advanced condensed matter physics, we are mainly going to learn quantum many body theory as its applied to various solid state systems or crystal lattices and other systems continuum systems, but this is the interacting version and it actually builds upon the first course of solid state physics and preliminary knowledge of quantum mechanics would be needed. This is the course is has a lot of mathematics embedded in it and the mathematics is to develop the formalism to deal with interacting systems and you may not have encountered interacting systems too much.

So, these course will give you a preliminary idea of how to deal with interacting systems and because interactions are very important, inter particle interactions are very important in condensed matter physics and so, we have to learn this technique and that is where all the mathematics comes and once when we learn it we will apply it to various things that we know such as magnetism, such as superconductivity and if there are time then we would go ead and discuss the keen Mele model and topological insulators the 2016 Nobel prize was awarded on the topology in condensed matter physics we briefly touch upon that.

(Refer Slide Time: 02:18)

Topics to be covered :

(i) Brief Recap of Quantum Mechanics

(ii) Second quantization

(iii) Application of Second quantization

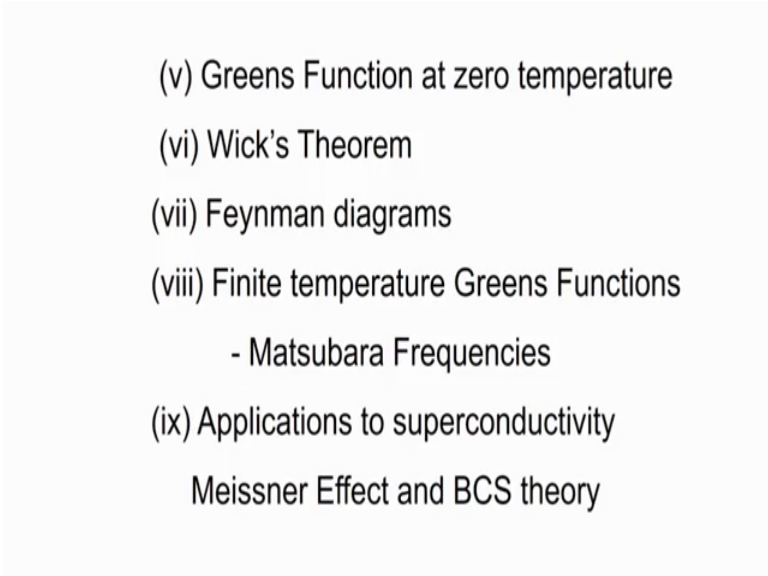
- Quantum Magnets
- Hubbard Model

(iv) Greens Functions

So, before we start talking about the contents of or rather the details of the course, let us talk about the topics that would be covered in the next few weeks t hat will be doing the course together. So, we will start with a brief recap of quantum mechanics and this is essential because we have to introduce concepts such as Hilbert spaces single particle Hilbert space and i you know many particle Hilbert space and so on and then we will talk about second quantization, this is in contrast to the first quantization which we see in quantum mechanics and this second quantization actually has the foundation of doing a quantum many body theory that we are going to show.

Then there will be applications of second quantization and how to write down a Hamiltonian particular, Hamiltonian for in the second quantized form and we apply to magnetism and a celebrated model called as Hobart model which has been used in the context of interacting condensed matter system to a very large extent. We will then talk about greens functions and these greens functions will be acting as if they are like wave functions work in single particle quantum mechanics and these greens functions have to be learned at 0 temperature.

(Refer Slide Time: 03:43)



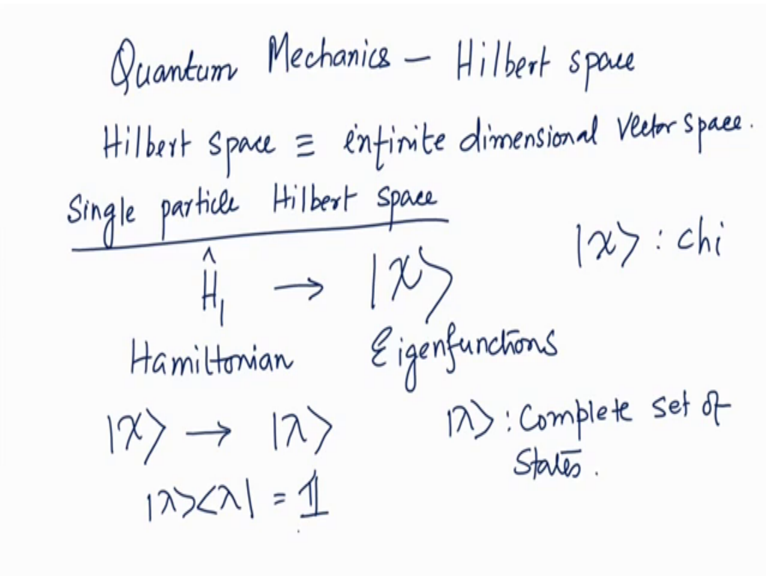
Where we would talk about wicks theorem and Feynman diagram and these greens function will be also learned in at finite temperature because as you know that all the condensed matter physics is done at finite temperature. So, and in that connection will learn Matsubara frequencies and finally, we will apply it to the theory of superconductivity and learn what are called as Meissner effect and MCS theory.

So, BCS theory is a celebrated theory in superconductivity, which explains all the phenomena related to the weak coupling superconductors or the so called conventional superconductors and maybe will briefly discuss the high temperature superconductors; which are the unconventional superconductors in some sense and that is where the course will stop.

So, technically speaking condensed matter physics deals with either 1 body problem or many body problems. The reason behind saying that is that a 2 body problem can always be reduced to a 1 body problem and 3 body problems are unsolvable, but physicists and chemists both they deal routinely with Avogadro number of particles, which means that 10 to the power 23 number of particles and when you talk about such large number of particles then you need to the, you must be talking about particles which are close to each other, such that they are coming within the de Broglie wavelength of each other.

Ah in that sense in order to describe such a system with so many particles, one really needs a quantum many body theory. Sometimes in this context it is advantageous to talk about instead of talking about a large number of non interacting particles, one can also talk about a few or relatively, few interacting particles and these particles are called as quasi particles and this description holds; however, that description would break down when these quasi particles, the time over which they are created if that time is shorter than the or rather longer than the time over which they decay, in which case the quasi particle descriptions will not hold.

(Refer Slide Time: 06:34)



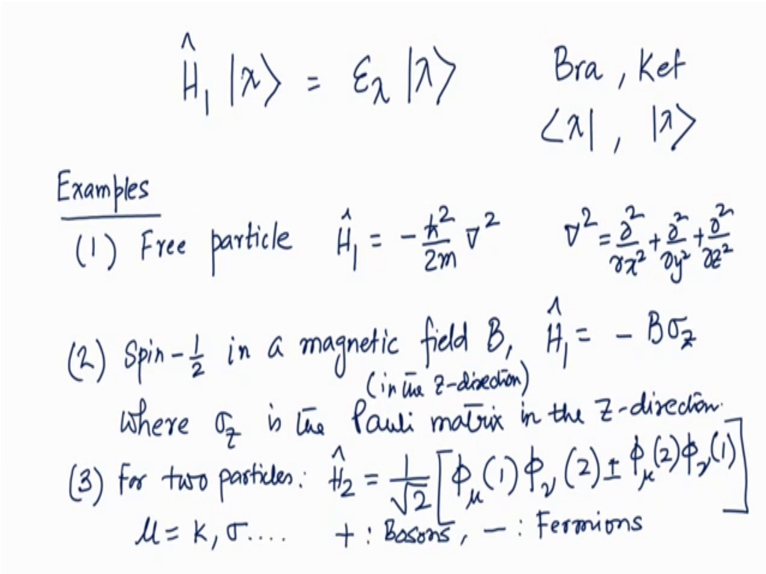
Now we shall begin our discussion with quantum mechanics and in particular we will talk about Hilbert spaces. So, the question is that what is a Hilbert space. So, a Hilbert space is infinite an infinite dimensional vector space and we will. So, a Hilbert space is infinite dimensional vector space.

Let us just talk about a single particle Hilbert space to begin with. So, let us assume that a single particle or a collection of particles which are non interacting. So, we are talking about 1 such particle is represented by Hamiltonian H1. So, this subscript 1 stands for 1 particle and it has a Eigen function. So, this is the Hamiltonian of the system and the Eigen functions are given by chi and this chi is actually formed of. So, this chi is written as or rather pronounced at chi, chi and this is formed of some complete set of states lambda.

So, lambda is the complete set of states here, set of states and obey lambda obeys are a relation which is. So, the outer product of lambda is equal to an identity matrix or a unit matrix which has only 1 as the diagonal elements and 0 for all the off diagonal elements and so these lambda form the complete set of states for the Eigen functions of H1.

So, which means that H1, when it acts on these lambda it gives an Eigen value equation which is epsilon lambda.

(Refer Slide Time: 09:41)



So, H1 acting on the Ket lambda. I just touch upon what we mean by Ket and so, it returns an energy Eigen value which is epsilon lambda and returns the state lambda. So, Dirac introduced this notation of Bra and Ket and all throughout quantum mechanics if you follow any book on quantum mechanics modern book on quantum mechanics, they write a Ket with like this and they write the Bra like this ok. So, these are the representations that are followed. So, that is just as we have written in the last slide. This was an outer product which is made out of the bras and now we are writing the Eigen value equation with the Ket here.

So, this will be made more clear as we go along and let us give some examples of such single particle Hamiltonian and let us talk about the most trivial example which is free particle and the by free particle what we mean is that the free particle in a continuum. The free particle Hamiltonian is represented, 1 particle Hamiltonian is represented by.

So, this minus H cross square over 2m is H square, where H cross is the planks constant which is H by 2 pi, m is the mass of the particle and this is the Laplacian which in

Cartesian coordinate system has a form del square, del x square plus del square, del y square plus del square, del z square ; however, often we go to another coordinate system in order to solve the problem and in which case we have to write the Laplacian or the del square operator in other coordinate systems such as spherical polar coordinate system or cylindrical coordinate system, which is usually slightly more complicated, but they are available everywhere.

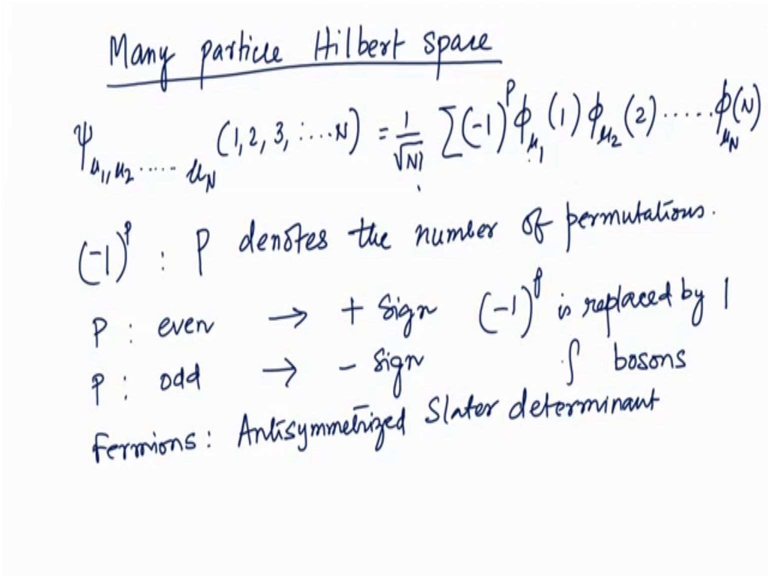
So, also let us write a spin half particle in a magnetic field b. So, H1 in this case is equal to B sigma z where. So, this magnetic field is in the z direction, it is assumed for simplicity. So, that is why we have taken the z component of the spinner matrix, which is a 2 by 2 matrix and is called as a Pauli matrix. There are 3 Pauli matrices, sigma x, sigma y and sigma z.

So, where sigma z is the Pauli matrix in the in the z direction and let me make things a little more involved and write down for 2 particles, these are non interacting particles will write down H2 because this involves 2 particles. So, we are writing it as H2, 1 over root 2 and there is a phi, I am writing it with a mu and this is at position one or you can write it as R1 if you like and there is a phi mu at 2 minus or rather we write plus, minus and then you have phi of mu 2 and phi of mu 1.

And so, this is the Hamiltonian for 2 particles where this phis are the functions or they are the Eigen functions, this mu represents an index which could be anything such as the momentum or the spin or for that matter any other thing that is appropriate for the description of the system.

So, in this case we have talked about the Hilbert space at the single particle level and written down the Eigen value equations

(Refer Slide Time: 15:35)



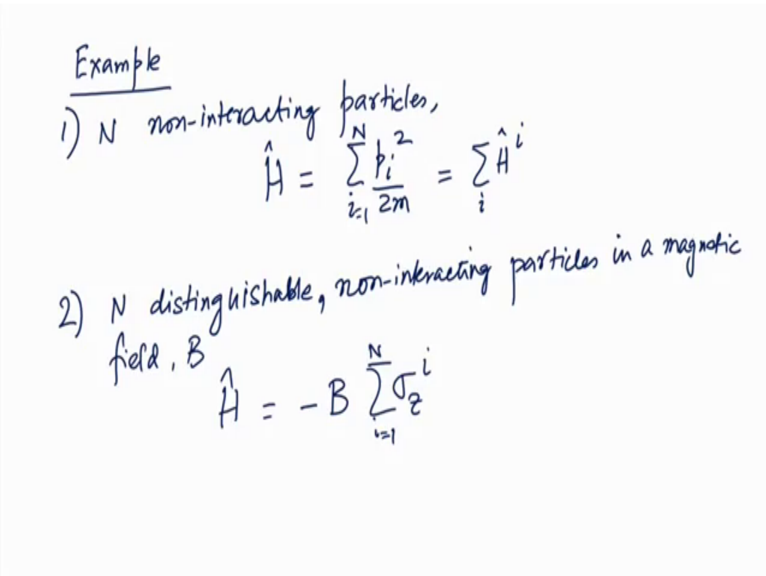
Now let us generalize this to the many particle Hilbert space. So, before we proceed, we have put a plus and a minus sign and we wish to assert that this plus sign is for Bosons after an Indian scientist called S N Bose and the minus sign is for Fermions after named after the scientist called Fermi, Enrico Fermi. So, to continue with the many particle Hilbert space, we can write down the wave function as. So, this is mu 1, mu 2.

Now, I no longer want to write mu, nu because there are several of these indices that will come and I am basically interested in writing down an N particle system and this has 1, 2 3 and so on and this is equal to 1 over N factorial and there is a minus 1 over P, phi of mu 1 at 1 phi of mu 2, at 2 and going all the way phi of mu n n and this is a many particle state there is a minus 1 to the power P, now minus 1 to the power P is where this P denotes the number of permutations and if P is even, then we there is no sign associated with it. So, there is a positive sign here because minus 1 to the power n even numbers a 2 n is even. So, we will simply write this without that minus 1 to the power P; however, we have when we have p equal to odd, then we have a negative sign ok.

So, just to go back to the 2 particle problem, you see that for fermions there is a negative sign. What I mean is that see here phi mu is for the particle at 1 and phi nu is for the particle at 2 and this has been swapped the indices have been swapped. So, that the phi mu is now for the particle at 2 and this phi nu is for the particle at 1 and there is a minus sign and because we have made 1 swaps in going from the first term to the second term, there is a negative sign coming which is apparent from this many body wave function as well and this is equal to, so this whole thing minus 1 to the power P is replaced by 1 for bosons. Also if you take a note of this for the fermions because of this minus 1 to the power P and there is a summation involved, you can this summation is over all the particles this for the fermions, one can write down this wave function in of the form of a matrix and this is called as the anti symmetrised Slater, symmetrised Slater determinant.

So, this wave function is the determinant of that matrix which you write and basically every time you make a swap of the particle visa we the index that you are using here you are getting a negative sign. So, there could be more examples.

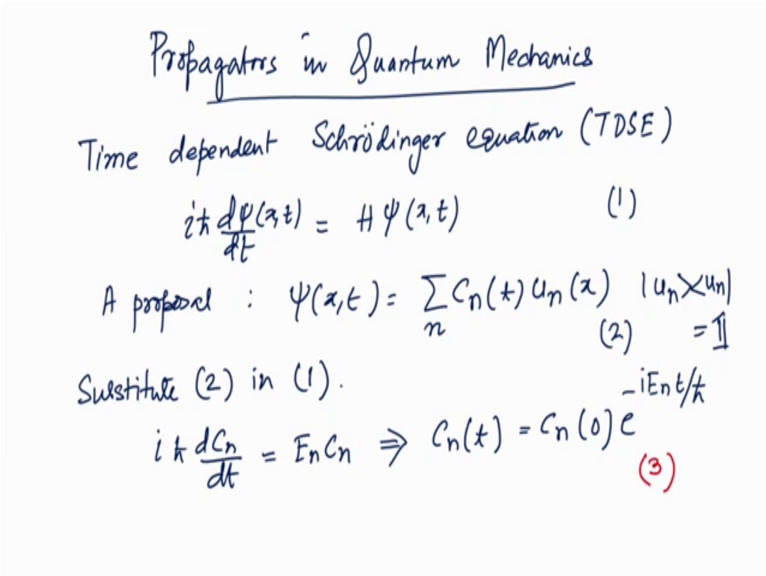
(Refer Slide Time: 20:54)



So, this is and Let us give an example of many particle system. So, there is n non interacting particles, in which case we will write the Hamiltonian. Now this the Hamiltonian is for many particle system even though they are non interacting this will be a summation over I and a Pi square over 2 m. So, that i is actually the index for each particle. So, this is equal to a summation over i and Hi, where Hi corresponds to a single particle Hamiltonian for written for a particle i.

And similarly when we have N distinguishable, non interacting particle in a magnetic field B, we can write that as H equal to minus band, then there is a sigma zi where i runs from 1 to N, similarly here also i runs from 1 to N and so, this is these are some of the examples of the many particle Hamiltonian and the many particle Hilbert space will be the here will be the product of the Hilbert space of the individual particles ok.

(Refer Slide Time: 23:11)



Let us now talk about propagators and how the propagators are interesting and useful in quantum mechanics. So, we will start with the description of propagators in quantum mechanics and we will see later on how this smoothly connects to the definition of greens function which as I said earlier is an important topic for us to learn in this course.

So, we start with a time dependent Schrodinger equation, which if at all we use later we call them as TDSE, Time Dependent Schrodinger Equation and which is written as iH cross and I will write it as d psi d t which is a function of x t this is equal to h psi x t. In principle I should have written it with a partial derivative this one for the d psi d t; however, I ignored that and wrote it as a full derivative, strictly speaking it should have been a partial derivative which is written as del psi del t, it will not affect too much our discussion that is that is going to flow. Now this can be solved by an a proposal of the form psi x t is equal to some C n t U n of x sum over n. So, that is the answers or the proposal that is for this problem take a note of this where U ns are the basis functions.

So, for writing every state or an Eigen function we need a basis, just like what we have introduced earlier lambda was the basis for the Eigen function Kai, here U n is the basis for this psi. So, the U ns would have this obey this relation and if you put call this as equation 1 and if you call this as equation 2, if you substitute 2 in 1, 1 is going to have a relation which is i H cross dCn dt equal to En Cn. Here you should also note 1 point in equation 2, that the time dependence of the wave function or the Eigen function psi on the left is carried only by the amplitudes.

So, these are the amplitudes which carry the information about time while they are independent of the of space and the space information is carried by the basis vectors which span the entire Hilbert space for the problem. So, if we substitute 2 in 1, we get an equation which is i H cross dCn n dt equal to En and Cn, this is just the recast of the form that appears in equation 1. So, it is the same as the Eigen for or rather Schrodinger equation written for the amplitudes Cn and the this will have a solution which is equal to a Cn of t which is equal to a Cn of 0 and an exponential minus i E n t over h cross.

It is also good to mention here that the Hamiltonian does not explicitly depend on time in this case, in which case we could not have written this because then E ns are not independent of time and the system loses its time translational or time reversal invariance, which will neglect at the moment and the solution comes in the form of this the amplitude Cn of t, that is as a function of t is C the value C of C n at t equal to 0, this 0 means at t equal to 0 and it is an exponential of minus iE and t over h cross and you can trivially verify that if you put this form in the equation that appears on the left, then this satisfies this equation.

(Refer Slide Time: 29:00)

$$\psi(x,t) = \sum_n C_n(0)\, e^{-iE_n t/\hbar}\, u_n(x) \qquad (4)$$

$$C_n(0) = \int \psi(x,0)\, u_n^*(x)\, dx = \langle u_n(x) | \psi(x,0) \rangle \qquad (5)$$

Putting (5) in (4)

$$\psi(x,t) = \sum_n \left[\int \psi(x',0)\, u_n^*(x')\, dx' \right] e^{-iE_n t/\hbar}\, u_n(x) \qquad (6)$$

$$\psi(x,t) = \int G(x,x',t)\, \psi(x',0)\, dx' \qquad (7)$$

$$G(x,x',t) = \sum_n u_n(x)\, u_n^*(x')\, e^{-iE_n t/\hbar} \qquad (8)$$

$$= \sum_n \langle u_n(x') | u_n(x) \rangle\, e^{-iE_n t/\hbar}$$

Let us call this as equation 3 and we will and then this equation 3, if its substituted in equation 2 and then we shall have the psi of x t that is written as Cn of 0 exponential minus iEn t over h cross and u n of x. Please note that this in this equation four Cn 0 is arbitrary and cannot be determined, unless the wave function psi is known at time t equal to 0. By that what I mean is that Cn 0 is actually found from the inner product of psi x 0 and u n star x and a. In the modern bracket notation this can be written as u n x psi x c.

So, if the wave function is specified for all x values that is all special values at time t equal to 0, then one can determine Cn 0, which is the value of the amplitude or the expression for the amplitude at t equal to 0. That tells that if we use this Cn 0 in 4. So, if you put 5 in 4, then my psi of x t, it is equal to sum over N and then I have a psi of x prime 0 and a U n star of x prime and a d x prime this into exponential minus iE n t by h cross and U n of x. Just to remind you that this U n star is actually the complex conjugate of Un and when we write this definition it is implicitly assumed that definition in 2 for a wave function it is implicitly assumed that the U ns are complex quantities.

So, they will have they can be. So, there is a Un and there is a U n star and both would be existing. So, if I have the psi of x t which is written as this, I can write this as g of x x prime t and psi prime psi of x prime 0 and a d x prime. Another thing that you should notice that in equation, let us call the top one of 6, we have used the x prime which is a dummy variable because this psi is a, is a function of x and now we are have introduced a dummy variable which is summed over.

So, this equation, let us call it we can call it as equation 7, introduces a propagator for psi of x d. So, if we know psi at t equal to 0, instead of solving the second order differential equation given by the Schrodinger equation, which is written as equation 1 here, instead of solving that we can actually solve this integral equation which is equation 7 and if we know psi of x at 0 at t equal to 0.

So, not only that, it takes contribution of psi at all the x prime points and builds up this entire integral from the contribution of psi from all the x prime points in order to have the value of psi at x d and of course, at a given space time point sigh of x 0 is or rather sigh of x t is proportional to psi of x 0. Now here my definition of the propagator is equal to sum over n and the Un x and Un star x prime and exponential minus iE n t over h cross.

So, that is the definition of propagator and this propagator is formed of the basis functions that we have used for writing down the Eigen functions psi. So, if you write it in the modern notation it is U n of x prime and U n of x and exponential minus iE n t over h cross. So, that is the form of the propagator and this propagator as I said derives contribution from all the x prime points and sums them up to arrive at psi of x t. So, once again I repeat that instead of solving equation 1 in order to obtain psi of x t, we can actually solve an integral equation which is equation 7 and which is for that one needs the knowledge of psi at x and time t equal to 0 and one also needs the knowledge of the propagator which can be obtained from the basis functions as its given in equation 8.