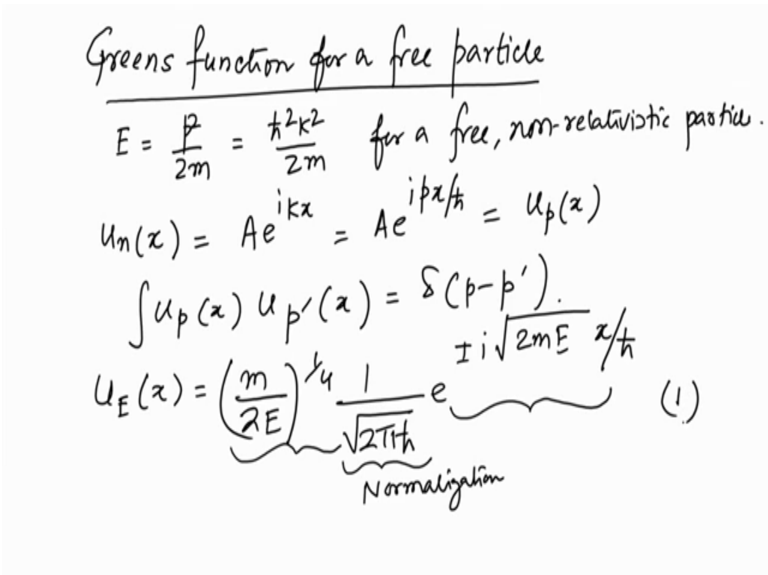
Advanced Condensed Matter Physics
Prof. Saurabh Basu
Department of Physics
Indian Institute of Technology, Guwahati

Lecture – 03
Second quantization I

To summarize what we have learned so far, we have defined what is a propagator which propagates a wave function from an initial time which could be at t equal to 0 or may be from a finite time t equal to t 1 and it propagates to a different time which is at t 2 which where t 2 is greater than t 1 and that is called as a propagator and we have also calculated the propagator or rather have related the propagator to the Green’s function for a particular problem. Now, we have to learn, how to compute a propagator for a given problem and we take the simplest possible example that is a free particle in continuum. So, we are going to calculate the propagator or the Green’s function.

(Refer Slide Time: 01:25)



So, Green’s function or equivalently the propagator for a free particle is what we are going to compute. So, just for your information free particle means that the energy momentum relationship is given by equal to p square over 2 m it is equal to h cross square k square over 2 m for a free non relativistic particle.

So, we are going to write the for this the basis function is a plane wave. So, it can be expressed in plane wave states and hence if you remember the basis states that we have written down earlier which now we can write it as A exponential i k x or which is equal to in terms of the momentum explicitly. It is i p x by h cross and hence, we shall replace this n index here by a u p of x where p is the momentum of the particle which is a well-defined quantity and the quantum number corresponding to the momentum is a good quantum number.

So, if we have these as the basis states the basis states also obey this orthogonality relation and. So, this is equal to delta of p minus p prime and my if I if I write down the in terms of the energy eigenstates then my u E x is equal to m over 2 E whole to the power one fourth and one divided by 2 p pi h cross and exponential plus minus i root over 2 m E by into x divided by h cross where if you note that this is the normalization factor and this is well. So, this is the normalization and this is the plane wave part written in the energy basis.

So, we will take this as the basis states and calculate the propagator or equivalently the Green's function.

(Refer Slide Time: 04:35)

Orthogonality relation:

$$\int u_E(x)\, u_{E'}(x)\, dx = \delta(E-E')$$

$$G(x,x';t) = \int dE\, u_E^*(x)\, u_E(x)\, e^{-iEt/\hbar} \qquad (2)$$

$$G(x,x';t) = \int dE \left(\frac{m}{2E}\right)^{1/2} \frac{1}{2\pi\hbar}\, e^{\pm i\sqrt{2mE}\,(x-x')/\hbar}\, e^{-iEt/\hbar}$$

$$K = \frac{\sqrt{2mE}}{\hbar} \Rightarrow dK = \frac{\sqrt{2m}}{\hbar} \cdot \frac{1}{2\sqrt{E}}\, dE$$

$$G(x,x';t) = \frac{1}{2\pi} \int dk\, e^{ik(x-x')}\, e^{-i\hbar k^2 t/2m} \qquad (3)$$

So, this will call it as equation one and now let us write down also the orthogonality relation for the basis states as u E u E prime or rather u E and u E x prime and there is a d x. So, this has to be erased. So, this is written as u E x u E prime x d x this is equal to delta e minus e prime ok.

So, these are the orthogonality relation that the basis states will follow and then the propagator or the Green's function can be written as d E and a u E x u E. So, there is a start over here and there is a exponential minus i e t by h cross and then we have if we put the values that we have or rather the expressions that we have taken in equation one then in this expression which is 2, then we get this as g x x prime t this is equal to a d E and there is a m over 2 E whole to the power half there is a one by 2 pi h cross and there is A exponential plus minus i root over 2 m E x minus x prime by h and exponential minus i e t by h cross.

So, this is the Green's function or the propagator for the free particle and we have solved this integral and to solve the integral one can make a substitution as k equal to root over 2 m E by h cross and that gives me a d k that is equal to root over 2 m by h cross 1 by 2 root over e d E and following that I can write down the g x x prime t which is equal to a 1 over 2 pi d k exponential i k x minus x prime exponential minus i h cross k square p by 2 m and this is the form that I have and I have to evaluate this evaluate this integral and this integral can be evaluated easily and one can write down g x x prime t.

(Refer Slide Time: 08:13)

$$\boxed{G(x,x';t) = \sqrt{\frac{m}{2\pi i\hbar t}}\; e^{-\frac{m(x-x')^2}{2i\hbar t}}} \qquad (4)$$

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

$G(x,x';t) \rightarrow$ Propagator

$\rightarrow$ Greens function (Retarded)

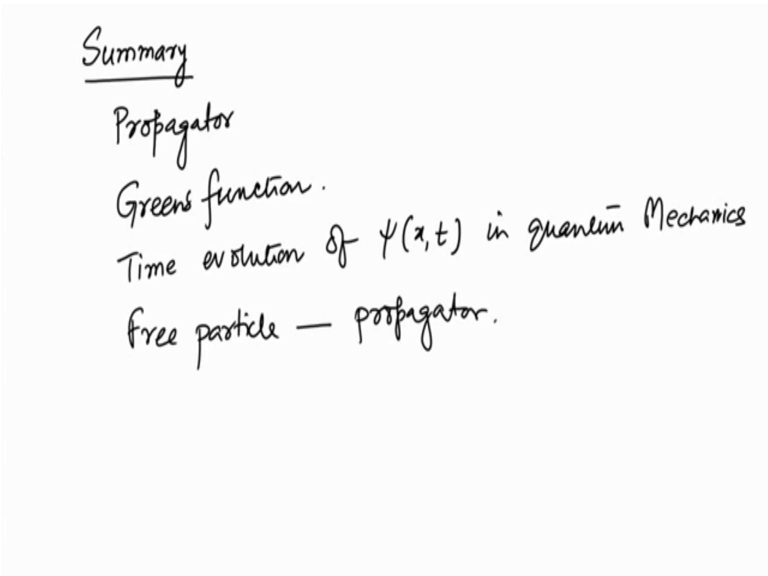
$$G_A(x,x';t) = G(x,x';t)\,\theta(-t)$$

So, which is equal to m over 2 pi i h cross t and exponential minus m x minus x prime square divided by 2 i h cross t. So, this is my equation 4 and this is the final form of the propagator. So, as we have said that for a particular problem such as this a free particle in a continuum, if we find this quantity this will take a wave function say from x equal to at t equal to 0 to t equal to some finite t by the operation of this propagator provided that my psi at x equal to 0 is known for all possible values of x.

So, just to repeat that is psi of x t is g of x x prime t and a psi of x prime 0 and we also have an integral over d x prime. So, for a given problem that is a free particle in a continuum g x x prime t denotes the propagator. So, g is the propagator and we also know how to link it to the Green's function and in particular we have learned for the retarded Green's function, but we can also write it for the advanced Green's function in a similar manner where we just need to write the advanced Green's function as x x prime t which is equal to g x x prime t and a theta of minus t.

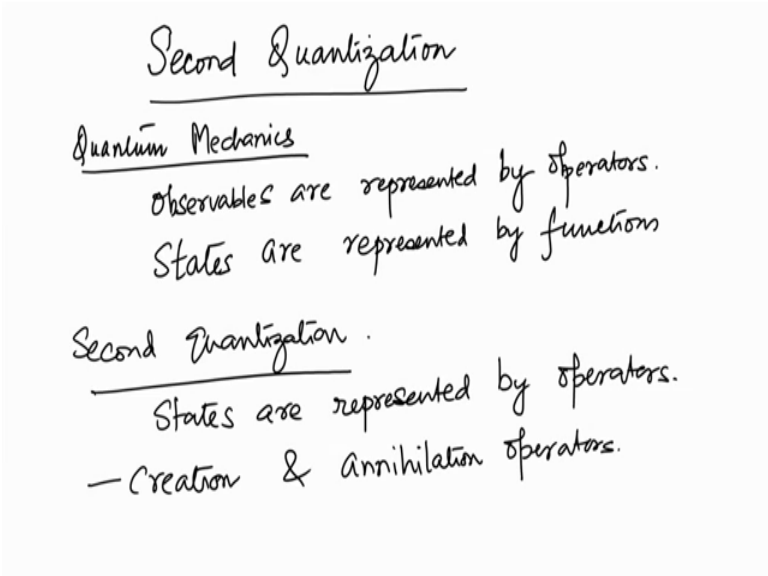
So, to remind you the theta function when minus t is greater than 0 then that is this theta function is equal to one and if it is not satisfied otherwise the theta function will give us 0. So, this is the definition of the advanced Green's function.

(Refer Slide Time: 11:00)



So, to summarize we have so far, whatever we have done is that we have defined a propagator and from the propagator we have learned how to calculate Green's function and how this propagator or the Green's function can talk about time evolution of wave function of psi of x t in quantum mechanics and then we have solved it for a for an easy problem rather easy problem here that is on the free particle and calculate it the propagator for the free particle.

(Refer Slide Time: 12:16)



So, the next thing that we have on the cards is to talk about second quantization and we would first define what is second quantization and then what do we do with this. In fact, we would write all the Hamiltonian in the second quantized formalism for us to attain to a problem in solid state physics. So, the second quantization is formalism or a technique which is different than the first quantization which is we all know as the quantum mechanics.

So, what happens in first quantization or rather, the conventional quantum mechanics ah? So, in quantum mechanics we have observables which are represented by observables are represented by operators and the state functions or the eigenstates states are represented as by functions which have continuous functions say that of the space variable x or x y and z or r theta and phi.

So, this is what we have learned in quantum mechanics recall your discussion that you have for the either the hydrogen atom or the harmonic oscillator in either of the cases we have written down a Hamiltonian in terms of operators which are the Laplacian operator and operators that go as it depends on space such as either x square in one dimension for the oscillator or it says one over r for the hydrogen atom and then when we solved a second order differential equation which goes by the name Schrodinger equation and then we have got the energy eigenvalues for the harmonic oscillator problem the energy eigenvalues came out as n plus half h cross omega where omega is equal to root over k by m and in the hydrogen atom problem.

The energy eigenvalues came out as minus 13 point psi 6 by n square electron volt and in both the cases n is the quantum number for the problem and n is quantized as either 0, 1, 2, etcetera for the harmonic oscillator and n equal to 1, 2, 3, etcetera for the hydrogen atom problem and the Eigen states that were computed from solving by solving the Schrodinger equation they are simple functions of r which are in the case of hydrogen atom they are known as polynomials in the name in the case of the harmonic oscillators they are known as Hermite polynomials.

So, this is what we are talking about that the states are represented by functions now in the second quantized formalism. So, second quantization we are going to represent the observable anyway by operators which were done in quantum mechanics as well; however, the states are now going to be represented by are represented now by operators as well operators and these operators are known as a creation and annihilation operator, they are also called as creation and destruction operators, but this destruction and annihilation they are used interchangeably we will also probably do that.

So, the commutation and the anti-commutation of the creation and then annihilation operators will define the property of the wave function and in the case of fermions this is an anti-symmetric wave function and whereas, in the case of bosons that is a symmetric wave function.

(Refer Slide Time: 17:05)

Commutation and anticommutation relations of the operators decide the symmetric (bosons) and antisym-metric (fermion) nature of the wavefunction.

Typical State is made up from a vacuum

$$|\Psi\rangle = \prod_{m=1}^{N} \left(a_\lambda^{\dagger}\right)^m |vac\rangle = \prod_{m=1}^{N} \left(a_\lambda^{\dagger}\right)^m |0\rangle$$

$$a_m |vac\rangle = 0$$

$a_m^{\dagger}, a_m$: Hermitian adjoints

Not self adjoint; distinct operators.

So, the commutation or the anti-commutation, rather, I will write and anti-commutation relation of the operators and what we mean by operators of the creation and the annihilation operators which you have seen in some form when you did the operator methods in quantum mechanics and so, we extend that to many particle system you have used it for the harmonic oscillator problem.

So, these are these operators they obey certain commutation relations or anti commutation relations which we are going to learn and these commutation or the anti-commutation relations they fix the nature of the wave function of the behaviour of the wave function; whether the wave function would be anti symmetric or symmetric with respect to interchange of particles that is known as anti-symmetric or symmetric property and these relations will actually decide that decide the symmetric as I said that is for bosons and anti-symmetric which is for fermions nature of the wave functions basically the typical state is made up from a vacuum where a state like this is made of from the product of the single particle states and where.

So, these are the creation operators the creation operators are always written with a dagger here and to the power m which is acting on vacuum. So, vacuum is a null state which has no particle. So, a lambda successively operating on this m times will create that many that is capital n number of particles. So, these are going to give me single particle states and I am going to get a full wave function starting from a single particle states by successively multiplying or rather operating the creation operator on the vacuum.

So, the vacuum is also written with a 0 and we can write it like this. So, that is my state and as I said that in the second quantized notation the states are formed by the creation operators or the annihilation operators the annihilation operators i have not written, but one can define the property of the annihilation operator as one which is not written with a dagger and which it acting on the vacuum gives me 0 which means that vacuum has no particles.

So, there is no way that one can annihilate a particle from there now one important thing is that that a m dagger and a m are Hermitian conjugate to each other Hermitian rather Hermitian adjoint to each other and they are distinct operators and they are not self adjoint. So, not a self adjoint and they are distinct operators. So, now, with this background let us go back and compute or rather at least initially define the states for both fermions and bosons and how they look like. So, we will the method of second quantization is what we are going to discuss.

(Refer Slide Time: 22:11)

Method of Second quantisation

Single particle Hamiltonian, H

$$H|\lambda\rangle = \varepsilon_\lambda |\lambda\rangle$$

Two particles (fermions/Bosons)

$$\psi_F(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle - \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right]$$

$$= \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)\right]$$

Now, keep in mind that there are a lot of books which they do this method of second quantization or write the Hamiltonian or any operator in the second quantized formalism. So, you need to actually focus on any one book because the notations that are used from one book to another very like which will be sometimes difficult for a reader to follow.

So, follow these notes along with a book that is going to be prescribed and then you will learn this thing better.

So, what we are trying to say is that lets take a single particle Hamiltonian H where H acting on a state lambda gives me a epsilon lambda and returns me the same state. So, this lambda can in principle be any quantum number for that which is suitable for that particular problem which could be momentum or energy and so on. So, we are uncommitted about that at this point and we write this as the eigenvalue equation now we can write for the wave function say for 2 particles and they could be. So, 2 particles, we want to generalize this equation and these 2 particles can be fermions or bosons.

So, and then one can write down psi for a fermion at two. So, these are say space variables x 1 and x 2 which is equal to one by root 2 and I can I will use both 2 notations which is x 1 lambda 1 and x 2 lambda 2. So, whatever that state lambda is. So, we are writing it in terms of the space variable. So, it is a. So, this would represent a state in the position space and this is equal to and there is a minus sign and there is an x 1 lambda 2 and there is a x 2 lambda one and that is the state and as I said that I will use another notation for that.

So, we can also write this as this is equal to psi 1 x 1 psi 2 x 2 minus psi 1 x 2 and psi 2 x 1 possibly this is a more simple notation for you because we are writing down the wave function psi is the quantum mechanical wave function and it is expressed in the position space and so, x 1 and x 2 refer to the positions of the 2 particles or the 2 fermions that we are talking about and there is a necessity and necessarily, there is a negative sign in between because we have swapped particle number one and particle number 2 while writing the second term as compared to the first term; however, this will not be there for a boson.

(Refer Slide Time: 26:05)

$$\psi_B(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle + \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right]$$

$$= \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)\right].$$

$$\psi_{F/B}(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) + P\,\psi_1(x_2)\psi_2(x_1)\right]$$

$P = -1$ for fermion

$= +1$ for Boson.

And one can write down the wave function for a boson equal to a 1 by root 2 and x 1 lambda 1 x 2 lambda 2 and there is a plus x 1 lambda 2 and the x 2 lambda 1 and this as earlier can be written down as psi 1 x 1 psi 2 x 2 plus psi 1 x 2 psi 2 x 1.

So, we can write it with. So, either for fermions or bosons we can write it with a in a more compact notation, we can write it with a psi 1 x 1 psi 2 x 2 plus p psi 1 x 2 psi 2 x 1 and this p equal to minus 1 for fermions and it is equal to plus 1 for bosons and in a similar fashion we can write down a many particle wave function.

(Refer Slide Time: 27:39)

$$\Psi = |\lambda_1, \lambda_2 \ldots \lambda_N\rangle = \frac{1}{\sqrt{N!\prod_{\lambda=0}^{\infty} n_\lambda!}} \sum_K P^{(1-\mathrm{Sgn}\,K)/2}\, |\lambda_{K_1}\rangle \otimes |\lambda_{K_2}\rangle \otimes \cdots\cdots \otimes |\lambda_{K_N}\rangle$$

$\mathrm{Sgn}\,K = 1$ or -1.

$+1$: for even number of transpositions

-1 : for odd number of transposition.

Let us now write it with a big psi which is nothing, but a lambda 1 lambda 2 and all the way for n particles and that is equal to.

So, there is a normalization that is used here which is n factorial and there is a lambda equal to 0 to infinity and n lambda factorial. So, this and there is a sum over k and there is a P which is 1 minus I will write it in S g n k divided by 2 and this is equal to all these single particle states lambda k 1 and product with lambda k 2 and product and all the way up to lambda k n as I said that this there is a particular index or the quantum number that is used here which are k 1 k 2 k n which can be either momentum or spin or position or energy depending upon the suitability of the problem.

So, the question is what is this p to the power one minus s g n k? So, just to say that that when we actually swap particles that is if we make transposition of particles that is move particles from one place to another which are these things are being swept this lambda one lambda 2 indices being swapped and in that case we have S g n k is equal to it is equal to one or minus 1. So, the 1 is plus 1 is for even number of transpositions number of transpositions and minus one is for odd number of transpositions.

So, it is clear that for sign of if it becomes plus 1, then I have p to the power 0 which means it is equal to 1. So, if you trans or rather swap particles even number of times then one does not pick up a sign for the fermionic wave function; while if it is done odd number of times, then one picks up a negative sign. However, this is only for fermion for bosons it is always equal to 1.