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

Lecture – 02
Propagators II

So, we have derived a formula for the propagator as we call it. So, it is G x x prime t which is expressed in terms of these basis functions.

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

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

Putting (5) in (4)

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

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

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

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

Which are u n x and u n x prime and it takes the system from some x to x prime at a given time t.

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$\psi(x,t) \rightarrow$ by solving $\underline{\text{TDSE}}$

$\rightarrow$ by solving the propagator

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

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)\psi(x,t) = \int \underbrace{\left(i\frac{\partial}{\partial t} - H\right)}\, G(x,x',t)\,\psi(x',0)\,dx' = 0 \quad (9)$$

$$\Rightarrow \left(i\hbar\frac{\partial}{\partial t} - H\right) G(x,x',t) = 0 \quad (10)$$

$\Rightarrow$ Schrödinger Equation for the propagator.

So, as I said earlier that we can get psi of x t by solving the Schrodinger equation, time dependent Schrodinger equation which we have written as TDSE or we can also get it by solving or rather computing the green of the propagator. So, what we want to show is that or rather emphasize is that this psi x t at a given point is the sum of contribution of coming from all the initial wave function, at all possible points x prime and that is taken into account and the contribution from a particular point is proportional to G of x x prime p and that is why it is called as the propagator.

So, it propagates the wave function from x to x prime at a given t, now let us try to cast this problem in terms of the propagator and. So, we have to find a equation of motion for the propagator, just like the wave function the equation of motion is given by the time dependent Schrodinger equation which we write it as TDSE and we should also be able to find corresponding equation rather the equation of motion for the propagator.

So, the way to do it is that if you go back to equations 7 where we have written the x psi of x t as an integral over G x x prime t and psi at x prime and 0 integrated over all x prime, I will simply multiply or rather operate this psi x t by this operator which is. So, we will do it as I del del t of and minus h that multiplied or rather operated upon psi x t will allow me to write I del del t minus h and there is a G x x prime p and there is a psi x prime 0 and there is a d x prime.

So, this tells me that this will act, this operator here will act on this function which is G x x prime t psi of x prime 0 and this operator will actually act on the psi of x prime 0 and will give me an equation which is equal to I del del t minus H G x x prime t equal to 0.

So, once again to iterate that in order to find out the equation of motion for the propagator which is G x x prime t I have taken this operator I h del del t minus H and operated on this psi which is basically the time dependent Schrodinger equation and that is put here and since that is equal to 0 we get this equation which is I del del t. There could be a h cross which is inadvertently I have missed that it could be there is the I h cross del del t minus h acting on the G x x prime t is equal to 0. So, let us call this as equation 9 and this as equation 10.

So, this is the Schrodinger equation for the propagate. So, far we have not done much accepting that we have written down the time dependent Schrodinger equation in terms of the propagator and one sort of similarity is very apparent is that in this problem we are trying to cast the G the propagator with the same role that it has in ordinary quantum mechanics.

And the reason we want to do would be apparent later or rather understood later in which we will connect this propagator with the greens function and this greens function will help us in formulating a number of things or rather compute the number of experimentally observed quantities in terms of the greens function so here we may like to actually talk about specifically t greater than 0.

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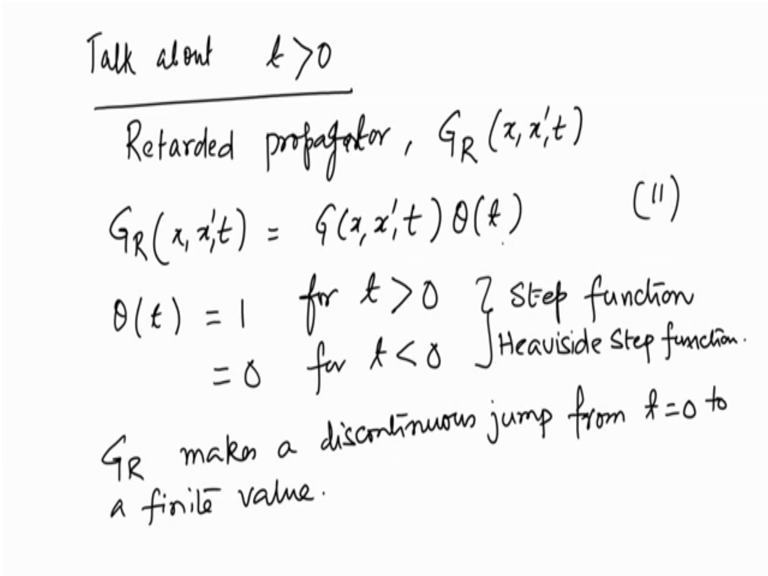

So, what I mean is that this t that appears in your these all these slides is only greater than 0. So, what happens to the wave function or the propagator as you move backward in time is not discussed or rather it will be discussed in a more general sense, but right now we want to concentrate on the fact that I only evolved a system positive in time. So, that t is greater than 0.

In which case I would define a propagator called as the retarded propagator and this propagator is written with a G R with the same indices as we have for G. So, a G R is defined as x x prime t which is equal to a G x x prime t and a theta function I will tell you the meaning of the theta function.

So, this is equation number 11 where this theta function is defined as it is equal to 1 for t greater than 0, it is equal to 0 for t less than 0 and this is also called as the step function or it also has a name which is called as a Heaviside step function and. So, this immediately makes it clear that a G x x prime t exists for all time positive and negative; however, G R which is also a function of x x prime and t exists or nonzero only for t greater than 0 and for t less than 0 it vanishes because of this theta function the way it is defined here.

So, this is my definition of G R. So, it is very clear that G R makes a discontinuous jump, jump from 0 from t equal to 0 to finite value. So, now the job of course, is trivial to find out a Schrodinger equation for G R, we have already found one for G now we will have to find the same thing for G R which is called as a retarded propagator. So, that is the job at hand. So, I need to do a time derivative, a partial time derivative on the G x x prime t and theta t more like a chain rule that we have for the derivatives for equation 1. So, let us see how one does that.

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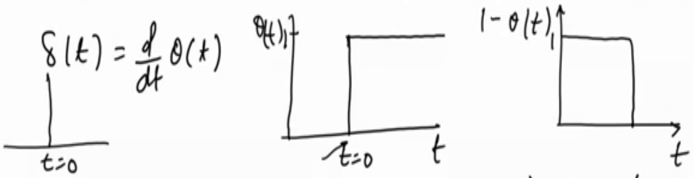
$$i\hbar \frac{\partial}{\partial t} G_R(x,x',t) = \theta(t)\, \underbrace{i\hbar \frac{\partial}{\partial t} G(x,x',t)} + i\hbar\, G(x,x',t)\,\delta(t)$$

$$\delta(t) = \frac{d}{dt}\theta(t)$$



$$i\hbar \frac{\partial}{\partial t} G_R(x,x',t) = \theta(t)\, H G(x,x',t) + i\hbar\, G(x,x',0).$$

$$\boxed{\left(i\hbar \frac{\partial}{\partial t} - H\right) G_R(x,x',t) = i\hbar\, \delta(x-x')\,\delta(t)} \quad 12$$

Sch. Eqn. for retarded propagator.

So, I have I h cross del del t of G R x x prime t I am only looking at the time derivative and that keeping theta function as constant I simply do that for the G and now keeping the G constant I have to do the same on the theta function, Now, what is the derivative time derivative of a theta function that can be easily understood if I plot this figure to actually graphically represent theta function. So, this is. So, this would be it is rather one minus theta function that I have drawn as a function of t and a theta function would look like theta of t versus t and it looks like. So, this is t equal to 0.

So, this is my theta function and I have to take a derivative of the theta function, look this function is 0 for t less than 0 anyway this function is equal to 1. So, this value is 1, this value is 1 as well and this value is constant for all t greater than t equal to 0 and it only has a discontinuity at t equal to 0. So, the derivative of the theta function is actually a delta function. So, which is d d t or a del del t if you write it more correctly.

So, this is the definition of the time derivative of the theta function. So, I will simply get a derivative so a delta function here which is a derivative of the theta function. Now, this if I recall the the Schrodinger equation that we have written down for G it becomes automatically I h cross del del t of G R x x prime t this is equal to a theta function and multiplied by a H and G x x prime t plus I h cross G x x prime. Now, in order to have a delta t being multiplied with it we need to this would only be non 0 a delta function is only non 0 at t equal to 0. In fact, it is infinite for t equal to 0 and at all other t it is 0. So, a delta function really looks like an infinite discontinuity at t equal to 0.

So, thus it make sense that there is an infinite a slope for the theta function at this point that is shown here. So, this, so to have t equal to 0 I will simply write this as. So, G x x prime 0. So, my equation for the greens function the retarded rather the retarded propagated which is what we were calling it is this and if I rearrange this if I bring it to the other side I will simply have I h cross del del t minus h and now acting on the G x x prime t this is equal to a I h cross a delta x minus x prime and a delta b ok.

So, this is just written notationally because that will be this is by if you go back then we have done this that the, actually this greens function from equation 8 or rather the propagator in equation 8 could actually be written as delta of x minus x prime and that is the delta function in time.

So, this is my Schrodinger equation for the retarded propagator. So, I will use a slightly shorthand notation for the Schrodinger equation for retarded propagator. So, this equation is what we need to solve for if we need to know the retarded propagator and this propagator needs to be computed for a given problem in order to know the time evolution of the wave function for that problem and this is going to be an important equation for our analysis just in a while. So, now, let us, let us look at that how we can connect this to a physically meaningful quantity such as a G x x prime omega.

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$G_R(x,x',\omega)$ $\quad$ ω: energy variable $= \frac{E}{\hbar}$

ω is conjugate to time.

$$\int \underbrace{G_R(x,x',t)}_{\sum_n u_n(x)\,u_n^*(x')\,e^{-iE_nt/\hbar}} e^{i\omega t}\,dt \rightarrow \text{Fourier transform of } G_R(x,x';t) \text{ is taken.}$$

$$\int_0^\infty e^{i(\hbar\omega - E_n)t/\hbar}\,dt \rightarrow \text{diverges}$$

$$\int_0^\infty e^{i(\hbar\omega - E_n \pm i\eta)t}\,dt \rightarrow \text{Convergent}$$

See omega is the energy variable rather it is the h cross omega is the energy. So, this is a energy variable that is written as, this is an energy variable and with just the H cross added to it it becomes a energy dimension of energy and since the it is, it is conjugate to time. So, omega is conjugate to time. In fact, the response of the system is often expressed in terms of G x x prime omega which is at a given omega value or other energy value one can compute the propagator.

So, we will we can write a G R here because this is what we are interested in and for getting this we will have to do an integral of the form which is x x prime t with exponential I omega t or one can write it. So, this is e over H cross then or you can write it as e over h cross into t and then you have to integrate over this.

So, basically this tells you that there is a Fourier transform of G R x x prime t is being taken, now remember that this has a form which is like u n of x prime let me just make sure that I use the same notation. So, it is u n x and u n star x prime it is u n x and a u n star x prime exponential minus I e n t over h cross and if i. So, there is a sum over n and if I use it there, then I will have an integral of the form which is exponential I could be h cross omega minus e n t by h cross and a d t and from 0 to infinity.

We are not going to minus infinity because we are using the retarded propagator which is only valid for all times t greater than 0 in which case we will have to solve this integral and this integral diverges as time goes to infinity. So, this divergence is removed by a trivial factor by introducing a small complex damping into this equation this will be done over and over again. So, I will simply do it mathematically here. So, I take a small imaginary part here and I will write it with a plus I eta for the moment and this integral is convergent. In physics we do not want to deal with divergent integrals and because this integral is it diverges as t goes to infinity we need to put a damping factor ideally a plus and my damping both would have been fine in this particular case we would discuss it with a plus sign and I will tell you the reason that we are taking a plus sign here and then my G x x prime omega it simply becomes.

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$$G_R(x,x',\omega) = -i\hbar \sum_n \frac{|u_n(x)\rangle\langle u_n(x')|}{\hbar\omega - E_n + i\eta} \qquad \eta \to 0 \text{ in the limit} \quad (13)$$

Relationship between propagator and Greens function.

$$G_+(x,x',\omega) = \int_0^\infty G_R(x,x',t)\, e^{i(\hbar\omega + i\eta)t}\, dt$$

G_+ : Retarded Green's function.

$$\boxed{(H - \hbar\omega - i\eta)\, G_+(x,x',\omega) = i\hbar\,\delta(x-x')} \quad (14).$$

I am skipping one step which should fill it up and this is equal to a u n x u n a h x prime you can write it with a notation that we have used and there is divided by divided by h cross omega minus e n and plus I eta where actually eta goes to 0 in the limiting case in the limit.

So, this would be my equation maybe this is my equation 12 and this I will write it as equation 13. So, this is my propagator rather the retarded propagator, we should put R there a retarded propagator written in the x omega space that is the this variables are kept, the space variables are kept intact and the time derivative time variable has been a Fourier transformed into the energy and we write it as a function of omega.

If you further want to get rid of this x and x prime variables in favour of the momentum variables one should write it with G R and k omega where k would be a momentum vector connecting the points x and x prime now what is the relationship between. So, the relationship between propagator and greens function, I have used it a couple of times, but in those all these situations we actually meant the propagator this G also represents a greens function. Right now we are talking about greens function in quantum mechanics or rather in a single particle description, but we will also talk about many particle greens function in our subsequent discussion.

So, this greens function is defined as. So, the so this G plus is the greens function and this greens function I will tell you what the plus means this is equal to 0 to infinity G R x x prime t exponential I H cross omega plus I, sorry this should be this will be just a plus I eta t and d t. So, G plus is called as the retarded greens function and we will take a specific example to compute retarded greens function aj say for the free particle or for that matter any case.

So, again the Schrodinger equation for the retarded greens function would simply be equal to minus h minus h cross omega minus I eta acting on a G plus and omega this is equal to a I h cross delta x minus x prime and this is our equation for the retarded greens function. So, we this is the equation or rather the equation of motion for the retarded greens function and it is also of importance.

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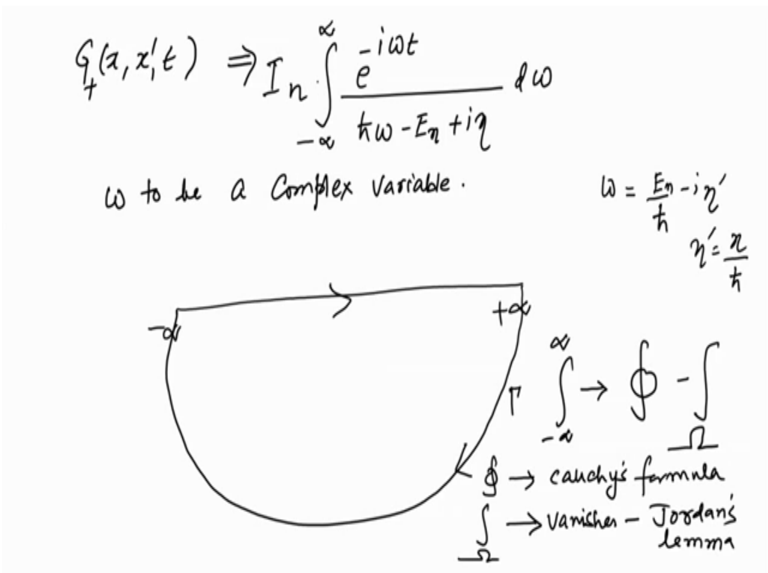

to calculate G plus x x prime t in which case you need to do a Fourier transform of G plus x x prime omega now that would involve an integral of the form which is exponential minus I omega t divided by h cross omega minus e n plus I eta and d omega.

Now, this integral can be a thought of or rather in order to compute this integral one can think of omega to be a complex variable now this limit of omega actually goes from minus infinity to plus infinity ok.

So, one really has omega going from minus infinity to plus infinity on a real line; however, because of this I eta one can think of omega to be a complex variable and there is a pole if you are conversant with complex integrals, There is a pole at e n minus I eta which means that it is in the lower half of the complex plane because your eta is a positive number an infinitesimal small positive number. So, we will have a pole at omega equal to e n over h cross and a minus I eta, it should be also divided by h cross let us call it then eta prime where eta prime equal to eta over h cross and. So, it is in the lower half plane.

So, it makes sense to actually do this complex integration by closing the contour from below and closing it like this in a clockwise sense and call this thing as the gamma the contour to be gamma. So, what I do is that in order to do this integral from minus infinity to plus infinity I convert this into a closed integral over this, over this entire loop that is shown and I will subtract out the curved portion from that.

So, that I get what I asked you want, this is the first term which is a closed loop integral can be found out from the Cauchy's formula and which is the 2 pi I into sum of residues and the second term will vanish because of the Jordan's lemma. So, I will write that briefly. So, this from the Cauchy's formula and this 1 vanishes because of Jordan's lemma.

So, in which case what one gets is that let us call this integral to be off. So, this involves an integral let us call that integral as I n.

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$$I_n = 2\pi i \, e^{-i(E_n - i\eta)t/\hbar} \qquad t > 0$$
$$= 0 \qquad t < 0.$$

$$G_R(x,x',t) = \frac{1}{2\pi\hbar}\int G_+(x,x',\omega)\, e^{-i\omega t}\, d\omega.$$

$$\boxed{G_R(x,x',t) = \frac{1}{2\pi\hbar}\sum_n u_n(x)\, u_n^*(x')\, I_n.}$$

$G_R \rightarrow$ retarded propagator ; G_A : Advanced Prop.

$G_+ \rightarrow$ retarded Greens function ; G_- : Advanced Greens function.

So, this I n if you use this prescription that I have shown one gets it as 2 pi I into the sum of residues which is e n minus I eta t over h cross this is of course, for t greater than 0 and this integral is equal to 0 for t less than 0. Now, to get back to our retarded issue had we added a minus I eta in this expression in order to make it a convergent integral in which case we had to actually talk about only t less than 0 which is called as the advanced propagator which would have given rise to an advance greens function.

So, right now we are talking about retarded propagator because most of our physical problems or the visible observables are related to the retarded greens function. So, then my G R which is the retarded propagator is related to the retarded greens function which I have written it with a positive sign is exponential minus I omega t, d omega and which is nothing, but 1 over 2 pi H sum over n u and x and a u and star x prime and this is multiplied by this I n and this is my either you call it a a. So, so this is how to get my retarded propagator or the retarded greens function for this problem where my G R is the retarded propagator and G plus is the retarded greens function.

So, this is in contrast with my advanced propagator which we will call it as G A as the advanced propagator and. So, and G minus is my advanced greens function and in the next we will give an example how to calculate this propagator for a given problem. Just once again to remind you that instead of solving a differential equation given by the Schrodinger equation you can solve an integral equation for the propagator or the greens function to have the same amount of information that is available by solving psi from the time dependent Schrodinger equation.